MATHEMATICAL THEORY AND NUMERICAL METHODS FOR GROSS-PITAEVSKII EQUATIONS AND APPLICATIONS

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Contents

Summary

Gross-Pitaevskii equation (GPE), first derived in early 1960s, is a widely used model in different subjects, such as quantum mechanics, condensed matter physics, nonlinear optics etc. Since 1995, GPE has regained considerable research interests due to the experimental success of Bose-Einstein condensates (BEC), which can be well described by GPE at ultra-cold temperature.

The purpose of this thesis is to carry out mathematical and numerical studies for GPE. We focus on the ground states and the dynamics of GPE. The ground state is defined as the minimizer of the energy functional associated with the corresponding GPE, under the constraint of total mass (L^2 norm) being normalized to 1. For the dynamics, the task is to solve the Cauchy problem for GPE.

This thesis mainly contains three parts. The first part is to investigate the dipolar GPE modeling degenerate dipolar quantum gas. For ground states, we prove the existence and uniqueness as well as non-existence. For dynamics, we discuss the well-posedness, possible finite time blow-up and dimension reduction. Convergence for this dimension reduction has been established in certain regimes. Efficient and accurate numerical methods are proposed to compute the ground states and the dynamics. Numerical results show the efficiency and accuracy of the numerical methods.

The second part is devoted to the coupled GPEs modeling a two component BEC. We show the existence and uniqueness as well as non-existence and limiting behavior of the ground states in different parameter regimes. Efficient and accurate numerical methods are designed to compute the ground states. Examples are shown to confirm the analytical analysis.

The third part is to understand the convergence of the finite difference discretizations for GPE. We prove the optimal convergence rates for the conservative Crank-Nicolson finite difference discretizations (CNFD) and the semi-implicit finite difference discretizations (SIFD) for rotational GPE, in two and three dimensions. We also consider the nonlinear Schrödinger equation perturbed by the wave operator, where the small perturbation causes high oscillation of the solution in time. This high oscillation brings significant difficulties in proving uniform convergence rates for CNFD and SIFD, independent of the perturbation. We overcome the difficulties and obtain uniform error bounds for both CNFD and SIFD, in one, two and three dimensions. Numerical results confirm our theoretical analysis.

Notations

t	time
i	imaginary unit
$\mathbf{x}$	spatial variable
$\mathbb{R}^d$	d dimensional Euclidean space
$\psi := \psi(\mathbf{x}, t)$	complex wave-function
$\hbar$	Planck constant
∇	gradient
$\nabla^2 = \nabla \cdot \nabla$, Δ	Laplace operator
$\bar{c}$	conjugate of c
$\mathrm{Re}(c)$	real part of c
$\mathrm{Im}(c)$	imaginary part of c
$L_z = -i(x\partial_y - y\partial_x)$	z-component of angular momentum
$\\|u\\|_p := \\|u\\|_{L^p(\mathbb{R}^d)}$	L^p ($p \in [1, \infty]$) norm of function $u(\mathbf{x})$, where there is no confusion about d
$\hat{f}(\xi) := \int_{\mathbb{R}^d} f(\mathbf{x}) e^{-i\mathbf{x}\cdot\xi}\, d\mathbf{x}$	Fourier transform of $f(\mathbf{x})$

Chapter 1

Introduction

The Gross-Pitaevskii equation (GPE), also known as the cubic nonlinear Schrödinger equation (NLSE), has various physics applications, such as quantum mechanics, condensate matter physics, nonlinear optics, water waves, etc. The equation was first developed to describe identical bosons by Eugene P. Gross [72] and Lev Petrovich Pitaevskii [116] in 1961, independently. Later, GPE has been found various applications in other areas, known as the cubic NLSE. Since 1995, the Gross-Pitaevskii theory of boson particles has regained great interest due to the successful experimental treatment of the dilute boson gas, which resulted in the remarkable discovery of Bose-Einstein condensate (BEC) [7, 36, 52]. Now, BEC has become one of the hottest research topics in physics, and motivates numerous mathematical and numerical studies on GPE.

1.1 The Gross-Pitaevskii equation

Many different physical applications lead to the Gross-Pitaevskii equation (GPE). For example, in BEC experiments, near absolute zero temperature, a large portion of the dilute atomic gas confined in an external trapping potential occupies the same lowest energy state and forms condensate. At temperature T much lower than the critical temperature T_c, using mean field approximation for this dilute many-body system, BEC can be described by a macroscopic wave function $\psi(\mathbf{x}, t)$, governed by GPE in the dimensionless form [16, 18, 117]

$$i\partial_t\psi(\mathbf{x}, t) = -\frac{1}{2}\nabla^2\psi(\mathbf{x}, t) + V_d(\mathbf{x})\psi(\mathbf{x}, t) + \beta_d|\psi(\mathbf{x}, t)|^2\psi(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^d,\ d = 1, 2, 3, \tag{1.1}$$

where t is time, $V_d(\mathbf{x})$ represents the confining trap and β_d represents the interaction between the particles in BEC (positive for repulsive interaction and negative for attractive interaction). The equation (1.1) can be generalized to arbitrary d dimensions, but we restrict our interests to $d = 1, 2, 3$ cases, which are the typical dimensions for the physical problems.

In nonlinear optics, GPE (1.1) describes the propagation of light in a Kerr medium (cubic nonlinearity) [89, 141]. The equation (1.1) also describes deep water wave motion [139]. Generally speaking, a wide range of nonlinear physical phenomenon can be modeled by NLSE when dissipation effects can be neglected and dispersion effects become dominant. As the cubic nonlinearity is one of the most common nonlinear effects in nature, GPE (cubic NLSE) has shown its great importance.

For GPE (1.1), there are two important conserved quantities for (1.1), i.e. the *mass*

$$N(\psi(\cdot,t)) := \int_{\mathbb{R}^d} |\psi(\mathbf{x},t)|^2 \, d\mathbf{x} \equiv N(\psi(\cdot,0)), \quad t \geq 0, \tag{1.2}$$

and the *energy*

$$E(t) := \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla\psi(\mathbf{x},t)|^2 + V_d(\mathbf{x}) \, |\psi(\mathbf{x},t)|^2 + \frac{\beta}{2} \, |\psi(\mathbf{x},t)|^4 \right] d\mathbf{x} \equiv E(0), \quad t \geq 0. \tag{1.3}$$

In view of the mass conservation, we assume that the wave function $\psi(\mathbf{x}, t)$ is always normalized such that $N(\psi(\cdot, t)) = 1$, when GPE is applied to BEC system. In this case, the normalization means that the total number of particles in BEC is unchanged during evolution.

In the study of GPE (1.1), it is important to choose proper function space. In this thesis, we will consider the equation (1.1) in the energy spaces defined as

$$\Xi_d = \left\{ u \in H^1(\mathbb{R}^d) \mid \|u\|^2_{\Xi_d} = \|u\|_2^2 + \|\nabla u\|_2^2 + \int_{\mathbb{R}^d} V_d(\mathbf{x}) |u(\mathbf{x})|^2 \, d\mathbf{x} < \infty \right\}, \tag{1.4}$$

and the potential $V_d(\mathbf{x})$ ($d = 1, 2, 3$) is assumed to be nonnegative without loss of generality. Noticing the L^2 normalization condition, it is convenient to introduce the unit sphere of Ξ_d to be

$$S_d = \Xi_d \bigcap \left\{ u \in L^2(\mathbb{R}^d) \middle| \, \|u\|_2 = 1 \right\}. \tag{1.5}$$

1.2 Ground state and dynamics

Concerning GPE (1.1), there are two basic issues, the ground state and the dynamics. Mathematically speaking, the dynamics include the time dependent behavior of GPE, such as the well-posedness of the Cauchy problem, finite time blow-up, stability of traveling waves, etc. The ground state is usually defined as the solution of the following minimization problem:

Find ($\phi_g \in S_d$), such that

$$E_g := E(\phi_g) = \min_{\phi \in S_d} E(\phi), \tag{1.6}$$

where S_d is a nonconvex set defined as (1.5), or equivalently as

$$S_d := \left\{ \phi \mid \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 d\mathbf{x} = 1,\ E(\phi) < \infty \right\}. \tag{1.7}$$

It is easy to show that the ground state ϕ_g satisfies the following Euler-Lagrange equation,

$$\mu\phi = \left[-\frac{1}{2}\nabla^2 + V_d(\mathbf{x}) + \beta|\phi|^2 \right] \phi, \tag{1.8}$$

under the constraint

$$\int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 \, d\mathbf{x} = 1, \tag{1.9}$$

with the eigenvalue μ being the Lagrange multiplier or chemical potential corresponding to the constraint (1.9), which can be computed as

$$\mu := \mu(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla\phi|^2 + V_d(\mathbf{x}) |\phi|^2 + \beta|\phi|^4 \right] d\mathbf{x} = E(\phi) + \frac{\beta}{2} \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^4 \, d\mathbf{x}. \tag{1.10}$$

In fact, the above Euler-Lagrange equation can be obtained from GPE (1.1) by substituting the ansatz

$$\psi(\mathbf{x}, t) = e^{-i\mu t}\phi(\mathbf{x}). \tag{1.11}$$

Hence, equation (1.8) is also called as the time-independent Gross-Pitaevskii equation.

The eigenfunctions of the nonlinear eigenvalue problem (1.8) under the normalization (1.9) are usually called as stationary states of GPE (1.1). Among them, the eigenfunction with minimum energy is the ground state and those whose energy are larger than that of the ground state are usually called as excited states.

In nonlinear optics, unlike BEC, there is no confining potential in this case, i.e. $V_d(\mathbf{x}) = 0$ or $\limsup_{|\mathbf{x}|\to\infty} |V_d(\mathbf{x})|$ is bounded, and the eigenfunctions of the nonlinear eigenvalue problem (1.8) without constraint (1.9) are usually called as bound states. Ground states in this case are defined in a different way [100]. In this study, we stick to the above definition in presence of the confining potential.

1.3 Existing results

Research on GPE has been greatly stimulated by the experimental success of BEC since 1995. For physical interest, there are two basic concerns. One is to justify when the system can be described by GPE accurately with mathematical proof. The other is to study the equation itself both analytically and numerically. In both cases, exploring the properties of the ground states and dynamics have been the most important tasks. Considerable theoretical analysis and numerical studies have been carried out in literature.

As stated before, in the derivation of GPE from BEC phenomenon, it is taken as the mean field limit of the quantum many-body system (BEC), which is a result of the quantum many-body theory. The quantum many-body theory was invented over fifty years ago to describe the many-body system and BEC becomes the first testing ground for it. Because of the coherent behavior, quantum behavior in BEC could be observed. Hence, it is possible to examine the quantum many-body theory in experiments. From the studies in literature, GPE has been found good agreement with experiments. Consequently, there have been some rigorous justifications of the equation from the many-body system BEC, in the mean field regime. For ground state, Lieb et al. [98] proved that the energy functional (1.3) correctly describes the energy of the many-body system (BEC). For dynamics, Erdős et al. [64] showed that GPE (1.1) can describe the dynamical behavior of BEC quite well for a large class of initial data. Near the critical temperature T_c, GPE approximation of the many-body BEC system becomes inaccurate. Other mean field models have been proposed [53, 111].

On the GPE itself, there have been extensive studies in recent years. For dynamics, along the theoretical front, well-posedness, blow-up and solitons of GPE have been discussed, see [43, 139] and references therein for an overview. Along the numerical front, a lot of numerical methods have been applied to GPE. Succi proposed a lattice Boltzmann method in [137, 138] and a particle-like scheme in [45]. Both schemes originated from the kinetic theory for the gas and the fluid. Different finite difference methods (FDM) have been adopted in numerical experiments, such as the explicit FDM [60], the leap-frog FDM [44], and the Crank-Nicolson FDM (CNFD) [3]. In addition, a symplectic spectral method was given in [146]. Explicit FDM is conditionally stable and has a restrict in its step size. However, it needs less computational time than Crank-Nicolson FDM scheme, while CNFD can conserve the mass and energy in the discretized level. Later, Adhikari et al. [107] proposed a Runge-Kutta spectral method with spectral discretization in space and Runge-Kutta type integration in time. Then Bao et al. proposed time-splitting spectral methods [16, 18–20]. Each numerical method has its own advantages and disadvantages. The most advantage of spectral method is the high accuracy with very limited grid points. For numerical comparisons between different numerical methods for GPE, or in a more general case, for the nonlinear Schrödinger equation (NLSE), we refer to [25, 47, 105, 144] and references therein.

For ground states, along the theoretical front, Lieb et al. [98] proved the existence and uniqueness of the positive ground state in three dimensions. Along the numerical front, various numerical methods have been proposed to compute the ground state. In [59], based on the Euler-Lagrange equation (1.8), a Runge-Kutta method was used. The technique involved a dimension reduction process from 3D to 2D by assuming the radial symmetry. Dodd [56] gave an analytical expansion of the energy $E(\phi)$ using the Hermite polynomial when the trap V_d is harmonic. By minimizing the energy in terms of the expansion, approximate ground state results were reported in [56]. In [50], Succi et al. used an imaginary time method to compute the ground states with centered finite-difference discretization in space and explicit forward discretization in time. Lin et al. designed an iterative method in [48]. After discretization in space, they transformed the problem to a minimization problem on finite dimensional vectors. Gauss-Seidel iteration methods were proposed to solve the corresponding problem. Bao and Tang proposed a finite element method to compute the ground state by directly minimizing the energy functional in [24]. In [9, 12, 15], Bao et al. developed a gradient flow with discrete normalization (GFDN) method to find the ground state, which contained a gradient flow and a projection at each step. Different discretizations have been discussed, including the finite difference discretization or spectral discretization in space, explicit (forward Euler) discretization or implicit (backward Euler) discretization in time. Among all the existing numerical methods and algorithms, Runge-Kutta method [59] is the simplest but only valid in 1D or 3D with radial symmetry. The analytical expansion approach [56] is valid for all dimensions (1D, 2D and 3D) but the approach relies on the spectrum of harmonic potential, which makes it impossible to extend to the general trapping potential cases. Moreover, the energy is modified and only an approximate problem is considered in this method. Gauss-Seidel iteration methods [48] are based on the optimization approach and do not use the properties of the GPE. The imaginary time method [50] is the same as the GFDN method, while the imaginary time is preferable in the physics community. The most popular method for computing the ground state for GPE is the GFDN method. Various numerical results have demonstrated the efficiency and accuracy of GFDN method.

1.4 The problems

In this thesis, we focus on the following three kinds of problems.

1. Dipolar Gross-Pitaevskii equation. Since 1995, BEC of ultracold atomic and molecular gases has attracted considerable interests. These trapped quantum gases are very dilute and most of their properties are governed by the interactions between particles in the condensate [117]. In the last several years, there has been a quest for realizing a novel kind of quantum gases with the dipolar interaction, acting between particles having a permanent magnetic or electric dipole moment. A major breakthrough has been very recently performed at Stuttgart University, where a BEC of ^{52}Cr atoms has been realized in experiment and it allows the experimental investigations of the unique properties of dipolar quantum gases [71]. In addition, recent experimental developments on cooling and trapping of molecules [63], on photoassociation [152], and on Feshbach resonances of binary mixtures open much more exciting perspectives towards a degenerate quantum gas of polar molecules [123]. These success of experiments have spurred great excitement in the atomic physics community and renewed interests in studying the ground states [69, 70, 85, 122, 125, 162] and dynamics [93, 115, 118, 164] of dipolar BECs.

Using the mean field approximation, when BEC system is in a rotational frame, the dipolar BEC is well described by the dipolar Gross-Pitaevskii equation given in the dimensionless form (see Chapter 2 and 3 for details) as

$$i\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) - \Omega L_z + \beta|\psi|^2 + \lambda\left(U_{\text{dip}} * |\psi|^2\right)\right]\psi,\ \mathbf{x}\in\mathbb{R}^3,\ t>0, \quad (1.12)$$

where $\mathbf{x} = (x,y,z)^T \in \mathbb{R}^3$, Ω represents the rotational speed of the laser beam, λ is a parameter representing the dipole-dipole interaction strength and other parameters are the same as in (1.1). L_z is the z-component of angular momentum defined as

$$L_z = -i(x\partial_y - y\partial_x), \quad (1.13)$$

and $U_{\text{dip}}(\mathbf{x})$ is given as

$$U_{\text{dip}}(\mathbf{x}) = \frac{3}{4\pi}\,\frac{1-3(\mathbf{x}\cdot\mathbf{n})^{\mathbf{2}}/|\mathbf{x}|^{\mathbf{2}}}{|\mathbf{x}|^3} = \frac{3}{4\pi}\,\frac{1-3\cos^2(\theta)}{|\mathbf{x}|^3}, \qquad \mathbf{x}\in\mathbb{R}^3, \quad (1.14)$$

with the dipolar axis $\mathbf{n} = (n_1,n_2,n_3)^T \in \mathbb{R}^3$ satisfying $|\mathbf{n}| = \sqrt{n_1^2+n_2^2+n_3^3} = 1$ and θ being the angle between $\mathbf{n}$ and $\mathbf{x}$. We will investigate the properties of dipolar GPE (1.12) both analytically and numerically.

2. Coupled Gross-Pitaevskii equations. Early experiments of BEC [7, 36, 52] have been using the magnetic field to trap the quantum gas and the spin degrees of freedom of the particles were frozen. Later, optical traps were used to replace the magnetic trap and the spin degree of freedom is then activated. This leads to the multiple component BEC. BEC with multiple species have been realized in experiments [74, 75, 100, 101, 108, 126, 133] and some interesting phenomenon absent in single-component BEC were observed in experiments and studied in theory [9, 21, 26, 38, 57, 83, 99]. The simplest multi-component BEC is the binary mixture, which can be used as a model for producing coherent atomic beams (also called as atomic laser) [127, 128]. The first experiment of two-component BEC was performed in JILA with $|F=2, m_f=2\rangle$ and $|1,-1\rangle$ spin states of ^{87}Rb [108]. Since then, extensive experimental and theoretical studies of two-component BEC have been carried out in the last several years [10, 40, 80, 102, 151, 167]. In the thesis, we will consider the coupled GPEs modeling a two-component BEC in optical resonators, given in the dimensionless form [75, 83, 117, 153, 167]

$$\begin{aligned} i\partial_t\psi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + (\beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2)\right]\psi_1 + (\lambda + \gamma P(t))\psi_2, \\ i\partial_t\psi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2)\right]\psi_2 + (\lambda + \gamma \bar{P}(t))\psi_1, \\ i\partial_t P(t) &= \int_{\mathbb{R}^d} \gamma\bar{\psi}_2(\mathbf{x},t)\psi_1(\mathbf{x},t)\,d\mathbf{x} + \nu P(t), \qquad \mathbf{x}\in\mathbb{R}^d. \end{aligned} \tag{1.15}$$

Here, $\Psi(\mathbf{x},t) := (\psi_1(\mathbf{x},t), \psi_2(\mathbf{x},t))^T$ is the complex-valued macroscopic wave function vector, $|P(t)|^2$ corresponds to the total number of photons in the cavity at time t, $V(\mathbf{x})$ is the real-valued external trapping potential, ν and γ describe the effective detuning strength and the coupling strength of the ring cavity respectively, λ is the effective Rabi frequency to realize the internal atomic Josephson junction (JJ) by a Raman transition, δ is the Raman transition constant, and $\beta_{jl} = \beta_{lj} = \frac{4\pi N a_{jl}}{a_0}$ $(j, l = 1, 2)$ are interaction constants with N being the total number of particle in the two-component BEC, a_0 being the dimensionless spatial unit and $a_{jl} = a_{lj}$ $(j, l = 1, 2)$ being the s-wave scattering lengths between the j-th and l-th component (positive for repulsive interaction and negative for attractive interaction).

Other multiple BEC such as spin-F BEC (F integer) can be modeled similarly using the mean field approximation. Generally speaking, a spin-F BEC has $2F+1$ spin states and thus can be described by $2F+1$ coupled GPEs. Here, we focus on the simplest two coupled GPEs.

3. Nonlinear Schrödinger equation with wave operator. GPE is a special NLSE with cubic nonlinearity and NLSE appears in a wide range of physical applications. For example, NLSE can be taken as the singular limit of the Klein-Gordon equation or the Zakharov system. Before taking the limits, there is a nonlinear Schrödinger equation with wave operator (NLSW) in some applications, such as the nonrelativistic limit of the Klein-Gordon equation [104, 129, 150], the Langmuir wave envelope approximation [31, 51] in plasma, and the modulated planar pulse approximation of the sine-Gordon equation for light bullets [14, 159]. The NLSW in the dimensionless form reads as

$$\begin{cases} i\partial_t u^\varepsilon(\mathbf{x},t) - \varepsilon^2\partial_{tt}u^\varepsilon(\mathbf{x},t) + \nabla^2 u^\varepsilon(\mathbf{x},t) + f(|u^\varepsilon|^2)u^\varepsilon(\mathbf{x},t) = 0, & \mathbf{x}\in\mathbb{R}^d,\ t>0, \\ u^\varepsilon(\mathbf{x},0) = u_0(\mathbf{x}), \qquad \partial_t u^\varepsilon(\mathbf{x},0) = u_1^\varepsilon(\mathbf{x}), & \mathbf{x}\in\mathbb{R}^d, \end{cases} \tag{1.16}$$

where $u^\varepsilon := u^\varepsilon(\mathbf{x},t)$ is a complex-valued function, $0 < \varepsilon \le 1$ is a dimensionless parameter,

$f : [0, +\infty) \to \mathbb{R}$ is a real-valued function. Formally, when $\varepsilon \to 0^+$, NLSW will converge to the standard NLSE [31, 129]. We will investigate the impact of the parameter ε in the convergence rates for the finite difference discretizations of NLSW (1.16).

1.5 Purpose of study and structure of thesis

This work is devoted to the mathematical analysis and numerical investigation for GPE. We focus on the ground states and the dynamics.

The thesis is organized as follows. In Chapter 2, 3 and 4, we consider the dipolar GPE (1.12) for modeling degenerate dipolar quantum gas, which involves a nonlocal term with a highly singular kernel. This highly singular kernel brings significant difficulties in analysis and simulation of the dipolar GPE. We reformulate the dipolar GPE into a Gross-Pitaevskii-Poisson system. Based on this new formulation, analytical results on ground states and dynamics are presented. Accurate and efficient numerical methods are proposed to compute the ground states and the dynamics. Then, we derive the lower dimensional equations (one and two dimensions) for the three dimensional GPE (1.12) with anisotropic trapping potential. Consequently, ground states and dynamics for the lower dimensional equations are analyzed and numerical methods are proposed to compute the ground states. On the other hand, rigorous convergence rates between the three dimensional GPE and lower dimensional equations are established in certain parameter regimes. Lastly, GPE (1.12) with a rotational term is considered.

In Chapter 5, we consider a system of two coupled GPEs modeling a two-component BEC. We prove the existence and uniqueness, as well as limiting behavior of the ground states in different parameter regimes. Furthermore, efficient and accurate numerical methods are designed for finding the ground states.

Chapter 6 is devoted to the numerical analysis for the finite difference discretizations applied to the rotational GPE ((1.12) with $\lambda = 0$), in two and three dimensions. The optimal convergence rates are obtained for conservative Crank-Nicolson finite difference (CNFD) method and semi-implicit finite difference (SIFD) method for discretizing GPE (1.12) without the nonlocal term, at the order $O(h^2 + \tau^2)$ with time step τ and mesh size h, in both discrete l^2 norm and discrete semi-H^1 norm. Moreover, we make numerical comparison between CNFD and SIFD and conclude that SIFD is preferable in practical computation.

In Chapter 7, we investigate the uniform convergence rates (resp. to ε) for finite difference methods applied to NLSW (1.16). The solution of NLSW (1.16) oscillates in time with $O(\varepsilon^2)$-wavelength at $O(\varepsilon^2)$ and $O(\varepsilon^4)$ amplitudes for ill-prepared and well-prepared initial data, respectively. This high oscillation in time brings significant difficulties in establishing error estimates uniformly in ε of the standard finite difference methods for NLSW, such as CNFD and SIFD. Using new technical tools, we obtain error bounds uniformly in ε, at the order of $O(h^2 + \tau^{2/3})$ and $O(h^2 + \tau)$ with time step τ and mesh size h for ill-prepared and well-prepared initial data, respectively, for both CNFD and SIFD in the l^2-norm and discrete semi-H^1 norm. In addition, our error bounds are valid for general nonlinearity $f(\cdot)$ (1.16) in one, two and three dimensions.

In Chapter 8, we draw some conclusion and discuss some future work.

Chapter 2

Gross-Pitaevskii equation for degenerate dipolar quantum gas

In this chapter, we consider GPE modeling degenerate dipolar quantum gas. Ground states and dynamics are analyzed rigorously. An efficient and accurate backward Euler sine pseudospectral method is designed to compute the ground states and a time-splitting sine pseudospectral method is proposed for dynamics.

2.1 Introduction

At temperature T much smaller than the critical temperature T_c, a dipolar BEC is well described by the macroscopic wave function $\psi = \psi(\mathbf{x}, t)$ whose evolution is governed by the three-dimensional (3D) Gross-Pitaevskii equation (GPE) [125, 162]

$$i\hbar\partial_t\psi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + U_0|\psi|^2 + \left(V_{\text{dip}} * |\psi|^2\right)\right]\psi, \quad \mathbf{x}\in\mathbb{R}^3,\ t>0, \tag{2.1}$$

where $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ is the Cartesian coordinates, m is the mass of a dipolar particle and $V(\mathbf{x})$ is an external trapping potential. When a harmonic trap potential is considered,

$$V(\mathbf{x}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \tag{2.2}$$

with ω_x, ω_y and ω_z being the trap frequencies in x-, y- and z-directions, respectively. $U_0 = \frac{4\pi\hbar^2 a_s}{m}$ describes local (or short-range) interaction between dipoles in the condensate with a_s the s-wave scattering length (positive for repulsive interaction and negative for attractive interaction). The long-range dipolar interaction potential between two dipoles is given by

$$V_{\rm dip}(\mathbf{x}) = \frac{\mu_0\mu_{\rm dip}^2}{4\pi}\,\frac{1-3(\mathbf{x}\cdot\mathbf{n})^2/|\mathbf{x}|^2}{|\mathbf{x}|^3} = \frac{\mu_0\mu_{\rm dip}^2}{4\pi}\,\frac{1-3\cos^2(\theta)}{|\mathbf{x}|^3}, \qquad \mathbf{x}\in\mathbb{R}^3, \tag{2.3}$$

where μ_0 is the vacuum magnetic permeability, $\mu_{\rm dip}$ is permanent magnetic dipole moment (e.g. $\mu_{\rm dip} = 6\mu_B$ for $^{52}\mathrm{C_r}$ with μ_B being the Bohr magneton), $\mathbf{n} = (n_1, n_2, n_3)^T \in \mathbb{R}^3$ is the dipole axis (or dipole moment) which is a given unit vector, i.e. $|\mathbf{n}| = \sqrt{n_1^2 + n_2^2 + n_3^3} = 1$, and θ is the angle between the dipole axis $\mathbf{n}$ and the vector $\mathbf{x}$. The wave function is normalized according to

$$\|\psi\|_2^2 := \int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|^2\, d\mathbf{x} = N, \tag{2.4}$$

where N is the total number of dipolar particles in the dipolar BEC.

By introducing the dimensionless variables, $t \to \frac{t}{\omega_0}$ with $\omega_0 = \min\{\omega_x, \omega_y, \omega_z\}$, $\mathbf{x} \to a_0\mathbf{x}$ with $a_0 = \sqrt{\frac{\hbar}{m\omega_0}}$, $\psi \to \frac{\sqrt{N}\psi}{a_0^{3/2}}$, we obtain the dimensionless GPE in 3D from (2.1) as [18, 117, 162, 163]:

$$i\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\psi|^2 + \lambda\left(U_{\rm dip} * |\psi|^2\right)\right]\psi, \qquad \mathbf{x}\in\mathbb{R}^3, \quad t>0, \tag{2.5}$$

where $\beta = \frac{NU_0}{\hbar\omega_0 a_0^3} = \frac{4\pi a_s N}{a_0}$, $\lambda = \frac{mN\mu_0\mu_{\rm dip}^2}{3\hbar^2 a_0}$, $V(\mathbf{x}) = \frac{1}{2}(\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2)$ is the dimensionless harmonic trapping potential with $\gamma_x = \frac{\omega_x}{\omega_0}$, $\gamma_y = \frac{\omega_y}{\omega_0}$ and $\gamma_z = \frac{\omega_z}{\omega_0}$, and the dimensionless long-range dipolar interaction potential $U_{\rm dip}(\mathbf{x})$ is given as

$$U_{\rm dip}(\mathbf{x}) = \frac{3}{4\pi}\,\frac{1-3(\mathbf{x}\cdot\mathbf{n})^2/|\mathbf{x}|^2}{|\mathbf{x}|^3} = \frac{3}{4\pi}\,\frac{1-3\cos^2(\theta)}{|\mathbf{x}|^3}, \qquad \mathbf{x}\in\mathbb{R}^3. \tag{2.6}$$

In fact, the above nondimensionlization is obtained by adopting a unit system where the units for length, time and energy are given by a_0, $1/\omega_0$ and $\hbar\omega_0$, respectively. As stated in section 1.1, there are two important invariants of (2.5), the *mass* (or normalization) of the wave function

$$N(\psi(\cdot,t)) := \|\psi(\cdot,t)\|^2 = \int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|^2\, d\mathbf{x} \equiv \int_{\mathbb{R}^3} |\psi(\mathbf{x},0)|^2\, d\mathbf{x} = 1, \qquad t\ge 0, \tag{2.7}$$

and the *energy* per particle

$$\begin{aligned} E(\psi(\cdot,t)) &:= \int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{\lambda}{2}\left(U_{\rm dip} * |\psi|^2\right)|\psi|^2\right] d\mathbf{x} \\ &\equiv E(\psi(\cdot,0)), \qquad t\ge 0. \end{aligned} \tag{2.8}$$

Analogous to the case of GPE (1.1), to find the stationary states including ground and excited states of a dipolar BEC, we take the ansatz

$$\psi(\mathbf{x},t) = e^{-i\mu t}\phi(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3, \quad t \geq 0, \tag{2.9}$$

where $\mu \in \mathbb{R}$ is the chemical potential and $\phi := \phi(\mathbf{x})$ is a time-independent function. Plugging (2.9) into (2.5), we get the time-independent GPE (or a nonlinear eigenvalue problem)

$$\mu\,\phi(\mathbf{x}) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\phi|^2 + \lambda\left(U_{\text{dip}} * |\phi|^2\right)\right]\phi(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3, \tag{2.10}$$

under the constraint

$$\|\phi\|_2^2 := \int_{\mathbb{R}^3} |\phi(\mathbf{x})|^2\, d\mathbf{x} = 1. \tag{2.11}$$

The ground state of a dipolar BEC is usually defined as the minimizer of the following nonconvex minimization problem for energy $E(\cdot)$ in (2.8) :

Find $\phi_g \in S_3$ and $\mu^g \in \mathbb{R}$ such that

$$E^g := E(\phi_g) = \min_{\phi \in S_3} E(\phi), \qquad \mu^g := \mu(\phi_g), \tag{2.12}$$

where the nonconvex set S_3 is defined in (1.5) and the chemical potential (or eigenvalue of (2.10)) is defined as

$$\begin{aligned} \mu(\phi) \;&:=\; \int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \beta|\phi|^4 + \lambda\left(U_{\text{dip}} * |\phi|^2\right)|\phi|^2\right] d\mathbf{x} \\ &\equiv\; E(\phi) + \frac{1}{2}\int_{\mathbb{R}^3}\left[\beta|\phi|^4 + \lambda\left(U_{\text{dip}} * |\phi|^2\right)|\phi|^2\right] d\mathbf{x}. \end{aligned} \tag{2.13}$$

In fact, the nonlinear eigenvalue problem (2.10) under the constraint (2.11) can be viewed as the Euler-Lagrangian equation of the nonconvex minimization problem (2.12). Any eigenfunction of the nonlinear eigenvalue problem (2.10) under the constraint (2.11) whose energy is larger than that of the ground state is usually called as an excited state in the physics literatures.

The theoretical study of dipolar BECs including ground states and dynamics as well as quantized vortices has been carried out in recent years based on the GPE (2.1). For the study in physics, we refer to [1,58,66,68,92,92,109,112,119,157,158,163,168] and references therein. For the mathematical studies, existence and uniqueness as well as the possible blow-up of solutions were studied in [42], and existence of solitary waves was proved in [8]. In most of the numerical methods used in the literatures for theoretically and/or numerically studying the ground states and dynamics of dipolar BECs, the way to deal with the convolution in (2.5) is usually to use the Fourier transform [33,69,93,122,147,160,165]. However, due to the high singularity in the dipolar interaction potential (2.6), there are two drawbacks in these numerical methods: (i) the Fourier transforms of the dipolar interaction potential (2.6) and the density function $|\psi|^2$ are usually carried out in the continuous level on the whole space $\mathbb{R}^3$ (see (2.18) for details) and in the discrete level on a bounded computational domain U, respectively, and due to this mismatch, there is a locking phenomena in practical computation as observed in [122]; (ii) the second term in the Fourier transform of the dipolar interaction potential is $\frac{0}{0}$-type for 0-mode, i.e when $\xi = 0$ (see (2.18) for details), and it is artificially omitted when $\xi = 0$ in practical computation [33, 70, 113, 122, 160, 163, 164] thus this may cause some numerical problems too. The main aim of this chapter is to propose new numerical methods for computing ground states and dynamics of dipolar BECs which can avoid the above two drawbacks and thus they are more accurate than those currently used in the literatures. The key step is to decouple the dipolar interaction potential into a short-range and a long-range interaction (see (2.17) for details) and thus we can reformulate the GPE (2.5) into a Gross-Pitaevskii-Poisson type system. In addition, based on the new mathematical formulation, we can prove existence and uniqueness as well as nonexistence of the ground states and discuss mathematically the dynamical properties of dipolar BECs in different parameter regimes.

2.2 Analytical results for ground states and dynamics

Let $r = |\mathbf{x}| = \sqrt{x^2 + y^2 + z^2}$ and denote

$$\partial_{\mathbf{n}} = \mathbf{n} \cdot \nabla = n_1 \partial_x + n_2 \partial_y + n_3 \partial_z, \qquad \partial_{\mathbf{nn}} = \partial_{\mathbf{n}}(\partial_{\mathbf{n}}). \tag{2.14}$$

Using the equality (see [115] and a mathematical proof in Appendix A)

$$\frac{1}{r^3}\left(1 - \frac{3(\mathbf{x}\cdot\mathbf{n})^2}{r^2}\right) = -\frac{4\pi}{3}\delta(\mathbf{x}) - \partial_{\mathbf{nn}}\left(\frac{1}{r}\right), \qquad \mathbf{x} \in \mathbb{R}^3, \tag{2.15}$$

with $\delta(\mathbf{x})$ being the Dirac distribution function and introducing a new function

$$\varphi(\mathbf{x}, t) := \left(\frac{1}{4\pi|\mathbf{x}|}\right) * |\psi(\cdot, t)|^2 = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{x}'|}|\psi(\mathbf{x}', t)|^2 \, d\mathbf{x}', \quad \mathbf{x} \in \mathbb{R}^3, \ t \geq 0, \tag{2.16}$$

we obtain

$$U_{\text{dip}} * |\psi(\cdot,t)|^2 = -|\psi(\mathbf{x},t)|^2 - 3\partial_{\mathbf{nn}} (\varphi(\mathbf{x},t)), \qquad \mathbf{x} \in \mathbb{R}^3, \quad t \geq 0. \tag{2.17}$$

In fact, the above equality decouples the dipolar interaction potential into a short-range and a long-range interaction which correspond to the first and second terms in the right hand side of (2.17), respectively. In fact, from (2.14)-(2.17), it is straightforward to get the Fourier transform of $U_{\text{dip}}(\mathbf{x})$ as

$$\widehat{(U_{\text{dip}})}(\xi) = -1 + \frac{3\,(\mathbf{n}\cdot\xi)^2}{|\xi|^2}, \qquad \xi \in \mathbb{R}^3. \tag{2.18}$$

Plugging (2.17) into (2.5) and noticing (2.16), we can reformulate the GPE (2.5) into a Gross-Pitaevskii-Poisson type system (GPPS)

$$i\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta-\lambda)|\psi(\mathbf{x},t)|^2 - 3\lambda\partial_{\mathbf{nn}}\varphi(\mathbf{x},t)\right]\psi(\mathbf{x},t), \tag{2.19}$$

$$\nabla^2\varphi(\mathbf{x},t) = -|\psi(\mathbf{x},t)|^2, \qquad \lim_{|\mathbf{x}|\to\infty}\varphi(\mathbf{x},t) = 0 \qquad \mathbf{x}\in\mathbb{R}^3, \quad t>0. \tag{2.20}$$

Note that the far-field condition in (2.20) makes the Poisson equation uniquely solvable. Using (2.20) and integration by parts, we can reformulate the energy functional $E(\cdot)$ in (2.8) as

$$E(\psi) = \int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{1}{2}(\beta-\lambda)|\psi|^4 + \frac{3\lambda}{2}\left|\partial_{\mathbf{n}}\nabla\varphi\right|^2\right]d\mathbf{x}\,, \tag{2.21}$$

where φ is defined through (2.20). This immediately shows that the decoupled short-range and long-range interactions of the dipolar interaction potential are attractive and repulsive, respectively, when $\lambda > 0$; and are repulsive and attractive, respectively, when $\lambda < 0$. Similarly, the nonlinear eigenvalue problem (2.10) can be reformulated as

$$\mu\,\phi(\mathbf{x}) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta-\lambda)\,|\phi|^2 - 3\lambda\partial_{\mathbf{nn}}\varphi(\mathbf{x})\right]\phi(\mathbf{x}), \tag{2.22}$$

$$\nabla^2\varphi(\mathbf{x}) = -|\phi(\mathbf{x})|^2, \quad \mathbf{x}\in\mathbb{R}^3, \qquad \lim_{|\mathbf{x}|\to\infty}\varphi(\mathbf{x}) = 0. \tag{2.23}$$

2.2.1 Existence and uniqueness for ground states

Under the new formulation for the energy functional $E(\cdot)$ in (2.21), we have

Lemma 2.1 *For the energy $E(\cdot)$ in (2.21), we have* *(i) For any $\phi \in S_3$, denote $\rho(\mathbf{x}) = |\phi(\mathbf{x})|^2$ for $\mathbf{x} \in \mathbb{R}^3$, then we have*

$$E(\phi) \geq E(|\phi|) = E\left(\sqrt{\rho}\right), \qquad \forall \phi \in S_3, \tag{2.24}$$

so the minimizer ϕ_g of (2.12) is of the form $e^{i\theta_0}|\phi_g|$ for some constant $\theta_0 \in \mathbb{R}$.

(ii) When $\beta \geq 0$ and $-\frac{1}{2}\beta \leq \lambda \leq \beta$, the energy $E(\sqrt{\rho})$ is strictly convex in ρ.

Proof: For any $\phi \in S_3$, denote $\rho = |\phi|^2$ and consider the Poisson equation

$$\nabla^2 \varphi(\mathbf{x}) = -|\phi(\mathbf{x})|^2 := -\rho(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \qquad \lim_{|\mathbf{x}|\to\infty} \varphi(\mathbf{x}) = 0. \tag{2.25}$$

Noticing (2.14) with $|\mathbf{n}| = 1$, we have the estimate

$$\|\partial_{\mathbf{n}} \nabla \varphi\|_2 \leq \|D^2 \varphi\|_2 = \|\nabla^2 \varphi\|_2 = \|\rho\|_2 = \|\phi\|_4^2, \qquad \text{with} \quad D^2 = \nabla\nabla. \tag{2.26}$$

(i) Write $\phi(\mathbf{x}) = e^{i\theta(\mathbf{x})}|\phi(\mathbf{x})|$, noticing (2.21) with $\psi = \phi$ and (2.25), we get

$$\begin{aligned} E(\phi) &= \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla|\phi||^2 + \frac{1}{2}|\phi|^2|\nabla\theta(\mathbf{x})|^2 + V(\mathbf{x})|\phi|^2 + \frac{1}{2}(\beta-\lambda)|\phi|^4 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla\varphi|^2\right] d\mathbf{x} \\ &\geq \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla|\phi||^2 + V(\mathbf{x})|\phi|^2 + \frac{1}{2}(\beta-\lambda)|\phi|^4 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla\varphi|^2\right] d\mathbf{x} \\ &= E(|\phi|) = E\left(\sqrt{\rho}\right), \qquad \forall \phi \in S_3, \end{aligned} \tag{2.27}$$

and the equality holds iff $\nabla\theta(\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{R}^3$, which means $\theta(\mathbf{x}) \equiv \theta_0$ is a constant.

(ii) From (2.21) with $\psi = \phi$ and noticing (2.25), we can split the energy $E\left(\sqrt{\rho}\right)$ into two parts, i.e.

$$E(\sqrt{\rho}) = E_1(\sqrt{\rho}) + E_2(\sqrt{\rho}), \tag{2.28}$$

where

$$E_1(\sqrt{\rho}) = \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\sqrt{\rho}|^2 + V(\mathbf{x})\rho\right] d\mathbf{x}, \tag{2.29}$$

$$E_2(\sqrt{\rho}) = \int_{\mathbb{R}^3} \left[\frac{1}{2}(\beta-\lambda)|\rho|^2 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla\varphi|^2\right] d\mathbf{x}. \tag{2.30}$$

As shown in [97], $E_1\left(\sqrt{\rho}\right)$ is convex (strictly) in ρ. Thus we only need to prove $E_2\left(\sqrt{\rho}\right)$ is convex too. In order to do so, consider $\sqrt{\rho_1} \in S_3$, $\sqrt{\rho_2} \in S_3$, and let φ_1 and φ_2 be the solutions of the Poisson equation (2.25) with $\rho = \rho_1$ and $\rho = \rho_2$, respectively. For any $\alpha \in [0,1]$, we have $\sqrt{\alpha\rho_1 + (1-\alpha)\rho_2} \in S_3$, and

$$\begin{aligned} &\alpha E_2(\sqrt{\rho_1}) + (1-\alpha)E_2(\sqrt{\rho_2}) - E_2\left(\sqrt{\alpha\rho_1 + (1-\alpha)\rho_2}\right) \\ &= \alpha(1-\alpha)\int_{\mathbb{R}^3} \left[\frac{1}{2}(\beta-\lambda)(\rho_1-\rho_2)^2 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla(\varphi_1-\varphi_2)|^2\right] d\mathbf{x}, \end{aligned} \tag{2.31}$$

which immediately implies that $E_2(\sqrt{\rho})$ is convex if $\beta \geq 0$ and $0 \leq \lambda \leq \beta$. If $\beta \geq 0$ and $-\frac{1}{2}\beta \leq \lambda < 0$, noticing that $\alpha\varphi_1 + (1-\alpha)\varphi_2$ is the solution of the Poisson equation (2.25) with $\rho = \alpha\rho_1 + (1-\alpha)\rho_2$, combining (2.26) with $\varphi = \varphi_1 - \varphi_2$ and (2.31), we obtain $E_2(\sqrt{\rho})$ is convex again. Combining all the results above together, the conclusion follows. □

Now, we are able to prove the existence and uniqueness as well as nonexistence results for the ground state of a dipolar BEC in different parameter regimes.

Theorem 2.1 *Assume $V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^3$ and $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ (i.e., confining potential), then we have:*

(i) If $\beta \geq 0$ and $-\frac{1}{2}\beta \leq \lambda \leq \beta$, there exists a ground state $\phi_g \in S_3$, and the positive ground state $|\phi_g|$ is unique. Moreover, $\phi_g = e^{i\theta_0}|\phi_g|$ for some constant $\theta_0 \in \mathbb{R}$.

(ii) If $\beta < 0$, or $\beta \geq 0$ and $\lambda < -\frac{1}{2}\beta$ or $\lambda > \beta$, there exists no ground state, i.e., $\inf_{\phi\in S_3} E(\phi) = -\infty$.

Proof: (i) Assume $\beta \geq 0$ and $-\frac{1}{2}\beta \leq \lambda \leq \beta$, we first show $E(\phi)$ is nonnegative in S_3, i.e.

$$E(\phi) = \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{1}{2}(\beta-\lambda)|\phi|^4 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla\varphi|^2\right] d\mathbf{x} \geq 0, \ \forall\phi \in S_3. \quad (2.32)$$

In fact, when $\beta \geq 0$ and $0 \leq \lambda \leq \beta$, noticing (2.21) with $\psi = \phi$, it is obvious that (2.32) is valid. When $\beta \geq 0$ and $-\frac{1}{2}\beta \leq \lambda < 0$, combining (2.21) with $\psi = \phi$, (2.25) and (2.26), we obtain (2.32) again as

$$\begin{aligned} E(\phi) &\geq \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{1}{2}(\beta-\lambda)|\phi|^4 + \frac{3\lambda}{2}|\phi|^4\right] d\mathbf{x} \\ &= \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{1}{2}(\beta+2\lambda)|\phi|^4\right] d\mathbf{x} \geq 0. \end{aligned} \quad (2.33)$$

Now, let $\{\phi^n\}_{n=0}^{\infty} \subset S_3$ be a minimizing sequence of the minimization problem (2.12). Then there exists a constant C such that

$$\|\nabla\phi^n\|_2 \leq C, \qquad \|\phi^n\|_4 \leq C, \qquad \int_{\mathbb{R}^3} V(\mathbf{x})|\phi^n(\mathbf{x})|^2 d\mathbf{x} \leq C, \qquad n \geq 0. \quad (2.34)$$

Therefore ϕ^n belongs to a weakly compact set in L^4, $H^1 = \{\phi \mid \|\phi\|_2 + \|\nabla\phi\|_2 < \infty\}$, and $L_V^2 = \{\phi \mid \int_{\mathbb{R}^3} V(\mathbf{x})|\phi(\mathbf{x})|^2 \, d\mathbf{x} < \infty\}$ with a weighted L^2-norm given by $\|\phi\|_V = [\int_{\mathbb{R}^3} |\phi(\mathbf{x})|^2 V(\mathbf{x}) d\mathbf{x}]^{1/2}$. Thus, there exists a $\phi^\infty \in H^1 \bigcap L_V^2 \bigcap L^4$ and a subsequence (which we denote as the original sequence for simplicity), such that

$$\phi^n \rightharpoonup \phi^\infty, \quad \text{in } L^2 \cap L^4 \cap L_V^2, \qquad \nabla\phi^n \rightharpoonup \nabla\phi^\infty, \quad \text{in } L^2. \quad (2.35)$$

Also, we can suppose that ϕ^n is nonnegative, since we can replace them with $|\phi^n|$, which also minimize the functional E. Similar as in [97], we can obtain $\|\phi^\infty\|_2 = 1$ due to the confining property of the potential $V(\mathbf{x})$. So, $\phi^\infty \in S_3$. Moreover, the L^2-norm convergence of ϕ^n and weak convergence in (2.35) would imply the strong convergence $\phi^n \to \phi^\infty \in L^2$. Thus, employing Hölder inequality and Sobolev inequality, we obtain

$$\begin{aligned}
\|(\phi^n)^2 - (\phi^\infty)^2\|_2 &\le C_1\|\phi^n - \phi^\infty\|_2^{1/2}(\|\phi^n\|_6^{1/2} + \|\phi^\infty\|_6^{1/2}) \\
&\le C_2(\|\nabla\phi^n\|_2^{1/2} + \|\nabla\phi^\infty\|_2^{1/2})\|\phi^n - \phi^\infty\|_2 \to 0, \qquad n \to \infty, \qquad (2.36)
\end{aligned}$$

which shows $\rho^n = (\phi^n)^2 \to \rho^\infty = (\phi^\infty)^2 \in L^2$. Since $E_2(\sqrt{\rho})$ in (2.30) is convex and lower semi-continuous in ρ, thus $E_2(\phi^\infty) \le \lim_{n\to\infty} E_2(\phi^n)$. For E_1 in (2.29), $E_1(\phi^\infty) \le \lim_{n\to\infty} E_1(\phi^n)$ because of the lower semi-continuity of the H^1- and L_V^2-norm. Combining the results together, we know $E(\phi^\infty) \le \lim_{n\to\infty} E(\phi^n)$, which proves that ϕ^∞ is indeed a minimizer of the minimization problem (2.12). The uniqueness follows from the strict convexity of $E(\sqrt{\rho})$ as shown in Lemma 2.1.

(ii) Assume $\beta < 0$, or $\beta \ge 0$ and $\lambda < -\frac{1}{2}\beta$ or $\lambda > \beta$. Without loss of generality, we assume $\mathbf{n} = (0, 0, 1)^T$ and choose the function

$$\phi_{\varepsilon_1,\varepsilon_2}(\mathbf{x}) = \frac{1}{(2\pi\varepsilon_1)^{1/2}} \cdot \frac{1}{(2\pi\varepsilon_2)^{1/4}} \exp\left(-\frac{x^2+y^2}{2\varepsilon_1}\right) \exp\left(-\frac{z^2}{2\varepsilon_2}\right), \qquad \mathbf{x} \in \mathbb{R}^3, \qquad (2.37)$$

with ε_1 and ε_2 two small positive parameters (in fact, for general $\mathbf{n} \in \mathbb{R}^3$ satisfies $|\mathbf{n}| = 1$, we can always choose $0 \ne \mathbf{n}_1 \in \mathbb{R}^3$ and $0 \ne \mathbf{n}_2 \in \mathbb{R}^3$ such that $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}\}$ forms an orthonormal basis of $\mathbb{R}^3$ and do the change of variables $\mathbf{x} = (x, y, z)^T$ to $\mathbf{y} = (\mathbf{x}\cdot\mathbf{n}_1, \mathbf{x}\cdot\mathbf{n}_2, \mathbf{x}\cdot\mathbf{n})^T$ on the right hand side of (2.21), the following computation is still valid). Taking the standard Fourier transform at both sides of the Poisson equation

$$-\nabla^2\varphi_{\varepsilon_1,\varepsilon_2}(\mathbf{x}) = |\phi_{\varepsilon_1,\varepsilon_2}(\mathbf{x})|^2 = \rho_{\varepsilon_1,\varepsilon_2}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \qquad \lim_{|\mathbf{x}|\to\infty} \varphi_{\varepsilon_1,\varepsilon_2}(\mathbf{x}) = 0, \qquad (2.38)$$

we get

$$|\xi|^2\widehat{\varphi_{\varepsilon_1,\varepsilon_2}}(\xi) = \widehat{\rho_{\varepsilon_1,\varepsilon_2}}(\xi), \qquad \xi \in \mathbb{R}^3. \qquad (2.39)$$

Using the Plancherel formula and changing of variables, we obtain

$$\begin{aligned}
\|\partial_{\mathbf{n}}\nabla\varphi_{\varepsilon_1,\varepsilon_2}\|_2^2 &= \frac{1}{(2\pi)^3}\|(\mathbf{n}\cdot\xi)\widehat{\varphi_{\varepsilon_1,\varepsilon_2}}(\xi)\|_2^2 = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \frac{|\xi_3|^2}{|\xi|^2}\left|\widehat{\rho_{\varepsilon_1,\varepsilon_2}}(\xi)\right|^2 d\xi \\
&= \frac{1}{(2\pi)^3\varepsilon_1\sqrt{\varepsilon_2}}\int_{\mathbb{R}^3} \frac{|\xi_3|^2\,|\widehat{\rho_{1,1}}(\xi)|^2}{(|\xi_1|^2+|\xi_2|^2)\cdot\frac{\varepsilon_2}{\varepsilon_1} + |\xi_3|^2}\, d\xi, \quad \varepsilon_1, \varepsilon_2 > 0. \qquad (2.40)
\end{aligned}$$

By the dominated convergence theorem, we get

$$\|\partial_{\mathbf{n}}\nabla\varphi_{\varepsilon_1,\varepsilon_2}\|_2^2 \to \left\{ \begin{array}{ll} 0, & \varepsilon_2/\varepsilon_1 \to +\infty, \\ \displaystyle\int_{\mathbb{R}^3} \frac{|\widehat{\rho_{1,1}}(\xi)|^2}{(2\pi)^3\varepsilon_1\sqrt{\varepsilon_2}}\,d\xi = \|\rho_{\varepsilon_1,\varepsilon_2}\|_2^2 = \|\phi_{\varepsilon_1,\varepsilon_2}\|_4^4, & \varepsilon_2/\varepsilon_1 \to 0^+. \end{array} \right. \tag{2.41}$$

When fixed $\varepsilon_1\sqrt{\varepsilon_2}$, the last integral in (2.40) is continuous in $\varepsilon_2/\varepsilon_1 > 0$. Thus, for any $\alpha \in (0,1)$, by adjusting $\varepsilon_2/\varepsilon_1 := C_\alpha > 0$, we could have $\|\partial_{\mathbf{n}}\nabla\varphi_{\varepsilon_1,\varepsilon_2}\|_2^2 = \alpha\|\phi_{\varepsilon_1,\varepsilon_2}\|_4^4$. Substituting (2.37) into (2.29) and (2.30) with $\sqrt{\rho} = \phi_{\varepsilon_1,\varepsilon_2}$ under fixed $\varepsilon_2/\varepsilon_1 > 0$, we get

$$E_1(\phi_{\varepsilon_1,\varepsilon_2}) = \int_{\mathbb{R}^3} \left[|\nabla\phi_{\varepsilon_1,\varepsilon_2}|^2 + V(\mathbf{x})|\phi_{\varepsilon_1,\varepsilon_2}|^2\right] d\mathbf{x} = \frac{C_1}{\varepsilon_1} + \frac{C_2}{\varepsilon_2} + \mathcal{O}(1), \tag{2.42}$$

$$E_2(\phi_{\varepsilon_1,\varepsilon_2}) = \frac{1}{2}\int_{\mathbb{R}^3} (\beta - \lambda + 3\alpha\lambda))|\phi_{\varepsilon_1,\varepsilon_2}|^4\,d\mathbf{x} = \frac{\beta - \lambda + 3\alpha\lambda}{2}\cdot\frac{C_3}{\varepsilon_1\sqrt{\varepsilon_2}}, \tag{2.43}$$

with some constants C_1, C_2, $C_3 > 0$ independent of ε_1 and ε_2. Thus, if $\beta < 0$, choose $\alpha = 1/3$; if $\beta \geq 0$ and $\lambda < -\frac{1}{2}\beta$, choose $1/3 - \frac{\beta}{3\lambda} < \alpha < 1$; and if $\beta \geq 0$ and $\lambda > \beta$, choose $0 < \alpha < \frac{1}{3}\left(1 - \frac{\beta}{\lambda}\right)$; as ε_1, $\varepsilon_2 \to 0^+$, we can get $\inf_{\phi\in S_3} E(\phi) = \lim_{\varepsilon_1,\varepsilon_2\to 0^+} E_1(\phi_{\varepsilon_1,\varepsilon_2}) + E_2(\phi_{\varepsilon_1,\varepsilon_2}) = -\infty$, which implies that there exists no ground state of the minimization problem (2.12). □

By splitting the total energy $E(\cdot)$ in (2.21) into kinetic, potential, interaction and dipolar energies, i.e.

$$E(\phi) = E_{\text{kin}}(\phi) + E_{\text{pot}}(\phi) + E_{\text{int}}(\phi) + E_{\text{dip}}(\phi), \tag{2.44}$$

where

$$\begin{aligned} E_{\text{kin}}(\phi) &= \frac{1}{2}\int_{\mathbb{R}^3} |\nabla\phi(\mathbf{x})|^2 d\mathbf{x},\; E_{\text{pot}}(\phi) = \int_{\mathbb{R}^3} V(\mathbf{x})|\phi(\mathbf{x})|^2 d\mathbf{x},\; E_{\text{int}}(\phi) = \frac{\beta}{2}\int_{\mathbb{R}^3} |\phi(\mathbf{x})|^4 d\mathbf{x}, \\ E_{\text{dip}}(\phi) &= \frac{\lambda}{2}\int_{\mathbb{R}^3} \left(U_{\text{dip}} * |\phi|^2\right)|\phi(\mathbf{x})|^2 d\mathbf{x} = \frac{\lambda}{2}\int_{\mathbb{R}^3} |\phi(\mathbf{x})|^2\left[-|\phi(\mathbf{x})|^2 - 3\partial_{\mathbf{nn}}\varphi\right] d\mathbf{x} \\ &= \frac{\lambda}{2}\int_{\mathbb{R}^3} \left[-|\phi(\mathbf{x})|^4 + 3(\nabla^2\varphi)(\partial_{\mathbf{nn}}\varphi)\right] d\mathbf{x} = \frac{\lambda}{2}\int_{\mathbb{R}^3} \left[-|\phi(\mathbf{x})|^4 + 3\left|\partial_{\mathbf{n}}\nabla\varphi\right|^2\right] d\mathbf{x}, \end{aligned} \tag{2.45}$$

with φ defined in (2.23), we have the following Viral identity:

Proposition 2.1 *Suppose ϕ_e is a stationary state of a dipolar BEC, i.e. an eigenfunction of the nonlinear eigenvalue problem (2.10) under the constraint (2.11), then we have*

$$2E_{\text{kin}}(\phi_e) - 2E_{\text{pot}}(\phi_e) + 3E_{\text{int}}(\phi_e) + 3E_{\text{dip}}(\phi_e) = 0. \tag{2.46}$$

Proof: Follow the analogous proof for a BEC without dipolar interaction [117] and we omit the details here for brevity. □

2.2.2 Analytical results for dynamics

The well-posedness of the Cauchy problem of (2.1) was discussed in [42] by analyzing the convolution kernel $U_{\text{dip}}(\mathbf{x})$ with detailed Fourier transform. Under the new formulation (2.19)-(2.20), here we present a simpler proof for the well-posedness and show finite time blow-up for the Cauchy problem of a dipolar BEC in different parameter regimes. We consider the energy space Ξ_3 defined in (1.4).

Theorem 2.2 *(Well-posedness) Suppose the real-valued trap potential* $V(\mathbf{x}) \in C^\infty(\mathbb{R}^3)$ *such that* $V(\mathbf{x}) \geq 0$ *for* $\mathbf{x} \in \mathbb{R}^3$ *and* $D^\alpha V(\mathbf{x}) \in L^\infty(\mathbb{R}^3)$ *for all* $\alpha \in \mathbb{N}_0^3$ *with* $|\alpha| \geq 2$. *For any initial data* $\psi(\mathbf{x}, t=0) = \psi_0(\mathbf{x}) \in \Xi_3$, *there exists* $T_{\max} \in (0, +\infty]$ *such that the problem (2.19)-(2.20) has a unique maximal solution* $\psi \in C\left([0, T_{max}), \Xi_3\right)$. *It is maximal in the sense that if* $T_{\max} < \infty$, *then* $\|\psi(\cdot,t)\|_{\Xi_3} \to \infty$ *when* $t \to T_{\max}^-$. *Moreover, the mass* $N(\psi(\cdot,t))$ *and energy* $E(\psi(\cdot,t))$ *defined in (2.7) and (2.8), respectively, are conserved for* $t \in [0, T_{\max})$. *Specifically, if* $\beta \geq 0$ *and* $-\frac{1}{2}\beta \leq \lambda \leq \beta$, *the solution to (2.19)-(2.20) is global in time, i.e.,* $T_{max} = \infty$.

Proof: For any $\phi \in \Xi_3$, let φ be the solution of the Poisson equation (2.25), denote $\rho = |\phi|^2$ and define

$$G(\phi, \bar{\phi}) := G(\rho) = \frac{1}{2}\int_{\mathbb{R}^3} |\phi(\mathbf{x})|^2 \partial_{\mathbf{nn}}\varphi(\mathbf{x})\, d\mathbf{x}, \qquad g(\phi) = \frac{\delta G(\phi,\bar{\phi})}{\delta \bar{\phi}} = \phi\, \partial_{\mathbf{nn}}\varphi. \tag{2.47}$$

Noticing (2.26), it is easy to show that $G(\phi) \in C^1(\Xi_3, \mathbb{R})$, $g(\phi) \in C(\Xi_3, L^p)$ for some $p \in (6/5, 2]$, and

$$\|g(u) - g(v)\|_{L^p} \leq C(\|u\|_{\Xi_3} + \|v\|_{\Xi_3})\|u - v\|_{L^r}, \text{ for some } r \in [2, 6),\ \forall u, v \in \Xi_3. \tag{2.48}$$

Applying the standard Theorems 9.2.1, 4.12.1 and 5.7.1 in [43, 139] for the well-posedness of the nonlinear Schrödinger equation, we can obtain the results immediately. □

Theorem 2.3 *(Finite time blow-up) If $\beta < 0$, or $\beta \geq 0$ and $\lambda < -\frac{1}{2}\beta$ or $\lambda > \beta$, and assume $V(\mathbf{x})$ satisfies $3V(\mathbf{x}) + \mathbf{x} \cdot \nabla V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^3$. For any initial data $\psi(\mathbf{x}, t = 0) = \psi_0(\mathbf{x}) \in \Xi_3$ to the problem (2.19)-(2.20), there exists finite time blow-up, i.e., $T_{max} < \infty$, if one of the following holds:*

(i) $E(\psi_0) < 0$;

(ii) $E(\psi_0) = 0$ and $\mathrm{Im}\left(\int_{\mathbb{R}^3} \bar{\psi}_0(\mathbf{x})\ (\mathbf{x} \cdot \nabla\psi_0(\mathbf{x}))\, d\mathbf{x}\right) < 0$;

(iii) $E(\psi_0) > 0$ and $\mathrm{Im}\left(\int_{\mathbb{R}^3} \bar{\psi}_0(\mathbf{x})\ (\mathbf{x} \cdot \nabla\psi_0(\mathbf{x}))\, d\mathbf{x}\right) < -\sqrt{3E(\psi_0)}\|\mathbf{x}\psi_0\|_{L^2}$.

Proof: Define the variance

$$\sigma_V(t) := \sigma_V(\psi(\cdot, t)) = \int_{\mathbb{R}^3} |\mathbf{x}|^2 |\psi(\mathbf{x}, t)|^2\, d\mathbf{x} = \delta_x(t) + \delta_y(t) + \delta_z(t), \qquad t \geq 0, \tag{2.49}$$

where

$$\sigma_\alpha(t) := \sigma_\alpha(\psi(\cdot, t)) = \int_{\mathbb{R}^3} \alpha^2 |\psi(\mathbf{x}, t)|^2\, d\mathbf{x}, \qquad \alpha = x,\ y,\ z. \tag{2.50}$$

For $\alpha = x$, or y or z, differentiating (2.50) with respect to t, noticing (2.19) and (2.20), integrating by parts, we get

$$\frac{d}{dt}\sigma_\alpha(t) = -i \int_{\mathbb{R}^3} \left[\alpha\bar{\psi}(\mathbf{x}, t)\partial_\alpha\psi(\mathbf{x}, t) - \alpha\psi(\mathbf{x}, t)\partial_\alpha\bar{\psi}(\mathbf{x}, t)\right]\, d\mathbf{x}, \qquad t \geq 0. \tag{2.51}$$

Similarly, we have

$$\frac{d^2}{dt^2}\sigma_\alpha(t) = \int_{\mathbb{R}^3} \left[2|\partial_\alpha\psi|^2 + (\beta - \lambda)|\psi|^4 + 6\lambda|\psi|^2\alpha\partial_\alpha\partial_{\mathbf{nn}}\varphi - 2\alpha|\psi|^2\partial_\alpha V(\mathbf{x})\right]\, d\mathbf{x}. \tag{2.52}$$

Noticing (2.20) and

$$-\int_{\mathbb{R}^3} \nabla^2\varphi\, (\mathbf{x} \cdot \nabla\partial_{\mathbf{nn}}\varphi)\ d\mathbf{x} = \frac{3}{2}\int_{\mathbb{R}^3} |\partial_{\mathbf{n}}\nabla\varphi|^2\, d\mathbf{x},$$

summing (2.52) for $\alpha = x$, y and z, using (2.49) and (2.8), we get

$$\begin{aligned}
\frac{d^2}{dt^2}\sigma_V(t) &= 2\int_{\mathbb{R}^3} \left(|\nabla\psi|^2 + \frac{3}{2}(\beta - \lambda)|\psi|^4 + \frac{9}{2}\lambda|\partial_{\mathbf{n}}\nabla\psi|^2 - |\psi|^2(\mathbf{x} \cdot \nabla V(\mathbf{x}))\right) d\mathbf{x} \\
&= 6E(\psi) - \int_{\mathbb{R}^3} |\nabla\psi(\mathbf{x}, t)|^2 - 2\int_{\mathbb{R}^3} |\psi(\mathbf{x}, t)|^2\, (3V(\mathbf{x}) + \mathbf{x} \cdot \nabla V(\mathbf{x}))\ d\mathbf{x} \\
&\leq 6E(\psi) \equiv 6E(\psi_0), \qquad t \geq 0.
\end{aligned} \tag{2.53}$$

Thus,

$$\sigma_V(t) \leq 3E(\psi_0)t^2 + \sigma_V'(0)t + \sigma_V(0), \qquad t \geq 0,$$

and the conclusion follows in the same manner as those in [43, 139] for the standard nonlinear Schrödinger equation. □

2.3 A numerical method for computing ground states

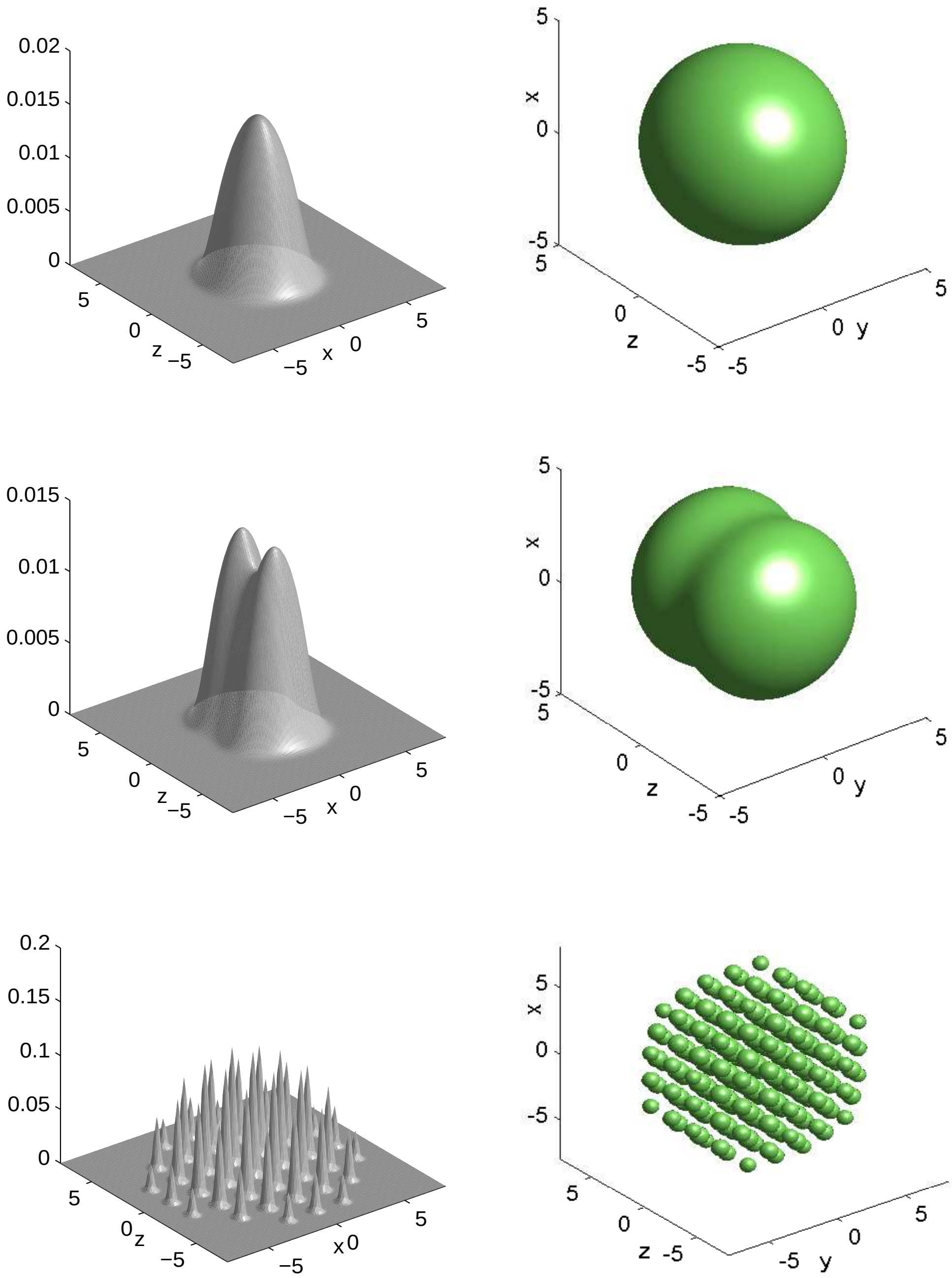

Figure 2.1: Surface plots of $|\phi_g(x,0,z)|^2$ (left column) and isosurface plots of $|\phi_g(x,y,z)| = 0.01$ (right column) for the ground state of a dipolar BEC with $\beta = 401.432$ and $\lambda = 0.16\beta$ for harmonic potential (top row), double-well potential (middle row) and optical lattice potential (bottom row).

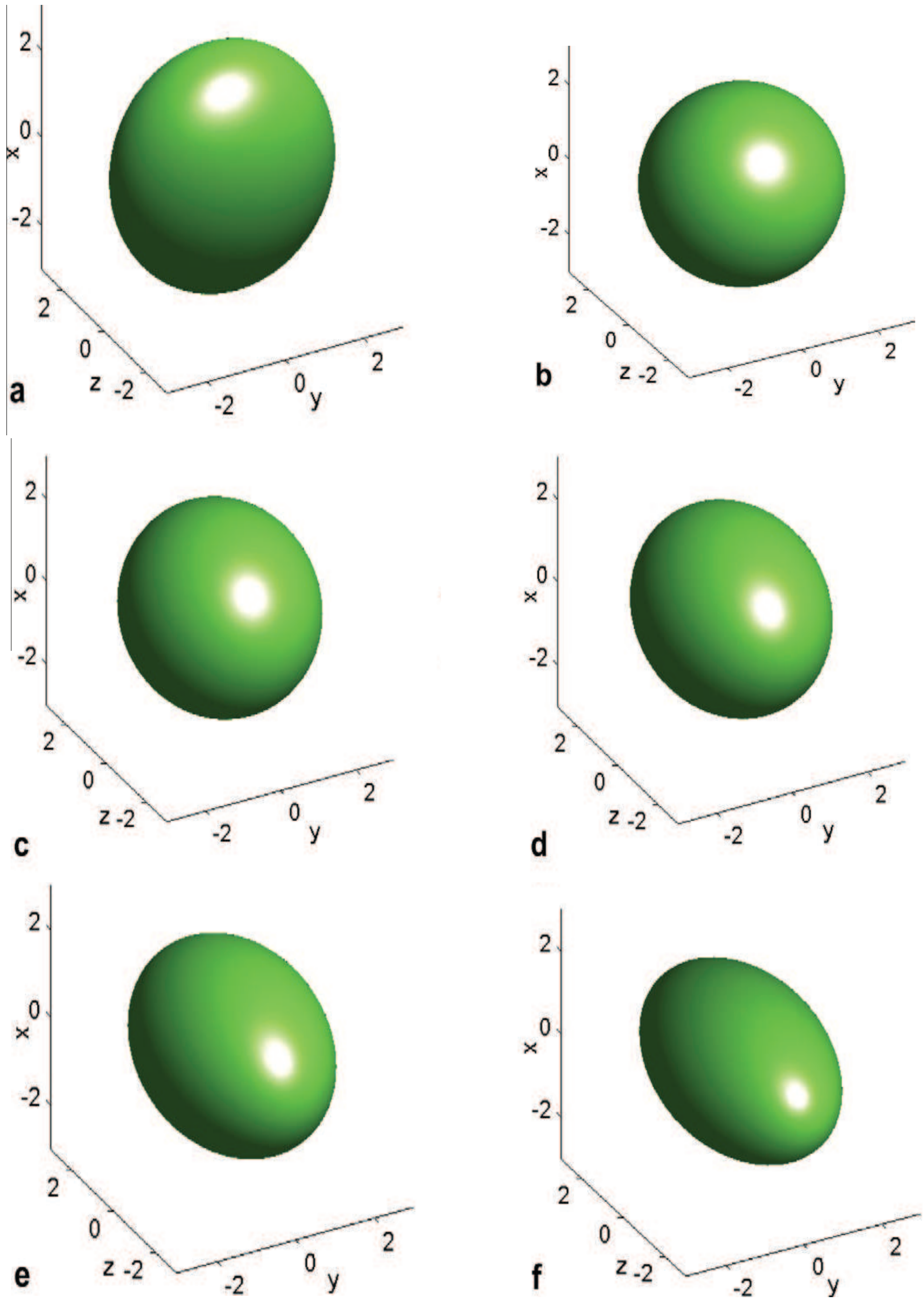

Figure 2.2: Isosurface plots of the ground state $|\phi_g(\mathbf{x})| = 0.08$ of a dipolar BEC with the harmonic potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2 + y^2 + z^2\right)$ and $\beta = 207.16$ for different values of $\frac{\lambda}{\beta}$: (a) $\frac{\lambda}{\beta} = -0.5$; (b) $\frac{\lambda}{\beta} = 0$; (c) $\frac{\lambda}{\beta} = 0.25$; (d) $\frac{\lambda}{\beta} = 0.5$; (e) $\frac{\lambda}{\beta} = 0.75$; (f) $\frac{\lambda}{\beta} = 1$.

Based on the new mathematical formulation for the energy in (2.21), we will present an efficient and accurate backward Euler sine pseudospectral method for computing the

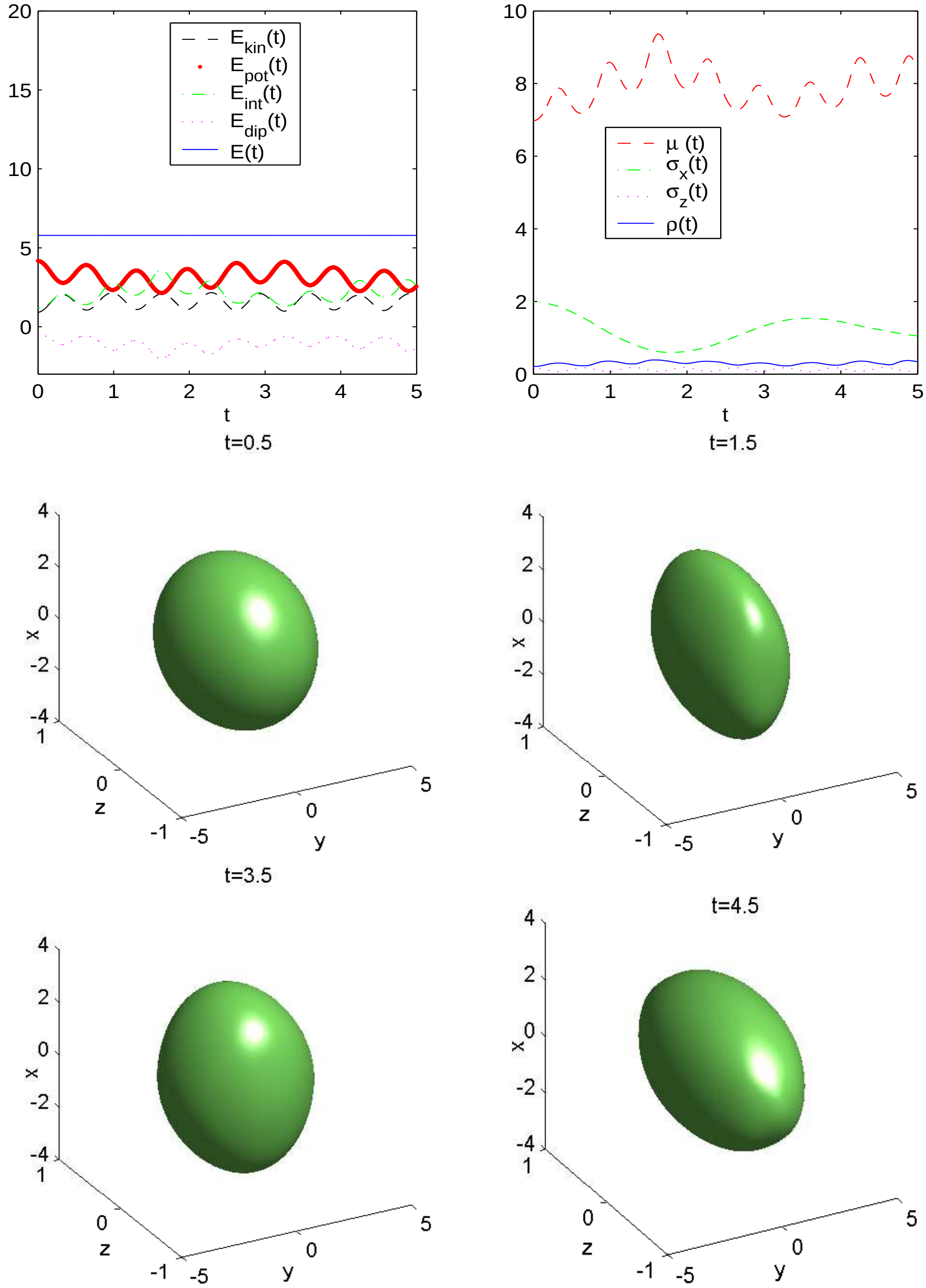

Figure 2.3: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at different times for a dipolar BEC when the dipolar direction is suddenly changed from $\mathbf{n} = (0, 0, 1)^T$ to $(1, 0, 0)^T$ at time $t = 0$.

ground states of a dipolar BEC.

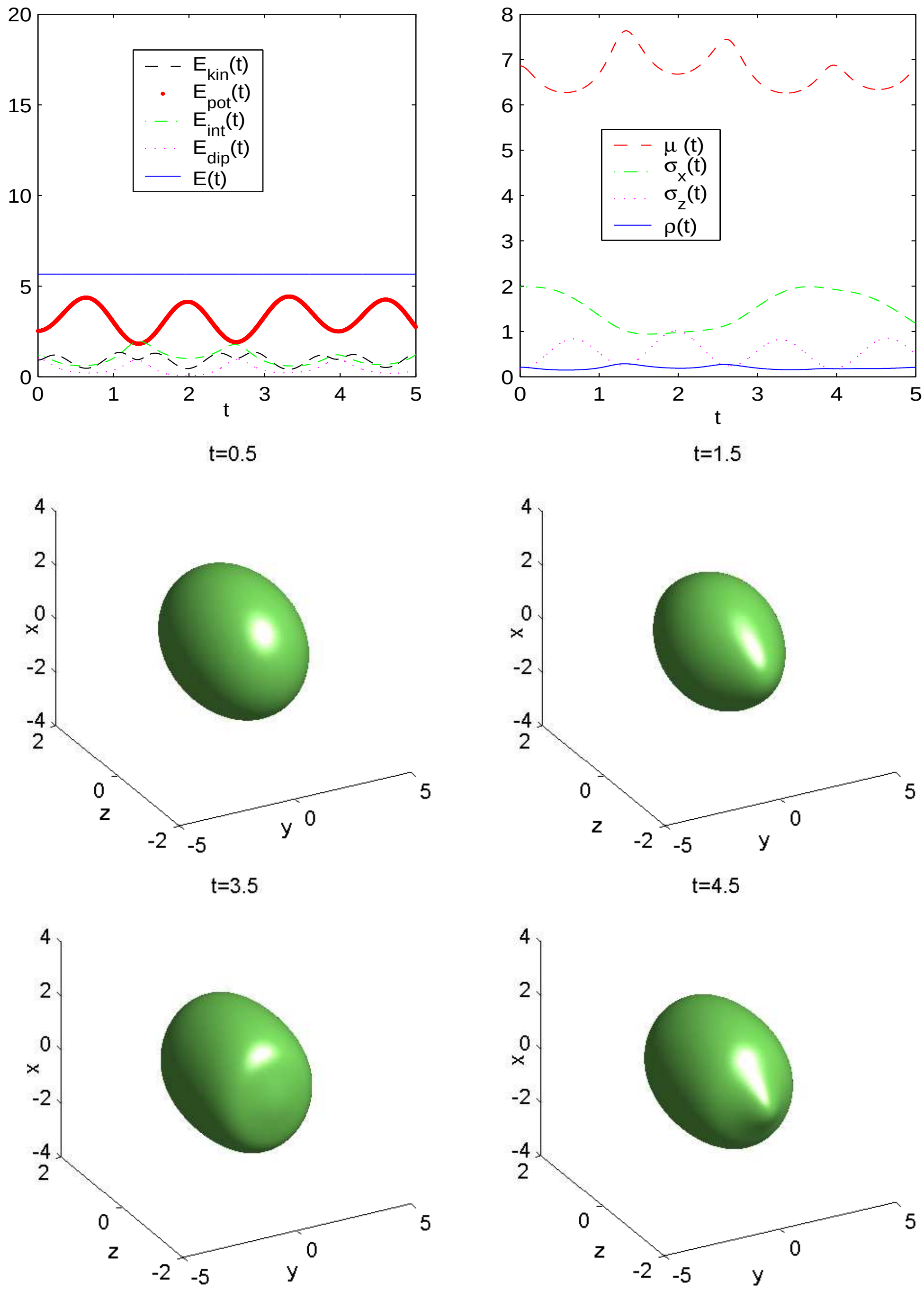

Figure 2.4: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at different times for a dipolar BEC when the trap potential is suddenly changed from from $\frac{1}{2}(x^2 + y^2 + 25z^2)$ to $\frac{1}{2}(x^2 + y^2 + \frac{25}{4}z^2)$ at time $t = 0$.

In practice, the whole space problem is usually truncated into a bounded computational domain $U = [a, b] \times [c, d] \times [e, f]$ with homogeneous Dirichlet boundary condition.

Various numerical methods have been proposed in the literatures for computing the ground states of BEC (see [10, 15, 18, 39, 48, 50, 126] and references therein). One of the popular and efficient techniques for dealing with the constraint (2.11) is through the following construction [10, 12, 15]: Choose a time step $\Delta t > 0$ and set $t_n = n\ \Delta t$ for $n = 0, 1, \ldots$ Applying the steepest decent method to the energy functional $E(\phi)$ in (2.21) without the constraint (2.11), and then projecting the solution back to the unit sphere S_3 at the end of each time interval $[t_n, t_{n+1}]$ in order to satisfy the constraint (2.11). This procedure leads to the fact that function $\phi(\mathbf{x}, t)$ is the solution of the following gradient flow with discrete normalization:

$$\partial_t \phi(\mathbf{x}, t) = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta - \lambda)|\phi(\mathbf{x}, t)|^2 + 3\lambda \partial_{\mathbf{nn}}\varphi(\mathbf{x}, t)\right]\phi(\mathbf{x}, t), \quad (2.54)$$

$$\nabla^2 \varphi(\mathbf{x}, t) = -|\phi(\mathbf{x}, t)|^2, \qquad \mathbf{x} \in U, \quad t_n \le t < t_{n+1}, \quad (2.55)$$

$$\phi(\mathbf{x}, t_{n+1}) := \phi(\mathbf{x}, t_{n+1}^+) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{\|\phi(\cdot, t_{n+1}^-)\|_2}, \qquad \mathbf{x} \in U, \quad n \ge 0, \quad (2.56)$$

$$\phi(\mathbf{x}, t)|_{\mathbf{x}\in\partial U} = \varphi(\mathbf{x}, t)|_{\mathbf{x}\in\partial U} = 0, \qquad t \ge 0, \quad (2.57)$$

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \qquad \text{with} \quad \|\phi_0\|_2 = 1; \quad (2.58)$$

where $\phi(\mathbf{x}, t_n^\pm) = \lim_{t \to t_n^\pm} \phi(\mathbf{x}, t)$.

Let M, K and L be even positive integers and define the index sets

$$\mathcal{T}_{MKL} = \{(j, k, l) \mid j = 1, 2, \ldots, M-1,\ k = 1, 2, \ldots, K-1,\ l = 1, 2, \ldots, L-1\},$$
$$\mathcal{T}_{MKL}^0 = \{(j, k, l) \mid j = 0, 1, \ldots, M,\ k = 0, 1, \ldots, K,\ l = 0, 1, \ldots, L\}.$$

Choose the spatial mesh sizes as $h_x = \frac{b-a}{M}$, $h_y = \frac{d-c}{K}$ and $h_z = \frac{f-e}{L}$ and define

$$x_j := a + j\ h_x, \qquad y_k = c + k\ h_y, \qquad z_l = e + l\ h_z, \qquad (j, k, l) \in \mathcal{T}_{MKL}^0.$$

Denote the space

$$Y_{MKL} = \text{span}\{\Phi_{jkl}(\mathbf{x}), \quad (j, k, l) \in \mathcal{T}_{MKL}\},$$

with

$$\Phi_{jkl}(\mathbf{x}) = \sin\left(\mu_j^x (x-a)\right) \sin\left(\mu_k^y (y-c)\right) \sin\left(\mu_l^z (z-e)\right), \quad \mathbf{x} \in U, \qquad (j, k, l) \in \mathcal{T}_{MKL},$$

$$\mu_j^x = \frac{\pi j}{b-a}, \qquad \mu_k^y = \frac{\pi k}{d-c}, \qquad \mu_l^z = \frac{\pi l}{f-e}, \qquad (j, k, l) \in \mathcal{T}_{MKL};$$

and $P_{MKL} : Y = \{\varphi \in C(U) \mid \varphi(\mathbf{x})|_{\mathbf{x}\in\partial U} = 0\} \to Y_{MKL}$ be the standard project operator [131], i.e.

$$(P_{MKL}v)(\mathbf{x}) = \sum_{p=1}^{M-1}\sum_{q=1}^{K-1}\sum_{s=1}^{L-1} \widehat{v}_{pqs}\ \Phi_{pqs}(\mathbf{x}), \quad \mathbf{x} \in U, \qquad \forall v \in Y,$$

with

$$\widehat{v}_{pqs} = \frac{8}{(b-a)(d-c)(f-e)} \int_U v(\mathbf{x})\ \Phi_{pqs}(\mathbf{x})\ d\mathbf{x}, \qquad (p,q,s) \in \mathcal{T}_{MKL}. \tag{2.59}$$

Then a backward Euler sine spectral discretization for (2.54)-(2.58) reads:
Find $\phi^{n+1}(\mathbf{x}) \in Y_{MKL}$ (i.e. $\phi^{+}(\mathbf{x}) \in Y_{MKL}$) and $\varphi^{n}(\mathbf{x}) \in Y_{MKL}$ such that

$$\frac{\phi^+(\mathbf{x}) - \phi^n(\mathbf{x})}{\Delta t} = \frac{1}{2}\nabla^2\phi^+(\mathbf{x}) - P_{MKL}\left\{\left[V(\mathbf{x}) + (\beta-\lambda)|\phi^n(\mathbf{x})|^2 - 3\lambda\partial_{\mathbf{nn}}\varphi^n(\mathbf{x})\right]\phi^+(\mathbf{x})\right\},$$
$$\nabla^2\varphi^n(\mathbf{x}) = -P_{MKL}\left(|\phi^n(\mathbf{x})|^2\right), \qquad \phi^{n+1}(\mathbf{x}) = \frac{\phi^+(\mathbf{x})}{\|\phi^+(\mathbf{x})\|_2}, \qquad \mathbf{x} \in U, \quad n \geq 0;$$

where $\phi^0(\mathbf{x}) = P_{MKL}\left(\phi_0(\mathbf{x})\right)$ is given.

The above discretization can be solved in phase space and it is not suitable in practice due to the difficulty of computing the integrals in (2.59). We now present an efficient implementation by choosing $\phi^0(\mathbf{x})$ as the interpolation of $\phi_0(\mathbf{x})$ on the grid points $\{(x_j, y_k, z_l),\ (j,k,l) \in \mathcal{T}^0_{MKL}\}$, i.e. $\phi^0(x_j,y_k,z_l) = \phi_0(x_j,y_k,z_l)$ for $(j,k,l) \in \mathcal{T}^0_{MKL}$, and approximating the integrals in (2.59) by a quadrature rule on the grid points. Let ϕ^n_{jkl} and φ^n_{jkl} be the approximations of $\phi(x_j,y_k,z_l,t_n)$ and $\varphi(x_j,y_k,z_l,t_n)$, respectively, which are the solution of (2.54)-(2.58); denote $\rho^n_{jkl} = |\phi^n_{jkl}|^2$ and choose $\phi^0_{jkl} = \phi_0(x_j,y_k,z_l)$ for $(j,k,l) \in \mathcal{T}^0_{MKL}$. For $n = 0, 1, \ldots$, a backward Euler sine pseudospectral discretization for (2.54)-(2.58) reads:

$$\frac{\phi^+_{jkl} - \phi^n_{jkl}}{\Delta t} = \frac{1}{2}\left(\nabla^2_s\phi^+\right)\big|_{jkl} - \left[V(x_j,y_k,z_l) + (\beta-\lambda)\left|\phi^n_{jkl}\right|^2 - 3\lambda\left(\partial^s_{\mathbf{nn}}\varphi^n\right)\big|_{jkl}\right]\phi^+_{jkl}, \tag{2.60}$$

$$-\left(\nabla^2_s\varphi^n\right)\big|_{jkl} = |\phi^n_{j,k,l}|^2 = \rho^n_{jkl}, \qquad \phi^{n+1}_{jkl} = \frac{\phi^+_{jkl}}{\|\phi^+\|_h}, \qquad (j,k,l) \in \mathcal{T}_{MKL}, \tag{2.61}$$

$$\phi^{n+1}_{0kl} = \phi^{n+1}_{Mkl} = \phi^{n+1}_{j0l} = \phi^{n+1}_{jKl} = \phi^{n+1}_{jk0} = \phi^{n+1}_{jkL} = 0, \qquad (j,k,l) \in \mathcal{T}^0_{MKL}, \tag{2.62}$$

$$\varphi^{n}_{0kl} = \varphi^{n}_{Mkl} = \varphi^{n}_{j0l} = \varphi^{n}_{jKl} = \varphi^{n}_{jk0} = \varphi^{n}_{jkL} = 0, \qquad (j,k,l) \in \mathcal{T}^0_{MKL}; \tag{2.63}$$

where ∇^2_s and $\partial^s_{\mathbf{nn}}$ are sine pseudospectral approximations of ∇^2 and $\partial_{\mathbf{nn}}$, respectively, defined as

$$\left(\nabla^2_s\phi^n\right)\big|_{jkl} = -\sum_{p=1}^{M-1}\sum_{q=1}^{K-1}\sum_{s=1}^{L-1}\left[(\mu^x_p)^2 + (\mu^y_q)^2 + (\mu^z_s)^2\right]\widetilde{(\phi^n)}_{pqs}\sin\left(\frac{jp\pi}{M}\right)\sin\left(\frac{kq\pi}{K}\right)\sin\left(\frac{ls\pi}{L}\right),$$
$$\left(\partial^s_{\mathbf{nn}}\varphi^n\right)\Big|_{jkl} = \sum_{p=1}^{M-1}\sum_{q=1}^{K-1}\sum_{s=1}^{L-1}\frac{\widetilde{(\rho^n)}_{pqs}}{(\mu^x_p)^2 + (\mu^y_q)^2 + (\mu^z_s)^2}\left(\partial_{\mathbf{nn}}\Phi_{pqs}(\mathbf{x})\right)\Big|_{(x_j,y_k,z_l)}, \tag{2.64}$$

for $(j,k,l) \in \mathcal{T}_{MKL}$ with $\widetilde{(\phi^n)}_{pqs}$ $((p,q,s) \in \mathcal{T}_{MKL})$ the discrete sine transform coefficients of the vector ϕ^n as

$$\widetilde{(\phi^n)}_{pqs} = \frac{8}{MKL} \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} \phi^n_{jkl} \sin\left(\frac{jp\pi}{M}\right) \sin\left(\frac{kq\pi}{K}\right) \sin\left(\frac{ls\pi}{L}\right), \quad (p,q,s) \in \mathcal{T}_{MKL}, \quad (2.65)$$

and the discrete h-norm is defined as

$$\|\phi^+\|_h^2 = h_x h_y h_z \sum_{j=1}^{M-1} \sum_{k=1}^{N-1} \sum_{l=1}^{L-1} |\phi^+_{jkl}|^2.$$

Similar as those in [19], the linear system (2.60)-(2.63) can be iteratively solved in phase space very efficiently via discrete sine transform and we omitted the details here for brevity.

2.4 A time-splitting pseudospectral method for dynamics

Similarly, based on the new Gross-Pitaevskii-Poisson type system (2.19)-(2.20), we will present an efficient and accurate time-splitting sine pseudospectral (TSSP) method for computing the dynamics of a dipolar BEC.

Again, in practice, the whole space problem is truncated into a bounded computational domain $U = [a,b] \times [c,d] \times [e,f]$ with homogeneous Dirichlet boundary condition. From time $t = t_n$ to time $t = t_{n+1}$, the Gross-Pitaevskii-Poisson type system (2.19)-(2.20) is solved in two steps. One solves first

$$i\partial_t \psi(\mathbf{x},t) = -\frac{1}{2}\nabla^2 \psi(\mathbf{x},t), \quad \mathbf{x} \in U, \qquad \psi(\mathbf{x},t)|_{\mathbf{x}\in\partial U} = 0, \qquad t_n \le t \le t_{n+1}, \quad (2.66)$$

for the time step of length Δt, followed by solving

$$i\partial_t \psi(\mathbf{x},t) = \left[V(\mathbf{x}) + (\beta - \lambda)|\psi(\mathbf{x},t)|^2 - 3\lambda \partial_{\mathbf{nn}} \varphi(\mathbf{x},t)\right] \psi(\mathbf{x},t), \quad (2.67)$$

$$\nabla^2 \varphi(\mathbf{x},t) = -|\psi(\mathbf{x},t)|^2, \qquad \mathbf{x} \in U, \qquad t_n \le t \le t_{n+1}; \quad (2.68)$$

$$\varphi(\mathbf{x},t)|_{\mathbf{x}\in\partial U} = 0, \qquad \psi(\mathbf{x},t)|_{\mathbf{x}\in\partial U} = 0, \qquad t_n \le t \le t_{n+1}; \quad (2.69)$$

for the same time step. Equation (2.66) will be discretized in space by sine pseudospectral method and integrated in time *exactly* [23]. For $t \in [t_n, t_{n+1}]$, the equations (2.67)-(2.69) leave $|\psi|$ and φ invariant in t [18, 23] and therefore they collapse to

$$i\partial_t \psi(\mathbf{x},t) = \left[V(\mathbf{x}) + (\beta - \lambda)|\psi(\mathbf{x},t_n)|^2 - 3\lambda \partial_{\mathbf{nn}} \varphi(\mathbf{x},t_n)\right] \psi(\mathbf{x},t), \quad \mathbf{x} \in U, \ t_n \le t \le t_{n+1}, \quad (2.70)$$

$$\nabla^2 \varphi(\mathbf{x},t_n) = -|\psi(\mathbf{x},t_n)|^2, \qquad \mathbf{x} \in U. \quad (2.71)$$

Again, equation (2.71) will be discretized in space by sine pseudospectral method [23,131] and the linear ODE (2.70) can be integrated in time *exactly* [18,23].

Let ψ^n_{jkl} and φ^n_{jkl} be the approximations of $\psi(x_j, y_k, z_l, t_n)$ and $\varphi(x_j, y_k, z_l, t_n)$, respectively, which are the solutions of (2.19)-(2.20); and choose $\psi^0_{jkl} = \psi_0(x_j, y_k, z_l)$ for $(j,k,l) \in \mathcal{T}^0_{MKL}$. For $n = 0, 1, \ldots$, a second-order TSSP method for solving (2.19)-(2.20) via the standard Strang splitting is [18,23,135]

$$\begin{aligned}
\psi^{(1)}_{jkl} &= \sum_{p=1}^{M-1}\sum_{q=1}^{K-1}\sum_{s=1}^{L-1} e^{-i\triangle t\left[(\mu^x_p)^2+(\mu^y_q)^2+(\mu^z_s)^2\right]/4}\,\widetilde{(\psi^n)}_{pqs}\sin\left(\frac{jp\pi}{M}\right)\sin\left(\frac{kq\pi}{K}\right)\sin\left(\frac{ls\pi}{L}\right),\\
\psi^{(2)}_{jkl} &= e^{-i\triangle t\left[V(x_j,y_k,z_l)+(\beta-\lambda)|\psi^{(1)}_{jkl}|^2-3\lambda\left(\partial^s_{\mathbf{nn}}\varphi^{(1)}\right)\big|_{jkl}\right]}\,\psi^{(1)}_{jkl}, \qquad (j,k,l)\in\mathcal{T}^0_{MKL}, \qquad (2.72)\\
\psi^{n+1}_{jkl} &= \sum_{p=1}^{M-1}\sum_{q=1}^{K-1}\sum_{s=1}^{L-1} e^{-i\triangle t\left[(\mu^x_p)^2+(\mu^y_q)^2+(\mu^z_s)^2\right]/4}\,\widetilde{(\psi^{(2)})}_{pqs}\sin\left(\frac{jp\pi}{M}\right)\sin\left(\frac{kq\pi}{K}\right)\sin\left(\frac{ls\pi}{L}\right);
\end{aligned}$$

where $\widetilde{(\psi^n)}_{pqs}$ and $\widetilde{(\psi^{(2)})}_{pqs}$ ($(p,q,s) \in \mathcal{T}_{MKL}$) are the discrete sine transform coefficients of the vectors ψ^n and $\psi^{(2)}$, respectively (defined similar as those in (2.65)); and $\left(\partial^s_{\mathbf{nn}}\varphi^{(1)}\right)\big|_{jkl}$ can be computed as in (2.64) with $\rho^n_{jkl} = \rho^{(1)}_{jkl} := |\psi^{(1)}_{jkl}|^2$ for $(j,k,l) \in \mathcal{T}^0_{MKL}$.

The above method is explicit, unconditionally stable, the memory cost is $O(MKL)$ and the computational cost per time step is $O\left(MKL\ln(MKL)\right)$. In fact, for the stability, we have

Lemma 2.2 *The TSSP method (2.72) is normalization conservation, i.e.*

$$\|\psi^n\|^2_h := h_x h_y h_z \sum_{j=1}^{M-1}\sum_{k=1}^{K-1}\sum_{l=1}^{L-1}|\psi^n_{jkl}|^2 \equiv h_x h_y h_z \sum_{j=1}^{M-1}\sum_{k=1}^{K-1}\sum_{l=1}^{L-1}|\psi^0_{jkl}|^2 = \|\psi^0\|^2_h, \;\; n \geq 0.$$

Proof: Follow the analogous proof in [18,23] and we omit the details here for brevity. □

2.5 Numerical results

In this section, we first compare our new methods and the standard method used in the literatures [33,147,160,163] to evaluate numerically the dipolar energy and then report ground states and dynamics of dipolar BECs by using our new numerical methods.

2.5.1 Comparison for evaluating the dipolar energy

Let

$$\phi := \phi(\mathbf{x}) = \pi^{-3/4}\gamma_x^{1/2}\gamma_z^{1/4}e^{-\frac{1}{2}\left(\gamma_x(x^2+y^2)+\gamma_z z^2\right)}, \qquad \mathbf{x}\in\mathbb{R}^3. \qquad (2.73)$$

Then the dipolar energy $E_{\rm dip}(\phi)$ in (2.45) can be evaluated analytically as [148]

$$E_{\rm dip}(\phi) = -\frac{\lambda\gamma_x\sqrt{\gamma_z}}{4\pi\sqrt{2\pi}} \begin{cases} \frac{1+2\kappa^2}{1-\kappa^2} - \frac{3\kappa^2 \arctan\left(\sqrt{\kappa^2-1}\right)}{(1-\kappa^2)\sqrt{\kappa^2-1}}, & \kappa > 1, \\ 0, & \kappa = 1, \\ \frac{1+2\kappa^2}{1-\kappa^2} - \frac{1.5\kappa^2}{(1-\kappa^2)\sqrt{1-\kappa^2}} \ln\left(\frac{1+\sqrt{1-\kappa^2}}{1-\sqrt{1-\kappa^2}}\right), & \kappa < 1, \end{cases} \tag{2.74}$$

with $\kappa = \sqrt{\frac{\gamma_z}{\gamma_x}}$. This provides a perfect example to test the efficiency of different numerical methods to deal with the dipolar potential. Based on our new formulation (2.45), the dipolar energy can be evaluated via discrete sine transform (DST) as

$$E_{\rm dip}(\phi) \approx \frac{\lambda h_x h_y h_z}{2} \sum_{j=1}^{M-1} \sum_{k=1}^{K-1} \sum_{l=1}^{L-1} |\phi(x_j, y_k, z_l)|^2 \left[-|\phi(x_j, y_k, z_l)|^2 - 3 \left(\partial^s_{\mathbf{nn}} \varphi^n\right)|_{jkl} \right],$$

where $(\partial^s_{\mathbf{nn}}\varphi^n)|_{jkl}$ is computed as in (2.64) with $\rho^n_{jkl} = |\phi(x_j, y_k, z_l)|^2$ for $(j,k,l) \in \mathcal{T}^0_{MKL}$. In the literatures [33, 147, 160, 163], this dipolar energy is usually calculated via discrete Fourier transform (DFT) as

$$E_{\rm dip}(\phi) \approx \frac{\lambda h_x h_y h_z}{2} \sum_{j=0}^{M-1} \sum_{k=0}^{K-1} \sum_{l=0}^{L-1} |\phi(x_j, y_k, z_l)|^2 \left[\mathcal{F}^{-1}_{jkl} \left(\widehat{(U_{\rm dip})}(2\mu^x_p, 2\mu^y_q, 2\mu^z_s) \cdot \mathcal{F}_{pqs}(|\phi|^2) \right) \right],$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are the discrete Fourier and inverse Fourier transforms over the grid points $\{(x_j, y_k, z_l),\ (j,k,l) \in \mathcal{T}^0_{MKL}\}$, respectively [160]. We take $\lambda = 24\pi$, the bounded computational domain $U = [-16, 16]^3$, $M = K = L$ and thus $h = h_x = h_y = h_z = \frac{32}{M}$. Tab. 2.1 lists the errors $e := \left|E_{\rm dip}(\phi) - E^h_{\rm dip}\right|$ with $E^h_{\rm dip}$ computed numerically via either (2.75) or (2.75) with mesh size h for three cases:

- Case I. $\gamma_x = 0.25$ and $\gamma_z = 1$ which implies $\kappa = 2.0$ and $E_{\rm dip}(\phi) = 0.0386708614$;
- Case II. $\gamma_x = \gamma_z = 1$ which implies $\kappa = 1.0$ and $E_{\rm dip}(\phi) = 0$;
- Case III. $\gamma_x = 2$ and $\gamma_z = 1$ which implies $\kappa = \sqrt{0.5}$ and $E_{\rm dip}(\phi) = -0.1386449741$.

From Tab. 2.1 and our extensive numerical results not shown here for brevity, we can conclude that our new method via discrete sine transform based on a new formulation is much more accurate than that of the standard method via discrete Fourier transform in the literatures for evaluating the dipolar energy.

	Case I		Case II		Case III	
	DST	DFT	DST	DFT	DST	DFT
$M = 32\&h = 1$	2.756E-2	2.756E-2	3.555E-18	1.279E-4	0.1018	0.1020
$M = 64\&h = 0.5$	1.629E-3	1.614E-3	9.154E-18	1.278E-4	9.788E-5	2.269E-4
$M = 128\&h = 0.25$	1.243E-7	1.588E-5	7.454E-17	1.278E-4	6.406E-7	1.284E-4

Table 2.1: Comparison for evaluating dipolar energy under different mesh sizes h.

2.5.2 Ground states of dipolar BECs

By using our new numerical method (2.60)-(2.63), here we report the ground states of a dipolar BEC (e.g., ^{52}Cr [115]) with different parameters and trapping potentials. In our computation and results, we always use the dimensionless quantities. We take $M = K = L = 128$, time step $\Delta t = 0.01$, dipolar direction $\mathbf{n} = (0,0,1)^T$ and the bounded computational domain $U = [-8,8]^3$ for all cases except $U = [-16,16]^3$ for the cases $\frac{N}{1000} = 1,\ 5,\ 10$ and $U = [-20,20]^3$ for the cases $\frac{N}{1000} = 50,\ 100$ in Tab. 2.2. The ground state ϕ_g is reached numerically when $\|\phi^{n+1}-\phi^n\|_\infty := \max_{0\le j\le M,\ 0\le k\le K,\ 0\le l\le L} |\phi_{jkl}^{n+1} - \phi_{jkl}^n| \le \varepsilon := 10^{-6}$ in (2.60)-(2.63). Tab. 2.2 shows the energy $E^g := E(\phi_g)$, chemical potential $\mu^g := \mu(\phi_g)$, kinetic energy $E^g_{\text{kin}} := E_{\text{kin}}(\phi_g)$, potential energy $E^g_{\text{pot}} := E_{\text{pot}}(\phi_g)$, interaction energy $E^g_{\text{int}} := E_{\text{int}}(\phi_g)$, dipolar energy $E^g_{\text{dip}} := E_{\text{dip}}(\phi_g)$, condensate widths $\sigma^g_x := \sigma_x(\phi_g)$ and $\sigma^g_z := \sigma_z(\phi_g)$ in (2.50) and central density $\rho_g(\mathbf{0}) := |\phi_g(0,0,0)|^2$ with harmonic potential $V(x,y,z) = \frac{1}{2}\left(x^2+y^2+0.25z^2\right)$ for different $\beta = 0.20716N$ and $\lambda = 0.033146N$ with N the total number of particles in the condensate; and Tab. 2.3 lists similar results with $\beta = 207.16$ for different values of $-0.5 \le \frac{\lambda}{\beta} \le 1$. In addition, Fig. 2.1 depicts the ground state $\phi_g(\mathbf{x})$, e.g. surface plots of $|\phi_g(x,0,z)|^2$ and isosurface plots of $|\phi_g(\mathbf{x})| = 0.01$, of a dipolar BEC with $\beta = 401.432$ and $\lambda = 0.16\beta$ for harmonic potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2+y^2+z^2\right)$, double-well potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2+y^2+z^2\right) + 4e^{-z^2/2}$ and optical lattice potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2+y^2+z^2\right) + 100\left[\sin^2\left(\frac{\pi}{2}x\right) + \sin^2\left(\frac{\pi}{2}y\right) + \sin^2\left(\frac{\pi}{2}z\right)\right]$; and Fig. 2.2 depicts the ground state $\phi_g(\mathbf{x})$, e.g. isosurface plots of $|\phi_g(\mathbf{x})| = 0.08$, of a dipolar BEC with the harmonic potential $V(\mathbf{x}) = \frac{1}{2}\left(x^2+y^2+z^2\right)$ and $\beta = 207.16$ for different values of $-0.5 \le \frac{\lambda}{\beta} \le 1$.

From Tabs. 2.2&2.3 and Figs. 2.1&2.2, we can draw the following conclusions: (i) For fixed trapping potential $V(\mathbf{x})$ and dipolar direction $\mathbf{n} = (0,0,1)^T$, when β and λ increase with the ratio $\frac{\lambda}{\beta}$ fixed, the energy E^g, chemical potential μ^g, potential energy

$\frac{N}{1000}$	E^g	μ^g	$E^g_{\rm kin}$	$E^g_{\rm pot}$	$E^g_{\rm int}$	$E^g_{\rm dip}$	σ^g_x	σ^g_z	$\rho_g(\mathbf{0})$
0.1	1.567	1.813	0.477	0.844	0.262	-0.015	0.796	1.299	0.06139
0.5	2.225	2.837	0.349	1.264	0.659	-0.047	0.940	1.745	0.02675
1	2.728	3.583	0.296	1.577	0.925	-0.070	1.035	2.009	0.01779
5	4.745	6.488	0.195	2.806	1.894	-0.151	1.354	2.790	0.00673
10	6.147	8.479	0.161	3.654	2.536	-0.204	1.538	3.212	0.00442
50	11.47	15.98	0.101	6.853	4.909	-0.398	2.095	4.441	0.00168
100	15.07	21.04	0.082	9.017	6.498	-0.526	2.400	5.103	0.00111

Table 2.2: Different quantities of the ground states of a dipolar BEC for $\beta = 0.20716N$ and $\lambda = 0.033146N$ with different number of particles N.

$\frac{\lambda}{\beta}$	E^g	μ^g	E^g_{kin}	E^g_{pot}	E^g_{int}	E^g_{dip}	σ^g_x	σ^g_z	$\rho_g(\mathbf{0})$
-0.5	2.957	3.927	0.265	1.721	0.839	0.131	1.153	1.770	0.01575
-0.25	2.883	3.817	0.274	1.675	0.853	0.081	1.111	1.879	0.01605
0	2.794	3.684	0.286	1.618	0.890	0.000	1.066	1.962	0.01693
0.25	2.689	3.525	0.303	1.550	0.950	-0.114	1.017	2.030	0.01842
0.5	2.563	3.332	0.327	1.468	1.047	-0.278	0.960	2.089	0.02087
0.75	2.406	3.084	0.364	1.363	1.212	-0.534	0.889	2.141	0.02536
1.0	2.193	2.726	0.443	1.217	1.575	-1.041	0.786	2.189	0.03630

Table 2.3: Different quantities of the ground states of a dipolar BEC with different values of $\frac{\lambda}{\beta}$ with $\beta = 207.16$.

$E^g_{\rm pot}$, interaction energy $E^g_{\rm int}$, condensate widths σ^g_x and σ^g_z of the ground states increase; and resp., the kinetic energy $E^g_{\rm kin}$, dipolar energy $E^g_{\rm dip}$ and central density $\rho_g(\mathbf{0})$ decrease (cf. Tab. 2.2). (ii) For fixed trapping potential $V(\mathbf{x})$, dipolar direction $\mathbf{n} = (0,0,1)^T$ and β, when the ratio $\frac{\lambda}{\beta}$ increases from -0.5 to 1, the kinetic energy $E^g_{\rm kin}$, interaction energy $E^g_{\rm int}$, condensate widths σ^g_z and central density $\rho_g(\mathbf{0})$ of the ground states increase; and resp., the energy E^g, chemical potential μ^g, potential energy $E^g_{\rm pot}$, dipolar energy $E^g_{\rm dip}$ and condensate widths σ^g_x decrease (cf. Tab. 2.3). (iii) Our new numerical method can compute the ground states accurately and efficiently (cf. Figs. 2.1&2.2).

2.5.3 Dynamics of dipolar BECs

Similarly, by using our new numerical method (2.72), here we report the dynamics of a dipolar BEC (e.g., ^{52}Cr [115]) under different setups. Again, in our computation and results, we always use the dimensionless quantities. We take the bounded computational domain $U = [-8,8]^2 \times [-4,4]$, $M = K = L = 128$, i.e. $h = h_x = h_y = 1/8, h_z = 1/16$, time step $\Delta t = 0.001$. The initial data $\psi(\mathbf{x},0) = \psi_0(\mathbf{x})$ is chosen as the ground state of a dipolar BEC computed numerically by our numerical method with $\mathbf{n} = (0,0,1)^T$, $V(\mathbf{x}) = \frac{1}{2}(x^2+y^2+25z^2)$, $\beta = 103.58$ and $\lambda = 0.8\beta = 82.864$.

The first case to study numerically is the dynamics of suddenly changing the dipolar direction from $\mathbf{n} = (0,0,1)^T$ to $\mathbf{n} = (1,0,0)^T$ at $t = 0$ and keeping all other quantities unchanged. Fig. 2.3 depicts time evolution of the energy $E(t) := E(\psi(\cdot,t))$, chemical potential $\mu(t) = \mu(\psi(\cdot,t)$, kinetic energy $E_{\text{kin}}(t) := E_{\text{kin}}(\psi(\cdot,t))$, potential energy $E_{\text{pot}}(t) := E_{\text{pot}}(\psi(\cdot,t))$, interaction energy $E_{\text{int}}(t) := E_{\text{int}}(\psi(\cdot,t))$, dipolar energy $E_{\text{dip}}(t) := E_{\text{dip}}(\psi(\cdot,t))$, condensate widths $\sigma_x(t) := \sigma_x(\psi(\cdot,t))$, $\sigma_z(t) := \sigma_z(\psi(\cdot,t))$, and central density $\rho(t) := |\psi(\mathbf{0},t)|^2$, as well as the isosurface of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ for different times. In addition, Fig. 2.4 show similar results for the case of suddenly changing the trapping potential from $V(\mathbf{x}) = \frac{1}{2}(x^2+y^2+25z^2)$ to $V(\mathbf{x}) = \frac{1}{2}(x^2+y^2+\frac{25}{4}z^2)$ at $t = 0$, i.e. decreasing the trapping frequency in z-direction from 5 to $\frac{5}{2}$, and keeping all other quantities unchanged; Fig. 2.5 show the results for the case of suddenly changing the dipolar interaction from $\lambda = 0.8\beta = 82.864$ to $\lambda = 4\beta = 414.32$ at $t = 0$ while keeping all other quantities unchanged, i.e. collapse of a dipolar BEC; and Fig. 2.6 show the results for the case of suddenly changing the interaction constant β from $\beta = 103.58$ to $\beta = -569.69$ at $t = 0$ while keeping all other quantities unchanged, i.e. another collapse of a dipolar BEC.

From Figs. 2.3, 2.4, 2.5 and 2.6, we can conclude that the dynamics of dipolar BEC can be very interesting and complicated. In fact, global existence of the solution is observed in the first two cases (cf. Figs. 2.3&2.4) and finite time blow-up is observed in the last two cases (cf. Figs. 2.5&2.6). The total energy is numerically conserved very well in our computation when there is no blow-up (cf. Figs. 2.3&2.4) and before blow-up happens (cf. Figs. 2.5&2.6). Of course, it is not conserved numerically near or after blow-up happens because the mesh size and time step are fixed which cannot resolve the solution. In addition, our new numerical method can compute the dynamics of dipolar BEC accurately and efficiently.

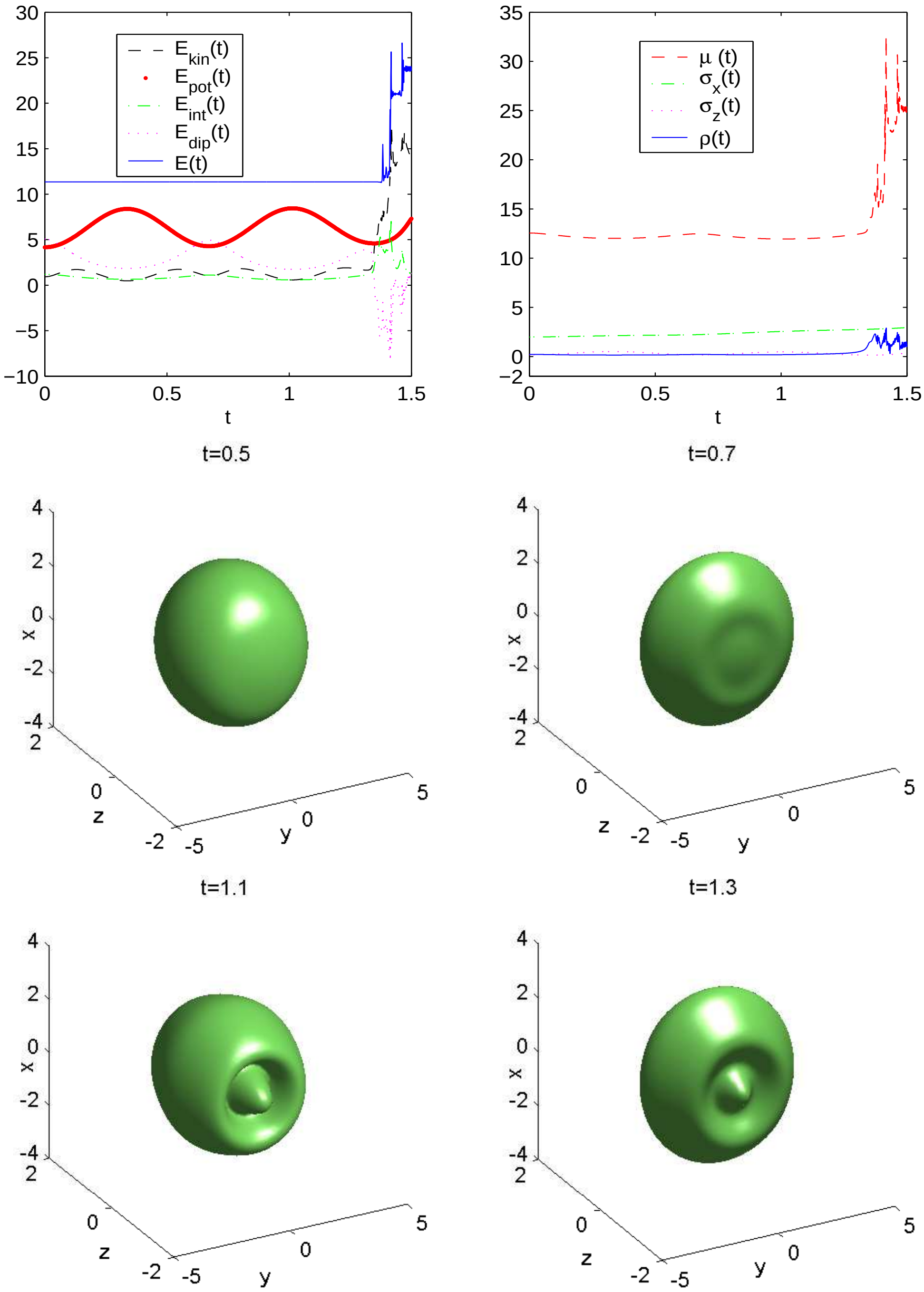

Figure 2.5: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at different times for a dipolar BEC when the dipolar interaction constant is suddenly changed from $\lambda = 0.8\beta = 82.864$ to $\lambda = 4\beta = 414.32$ at time $t = 0$.

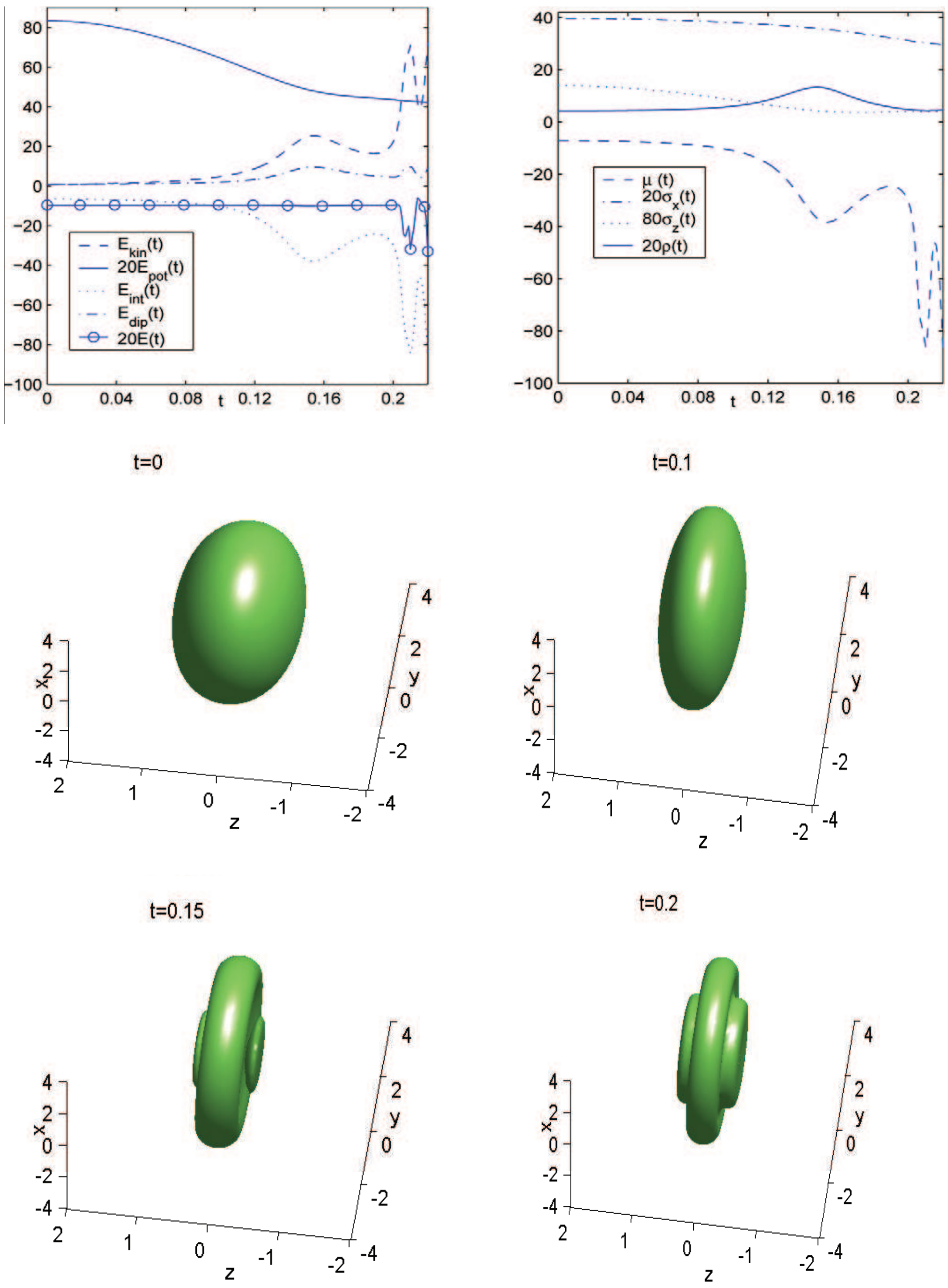

Figure 2.6: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at different times for a dipolar BEC when the interaction constant β is suddenly changed from $\beta = 103.58$ to $\beta = -569.69$ at time $t = 0$.

Chapter 3

Dipolar Gross-Pitaevskii equation with anisotropic confinement

In this chapter, we continue the study of 3D dipolar GPE (2.5). With strongly anisotropic confining potential, spatial degrees of freedom of BEC can be frozen in one or two directions. Then the corresponding 3D dipolar GPE (2.5) can be reduced to lower dimensional equations. We derive the effective equations in lower dimensions for these cases. The corresponding properties of ground states and dynamics are analyzed and the convergence rate of such dimension reduction is proved in certain parameter regimes. Numerical methods are proposed to compute the ground states for reduced equations.

3.1 Lower dimensional models for dipolar GPE

For the 3D dipolar GPE (2.5) which is reformulated into GPPS (2.19)-(2.20), we consider the following two cases where $V(\mathbf{x})$ ($\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$) is anisotropic:

Case I, potential is highly confined in vertical z direction, where

$$V(\mathbf{x}) = V_2(x, y) + \frac{z^2}{2\varepsilon^4}. \tag{3.1}$$

Case II, potential is highly confined in horizon $x - y$ plane, where

$$V(\mathbf{x}) = V_1(z) + \frac{x^2 + y^2}{2\varepsilon^4}. \tag{3.2}$$

In both cases, $\varepsilon > 0$ is a small parameter describing the strength of confinement.

In **Case I**, when $\varepsilon \to 0^+$, evolution of the solution $\psi(\mathbf{x},t)$ of GPPS (2.19)-(2.20) would essentially occur in the ground state mode of $-\frac{1}{2}\partial_{zz} + \frac{z^2}{2\varepsilon^4}$, which is spanned by $w_\varepsilon(z) = \varepsilon^{-1/2}\pi^{-1/4}e^{-\frac{z^2}{2\varepsilon^2}}$. By taking ansatz

$$\psi(\mathbf{x},t) = e^{-it/2\varepsilon^2}\varepsilon^{-1/2}\phi(x,y,t)w_\varepsilon(z), \quad (x,y,z) \in \mathbb{R}^3, \quad t \geq 0, \tag{3.3}$$

the three dimensional (3D) GPPS (2.19)-(2.20) will be formally reduced to a **quasi-2D equation I** (shown in Appendix B):

$$i\partial_t\phi = \left[-\frac{1}{2}\Delta + V_2 + \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi|^2 - \frac{3\lambda}{2}(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi^{2D}\right]\phi, \quad \mathbf{x} \in \mathbb{R}^2, \, t \geq 0, \tag{3.4}$$

where $\mathbf{x} = (x,y)^T$, $\mathbf{n}_\perp = (n_1,n_2)^T$, $\partial_{\mathbf{n}_\perp} = \mathbf{n}_\perp \cdot \nabla$, $\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} = \partial_{\mathbf{n}_\perp}(\partial_{\mathbf{n}_\perp})$, $\Delta = \partial_{xx} + \partial_{yy}$ and

$$\varphi^{2D}(\mathbf{x},t) = U_\varepsilon^{2D} * |\phi|^2, \, U_\varepsilon^{2D}(\mathbf{x}) = \frac{1}{2\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}} \frac{e^{-s^2/2}}{\sqrt{x^2+y^2+\varepsilon^2 s^2}}\, ds, \, \mathbf{x} \in \mathbb{R}^2, \, t \geq 0. \tag{3.5}$$

In addition, as $\varepsilon \to 0^+$, φ^{2D} can be approximated by

$$\varphi^{2D}(\mathbf{x},t) = U_{\text{dip}}^{2D} * |\phi|^2, \quad \text{with} \quad U_{\text{dip}}^{2D}(\mathbf{x}) = \frac{1}{2\pi\sqrt{x^2+y^2}}, \qquad \mathbf{x} \in \mathbb{R}^2, \quad t \geq 0, \tag{3.6}$$

which can be re-written as a fractional Poisson equation

$$(-\Delta)^{1/2}\varphi^{2D}(\mathbf{x},t) = |\phi(\mathbf{x},t)|^2, \quad \mathbf{x} \in \mathbb{R}^2, \quad \lim_{|\mathbf{x}|\to\infty}\varphi^{2D}(\mathbf{x},t) = 0, \qquad t \geq 0. \tag{3.7}$$

Thus an alternative **quasi-2D equation II** can be obtained as :

$$i\partial_t\phi = \left[-\frac{1}{2}\Delta + V_2 + \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi|^2 - \frac{3\lambda}{2}(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)(-\Delta)^{-1/2}(|\phi|^2)\right]\phi. \tag{3.8}$$

Similarly, in **Case II**, evolution of the solution $\psi(\mathbf{x},t)$ of GPPS (2.19)-(2.20) in x-, y-directions would essentially occur in the ground state mode of $-\frac{1}{2}(\partial_{xx} + \partial_{yy}) + \frac{x^2+y^2}{2\varepsilon^4}$, which is spanned by $w_\varepsilon(x,y) = \varepsilon^{-1}\pi^{-1/2}e^{-\frac{x^2+y^2}{2\varepsilon^2}}$. Again, by taking the ansatz

$$\psi(\mathbf{x},t) = e^{-it/\varepsilon^2}\phi(z,t)w_\varepsilon(x,y), \qquad \mathbf{x} = (x,y,z) \in \mathbb{R}^3, \quad t \geq 0, \tag{3.9}$$

the 3D GPPS (2.19)-(2.20) will be formally reduced to a **quasi-1D equation** :

$$i\partial_t\phi = \left[-\frac{1}{2}\partial_{zz} + V_1 + \frac{2\beta + \lambda(1-3n_3^2)}{2\pi\varepsilon^2}|\phi|^2 - \frac{3\lambda(3n_3^2-1)}{8\sqrt{2\varepsilon^2\pi}}\partial_{zz}\varphi^{1D}\right]\phi, \; z \in \mathbb{R}, \; t > 0, \tag{3.10}$$

where

$$\varphi^{1D}(z,t) = U_\varepsilon^{1D} * |\phi|^2, \quad U_\varepsilon^{1D}(z) = \frac{\sqrt{2}e^{z^2/2\varepsilon^2}}{\sqrt{\pi}\,\varepsilon}\int_{|z|}^{\infty} e^{-s^2/2\varepsilon^2}\, ds, \quad z \in \mathbb{R}, t \geq 0. \tag{3.11}$$

The above effective lower dimensional models in 2D and 1D are very useful in the study of dipolar BEC since the reduced equations retain the full structure information while they are much easier and cheaper to be simulated in practical computation. In fact, for the GPE without the dipolar term, i.e. $\lambda = 0$, there have been extensive studies on this subject. For formal analysis and numerical simulation, the convergence rate of such dimension reduction was investigated numerically in [17, 22] and a nonlinear Schrödinger equation with polynomial nonlinearity in reduced dimensions was proposed in [124]. For rigorous analysis, convergence of the dimension reduction under anisotropic confinement has been proven in the weak interaction regime [29,30], i.e. $\beta = O(\varepsilon)$ in 2D and $\beta = O(\varepsilon^2)$ in 1D. However, with the dipolar term, i.e. $\lambda \neq 0$, there were few works towards the mathematical analysis for this dimension reduction except some preliminary results in [42].

The main aim of this chapter is to establish existence and uniqueness of the ground states and well-posedness of the Cauchy problems associated to the quasi-2D equations I and II and the quasi-1D equation, and to analyze the convergence and convergence rate of the dimension reduction from 3D to 2D and 1D. Another goal is to propose numerical methods for computing the ground states of the quasi-2D equation I and the quasi-1D equation.

We will investigate the quasi-2D equations I, II and the quasi-1D equation in the energy space Ξ_d ($d = 1, 2$) defined in (1.4).

3.2 Results for the quasi-2D equation I

In this section, we discuss the existence, uniqueness as well as nonexistence of ground states for the quasi-2D equation I and local (global) existence for Cauchy problem. When considering the ground state in 2D case, the following best constant C_b [155] in the following inequality is crucial,

$$\int_{\mathbb{R}^2} |f(\mathbf{x})|^4 \, d\mathbf{x} \leq \frac{1}{C_b} \int_{\mathbb{R}^2} |\nabla f|^2 \, d\mathbf{x} \cdot \int_{\mathbb{R}^2} |f|^2 \, d\mathbf{x}, \quad f \in H^1(\mathbb{R}^2). \tag{3.12}$$

For simplification of notation, in this and the next section, we also denote $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$.

3.2.1 Existence and uniqueness of ground state

Associated to the quasi-2D equation I (3.4)-(3.5), the energy is

$$E_{2D}(\phi) = \frac{1}{2}\int_{\mathbb{R}^2}\left[|\nabla\phi|^2 + 2V_2(\mathbf{x})|\phi|^2 + \frac{\beta-\lambda+3n_3^2\lambda}{\varepsilon\sqrt{2\pi}}|\phi|^4 - \frac{3}{2}\lambda|\phi|^2\widetilde{\varphi^{2D}}\right]d\mathbf{x}, \qquad (3.13)$$

for $\phi \in \Xi_2$, where

$$\widetilde{\varphi^{2D}} = \left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta\right)\varphi^{2D}, \quad \varphi^{2D} = U_\varepsilon^{2D} * |\phi|^2. \qquad (3.14)$$

The ground state $\phi_g \in S_2$ of (3.4) is then the solution of the minimization problem:

$$\text{Find } \phi_g \in S_2, \quad \text{such that } E_{2D}(\phi_g) = \min_{\phi\in S_2} E_{2D}(\phi). \qquad (3.15)$$

We have the following results on the ground state.

Theorem 3.1 *(Existence and uniqueness of the ground state) Assume* $0 \le V_2(\mathbf{x}) \in L^\infty_{loc}(\mathbb{R}^2)$ *satisfying* $\lim_{|\mathbf{x}|\to\infty} V_2(\mathbf{x}) = \infty$.
(i) There exists a ground state $\phi_g \in S_2$ *of the system (3.4)-(3.5) if one of the following conditions holds,*

(A1) $\lambda \ge 0$, $\beta - \lambda > -\varepsilon\sqrt{2\pi}C_b$;

(A2) $\lambda < 0$, $\beta + (\frac{1}{2} + 3|n_3^2 - \frac{1}{2}|)\lambda > -\varepsilon\sqrt{2\pi}C_b$.

(ii) The positive ground state $|\phi_g|$ *is unique under one of the following conditions:*

(A1′) $\lambda \ge 0$, $\beta - \lambda \ge 0$;

(A2′) $\lambda < 0$, $\beta + (\frac{1}{2} + 3|n_3^2 - \frac{1}{2}|)\lambda \ge 0$.

Moreover, $\phi_g = e^{i\theta_0}|\phi_g|$ *for some constant* $\theta_0 \in \mathbb{R}$.
(iii) If $\beta + \frac{1}{2}\lambda(1 - 3n_3^2) < -\varepsilon\sqrt{2\pi}C_b$, *there exists no ground state of the equation (3.4).*

In order to prove this theorem, we first study the property of the nonlocal term.

Lemma 3.1 *(Kernel* U_ε^{2D} *in (3.5)) For any real function* $f(\mathbf{x})$ *in the Schwartz space* $\mathcal{S}(\mathbb{R}^2)$, *we have*

$$\widehat{U_\varepsilon^{2D} * f}(\xi) = \hat{f}(\xi)\,\widehat{U_\varepsilon^{2D}}(\xi) = \frac{\hat{f}(\xi)}{\pi}\int_{\mathbb{R}}\frac{e^{-\varepsilon^2 s^2/2}}{|\xi|^2 + s^2}ds, \qquad f \in \mathcal{S}(\mathbb{R}^2). \qquad (3.16)$$

Moreover, define the operator

$$T_{jk}(f) = \partial_{x_j x_k}(U_\varepsilon^{2D} * f), \qquad j,k = 1,2,$$

then we have

$$\|T_{jk}f\|_2 \le \frac{\sqrt{2}}{\sqrt{\pi}\,\varepsilon}\|f\|_2, \qquad \|T_{jk}f\|_2 \le \|\nabla f\|_2, \tag{3.17}$$

hence T_{jk} *can be extended to a bounded linear operator from* $L^2(\mathbb{R}^2)$ *to* $L^2(\mathbb{R}^2)$*.*

Proof: From (3.5), we have

$$|U_\varepsilon^{2D}(\mathbf{x})| = \left|\frac{1}{2\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}}\frac{e^{-s^2/2}}{\sqrt{|\mathbf{x}|^2+\varepsilon^2 s^2}}\,ds\right| \le \frac{1}{2\pi|\mathbf{x}|}, \quad |\mathbf{x}|\neq 0. \tag{3.18}$$

This immediately implies that $U_\varepsilon^{2D} * g$ is well-defined for any $g \in L^1(\mathbb{R}^2)\bigcap L^2(\mathbb{R}^2)$ since the right hand side in the above inequality is the singular kernel of Riesz potential. Re-write $U_\varepsilon^{2D}(\mathbf{x})$ as

$$U_\varepsilon^{2D}(\mathbf{x}) = \frac{1}{2\pi}\int_{\mathbb{R}^2}\varepsilon^{-2}\frac{w_0^2(z/\varepsilon)w_0^2(z'/\varepsilon)}{\sqrt{|\mathbf{x}|^2+(z-z')^2}}dzdz',$$

with $w_0(z) = \frac{1}{\pi^{1/4}}e^{-z^2/2}$, using the Plancherel formula, we get

$$\widehat{U_\varepsilon^{2D}}(\xi_1,\xi_2) = \frac{1}{\pi}\int_{\mathbb{R}}\frac{\widehat{w_0^2}(\varepsilon\xi_3)\overline{\widehat{w_0^2}}(\varepsilon\xi_3)}{\xi_1^2+\xi_2^2+\xi_3^2}d\xi_3 = \frac{1}{\pi}\int_{\mathbb{R}}\frac{e^{-\varepsilon^2 s^2/2}}{|\xi|^2+s^2}ds, \qquad \xi = (\xi_1,\xi_2)^T \in \mathbb{R}^2,$$

which immediately implies (3.16). For T_{jk}, we have

$$\left|\widehat{T_{jk}f}(\xi)\right| = \left|\frac{\hat{f}(\xi)}{\pi}\int_{\mathbb{R}}\frac{e^{-\varepsilon^2 s^2/2}\xi_j\xi_k}{|\xi|^2+s^2}ds\right| \le \frac{\left|\hat{f}(\xi)\right|}{\pi}\int_{\mathbb{R}}e^{-\varepsilon^2 s^2/2}ds = \frac{\sqrt{2}}{\sqrt{\pi}\,\varepsilon}\left|\hat{f}(\xi)\right|, \quad \xi\in\mathbb{R}^2.$$

Thus we can get the first inequality in (3.17) and know that $T_{jk}:\ L^2 \to L^2$ is bounded. Moreover, from

$$\left|\widehat{T_{jk}f}(\xi)\right| = \left|\frac{\hat{f}(\xi)}{\pi}\int_{\mathbb{R}}\frac{e^{-\varepsilon^2 s^2/2}\xi_j\xi_k}{|\xi|^2+s^2}ds\right| \le \frac{|\hat{f}(\xi)|\ |\xi_j\xi_k|}{\pi}\int_{\mathbb{R}}\frac{1}{|\xi|^2+s^2}ds \le |\xi|\ |\hat{f}(\xi)|, \tag{3.19}$$

we can obtain the second inequality in (3.17) and know that $T_{jk}:\ H^1 \to L^2$ is bounded too.

□

Remark 3.1 *In fact,* T_{jk} *is bounded from* $L^p \to L^p$*, i.e., there exists* $C_p > 0$ *independent of* ε*, such that*

$$\|T_{jk}(f)\|_{L^p(\mathbb{R}^2)} \le \frac{C_p}{\varepsilon}\|f\|_{L^p(\mathbb{R}^2)}, \quad p\in(1,\infty). \tag{3.20}$$

This can be obtained using L^p *estimate for Poisson equation and Minkowski inequality.*

Lemma 3.2 *For the energy $E_{2D}(\cdot)$ in (3.13), we have*

(i) For any $\phi \in S_2$, denote $\rho(\mathbf{x}) = |\phi(\mathbf{x})|^2$, then we have

$$E_{2D}(\phi) \geq E_{2D}(|\phi|) = E_{2D}\left(\sqrt{\rho}\right), \qquad \forall \phi \in S_2, \tag{3.21}$$

so the ground state ϕ_g of (3.13) is of the form $e^{i\theta_0}|\phi_g|$ for some constant $\theta_0 \in \mathbb{R}$.

(ii) Under the condition (A1) or (A2) in Theorem 3.1, $E_{2D}(\sqrt{\rho})$ is bounded below.

(iii) Under the condition (A1′) or (A2′) in Theorem 3.1, $E_{2D}(\sqrt{\rho})$ is strictly convex.

Proof: (i) For $\phi(\mathbf{x}) \in S_2$, $|\phi(\mathbf{x})| \in S_2$. A simple calculation shows

$$E_{2D}(\phi(\mathbf{x})) - E_{2D}(|\phi(\mathbf{x})|) = \frac{1}{2}\|\nabla\phi\|_2^2 - \frac{1}{2}\|\nabla|\phi|\|_2^2 \geq 0, \tag{3.22}$$

where the equality holds iff [97]

$$|\nabla\phi(\mathbf{x})| = \nabla|\phi(\mathbf{x})|, \quad \text{a.e. } \mathbf{x} \in \mathbb{R}^2, \tag{3.23}$$

which is equivalent to

$$\phi(\mathbf{x}) = e^{i\theta}|\phi(\mathbf{x})|, \qquad \text{for some } \theta \in \mathbb{R}. \tag{3.24}$$

Then the conclusion follows.

(ii) For $\sqrt{\rho} = \phi \in S_2$, we separate the energy E_{2D} into two parts:

$$E_{2D}(\phi) = E_1(\phi) + E_2(\phi) = E_1(\sqrt{\rho}) + E_2(\sqrt{\rho}), \tag{3.25}$$

where

$$E_1(\sqrt{\rho}) = \frac{1}{2}\int_{\mathbb{R}^2}\left[|\nabla\sqrt{\rho}|^2 + 2V_2(\mathbf{x})\rho\right]d\mathbf{x}, \tag{3.26}$$

$$E_2(\sqrt{\rho}) = \frac{1}{2}\int_{\mathbb{R}^2}\left[\frac{\beta - \lambda + 3n_3^2\lambda}{\varepsilon\sqrt{2\pi}}|\rho|^2 - \frac{3}{2}\lambda\rho\widetilde{\varphi^{2D}}\right]d\mathbf{x}, \tag{3.27}$$

with

$$\widetilde{\varphi^{2D}} = \left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta_\perp\right)U_\varepsilon^{2D} * \rho. \tag{3.28}$$

Applying Plancherel formula and Lemma 3.1, there holds

$$\begin{aligned}\int_{\mathbb{R}^2}\widetilde{\varphi^{2D}}(\mathbf{x})\rho(\mathbf{x})\,d\mathbf{x} &= \frac{1}{4\pi^2}\int_{\mathbb{R}^2}\widehat{\widetilde{\varphi^{2D}}}(\xi)\bar{\hat{\rho}}(\xi)d\xi \\ &= \frac{-1}{4\pi^3}\int_{\mathbb{R}^3}\frac{\left((n_1\xi_1 + n_2\xi_2)^2 - n_3^2|\xi|^2\right)e^{-\varepsilon^2s^2/2}}{|\xi|^2 + s^2}|\hat{\rho}|^2 ds d\xi.\end{aligned} \tag{3.29}$$

Recalling Cauchy inequality and $n_1^2+n_2^2+n_3^2=1$, we have

$$-n_3^2|\xi|^2 \le (n_1\xi_1+n_2\xi_2)^2 - n_3^2|\xi|^2 \le (1-2n_3^2)|\xi|^2. \tag{3.30}$$

Let $C_0=\max\{|n_3^2|,|1-2n_3^2|\}$, we can derive that

$$\left|\int_{\mathbb{R}^2}\widetilde{\varphi^{2D}}(\mathbf{x})\rho(\mathbf{x})\,d\mathbf{x}\right| \le \frac{C_0}{4\pi^3}\int_{\mathbb{R}^3} e^{-\varepsilon^2 s^2/2}|\hat{\rho}|^2 ds d\xi = \frac{\sqrt{2}C_0}{\varepsilon\sqrt{\pi}}\|\rho\|_2^2. \tag{3.31}$$

Hence, $E_2(\sqrt{\rho})$ could be bounded by $\|\rho\|_2^2$. In detail, under the condition (A1) $\lambda\ge 0$, $\beta-\lambda\ge -\varepsilon\sqrt{2\pi}C_b$, we have

$$E_2(\sqrt{\rho}) \quad \ge \quad \frac{\beta-\lambda+3n_3^2\lambda}{\varepsilon 2\sqrt{2\pi}}\|\rho\|_2^2 - \frac{3\sqrt{2}n_3^2\lambda}{4\varepsilon\sqrt{\pi}}\|\rho\|_2^2 \ge -\frac{C_b}{2}\|\rho\|_2^2. \tag{3.32}$$

Under the condition (A2), if $\lambda<0$ and $n_3^2\ge\frac{1}{2}$, then

$$E_2(\sqrt{\rho}) \ge \frac{\beta-\lambda+3n_3^2\lambda}{\varepsilon 2\sqrt{2\pi}}\|\rho\|_2^2 \ge -\frac{C_b}{2}\|\rho\|_2^2; \tag{3.33}$$

if $\lambda<0$ and $n_3^2<\frac{1}{2}$, then

$$E_2(\sqrt{\rho}) \ge \frac{\beta-\lambda+3n_3^2\lambda}{\varepsilon 2\sqrt{2\pi}}\|\rho\|_2^2 + \frac{3\sqrt{2}(1-2n_3^2)\lambda}{4\varepsilon\sqrt{\pi}}\|\rho\|_2^2 \ge -\frac{C_b}{2}\|\rho\|_2^2. \tag{3.34}$$

Recalling the choice of best constant C_b, under either condition (A1) or (A2), the energy

$$E_{2D}(\sqrt{\rho}) = E_1(\sqrt{\rho}) + E_2(\sqrt{\rho}) \ge \frac{1}{2}\|\nabla\sqrt{\rho}\|_2^2 - \frac{C_b}{2}\|\rho\|_2^2 \ge 0. \tag{3.35}$$

(iii) Again, we split the energy as (3.25). It is well known that $E_1(\sqrt{\rho})$ is strictly convex in ρ [97]. It remains to show that $E_2(\sqrt{\rho})$ is convex in $\sqrt{\rho}$. For any real function $u\in L^1(\mathbb{R}^2)\cap L^2(\mathbb{R}^2)$, let

$$H(u) = \frac{1}{2}\int_{\mathbb{R}^2}\left[\frac{\beta-\lambda+3n_3^2\lambda}{\varepsilon\sqrt{2\pi}}|u|^2 - \frac{3}{2}\lambda u\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta_\perp\right)(U_\varepsilon^{2D}*u)\right]d\mathbf{x}. \tag{3.36}$$

Then $E_2(\sqrt{\rho}) = H(\rho)$. It suffices to show $H(\rho)$ is convex in ρ. For this purpose, let $\sqrt{\rho_1}=\phi_1\in S_2$ and $\sqrt{\rho_2}=\phi_2\in S_2$, for any $\theta\in[0,1]$, consider $\rho_\theta=\theta\rho_1+(1-\theta)\rho_2$ and $\sqrt{\rho_\theta}\in S_2$, then we compute directly and get

$$\theta H(\rho_1) + (1-\theta)H(\rho_2) - H(\rho_\theta) = \theta(1-\theta)H(\rho_1-\rho_2). \tag{3.37}$$

Similar as (3.29), looking at the Fourier domain, we could obtain the lower bounds for $H(\rho_1-\rho_2)$ under the condition (A1′) or (A2′), while replacing C_b with 0 in the above proof of (ii), i.e.,

$$H(\rho_1-\rho_2) \ge 0. \tag{3.38}$$

This shows that $H(\rho)$, i.e. $E_2(\sqrt{\rho})$, is convex in ρ. Thus $E_{2D}(\sqrt{\rho})$ is strictly convex. $\square$

Proof of Theorem 3.1: (i) We first prove the existence results. Lemma 3.2 ensures that there exists a minimizing sequence of positive function $\{\phi^n\}_{n=0}^{\infty} \subset S_2$, such that $\lim_{n\to\infty} E_{2D}(\phi^n) = \inf_{\phi\in S_2} E_{2D}(\phi)$. Then, under condition (A1) or (A2), there exists a constant C such that

$$\|\nabla\phi^n\|_2 + \|\phi^n\|_4 + \int_{\mathbb{R}^2} V_2(\mathbf{x})|\phi^n(\mathbf{x})|^2 d\mathbf{x} \le C, \qquad n \ge 0. \tag{3.39}$$

Therefore ϕ^n belongs to a weakly compact set in $L^4(\mathbb{R}^2)$, $H^1(\mathbb{R}^2)$, and $L^2_{V_2}(\mathbb{R}^2)$ with a weighted L^2-norm given by $\|\phi\|_{L_{V_2}} = [\int_{\mathbb{R}^2} |\phi(\mathbf{x})|^2 V_2(\mathbf{x}) d\mathbf{x}]^{1/2}$. Thus, there exists a $\phi^\infty \in H^1 \bigcap L^2_{V_2} \bigcap L^4$ and a subsequence of $\{\phi^n\}_{n=0}^{\infty}$ (which we denote as the original sequence for simplicity), such that

$$\phi^n \rightharpoonup \phi^\infty, \quad \text{in } L^2 \cap L^4 \cap L^2_{V_2}, \qquad \nabla\phi^n \rightharpoonup \nabla\phi^\infty, \quad \text{in } L^2. \tag{3.40}$$

The confining condition $\lim_{|\mathbf{x}|\to\infty} V_2(\mathbf{x}) = \infty$ will give that $\|\phi^\infty\|_2 = 1$ [10,96]. Hence $\phi^\infty \in S_2$ and $\phi^n \to \phi^\infty$ in $L^2(\mathbb{R}^2)$ due to the L^2-norm convergence and weak convergence of $\{\phi^n\}_{n=0}^{\infty}$. By the lower semi-continuity of the H^1- and $L^2_{V_2}$-norm, for E_1 in (3.26), we know

$$E_1(\phi^\infty) \le \liminf_{n\to\infty} E_1(\phi^n). \tag{3.41}$$

By Sobolev inequality, there exists $C(p) > 0$ depending on $p \ge 2$, such that $\|\phi^n\|_p \le C(p)(\|\nabla\phi^n\|_2 + \|\phi^n\|_2) \le C(p)(1+C)$, uniformly for $n \ge 0$, applying Hölder's inequality, we have

$$\|(\phi^n)^2 - (\phi^\infty)^2\|_2^2 \le C_1(\|\phi^n\|_6^3 + \|\phi^n\|_6^3)\|\phi^n - \phi^\infty\|_2, \tag{3.42}$$

which shows $\rho^n = (\phi^n)^2 \to \rho^\infty = (\phi^\infty)^2 \in L^2(\mathbb{R}^2)$. Using the Fourier transform of U_ε^{2D} in Lemma 3.1 and (3.31), it is easy to derive the convergence for E_2 in (3.27)

$$E_2(\phi^\infty) = \lim_{n\to\infty} E_2(\phi^n). \tag{3.43}$$

Hence,

$$E_{2D}(\phi^\infty) = E_1(\phi^\infty) + E_2(\phi^\infty) \le \liminf_{n\to\infty} E_{2D}(\phi^n). \tag{3.44}$$

Now, we see that ϕ^∞ is indeed a minimizer. For the uniqueness part, it is straightforward by the strict convexity of $E_{2D}(\sqrt{\rho})$ in Lemma 3.2.

(ii) Since the nonlinear term in the equation behaviors as a cubic nonlinearity, it is natural to consider the following. Let $\phi(\mathbf{x}) \in S_2$ be a real function that attains the best constant C_b [155], then $\phi(\mathbf{x})$ is radial symmetric. Choose $\phi_\delta(\mathbf{x}) = \delta^{-1}\phi(\delta^{-1}\mathbf{x})$, $\delta > 0$, then $\phi_\delta \in S_2$. Denote $\varphi_\delta = \left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta_\perp\right)(U_\varepsilon^{2D} * |\phi_\delta|^2)$, by the same computation as in Lemma 3.2, there holds

$$\begin{aligned}\int_{\mathbb{R}^2} \varphi_\delta|\phi_\delta|^2\,d\mathbf{x} &= \frac{-1}{4\pi^3}\int_{\mathbb{R}^3} \frac{(n_1\xi_1+n_2\xi_2)^2 - n_3^2|\xi|^2}{|\xi|^2+s^2} e^{-\varepsilon^2 s^2/2}|\widehat{|\phi|^2}(\delta\xi)|^2\,dsd\xi \\ &= \frac{-1}{4\delta^2\pi^3}\int_{\mathbb{R}^3} \frac{(n_1\xi_1+n_2\xi_2)^2 - n_3^2|\xi|^2}{|\xi|^2+\delta^2 s^2} e^{-\varepsilon^2 s^2/2}|\widehat{|\phi|^2}(\xi)|^2\,dsd\xi,\end{aligned}$$

using the fact that $\phi(\mathbf{x})$ is radial symmetric, $\widehat{|\phi|^2}(\xi)$ is also radial symmetric. Thus, we would obtain

$$\int_{\mathbb{R}^2} \varphi_\delta|\phi_\delta|^2\,d\mathbf{x} = -\frac{(n_1^2+n_2^2-2n_3^2)+o(1)}{\sqrt{2\pi}\varepsilon\delta^2}\|\phi\|_4^4, \quad \text{as } \delta\to 0^+. \tag{3.45}$$

Hence, let $\delta \to 0^+$,

$$E_{2D}(\phi_\delta) = \frac{1}{2\delta^2}\left(\|\nabla\phi\|_2^2 + \left(\frac{\beta+\frac{1}{2}\lambda(1-3n_3^2)+o(1)}{\sqrt{2\pi}\varepsilon}\right)\|\phi\|_4^4\right) + \int_{\mathbb{R}^2} V_2(\delta\mathbf{x})|\phi|^2(\mathbf{x})d\mathbf{x}.$$

Recalling that $\|\nabla\phi\|_2^2 = C_b\|\phi\|_4^4$, we know $\lim_{\delta\to 0^+} E_{2D}(\phi_\delta) = -\infty$ if $\beta + \frac{1}{2}\lambda(1-3n_3^2) < -\sqrt{2\pi}\varepsilon C_b$, i.e. there is no ground state in this case. $\square$

3.2.2 Well-posedness for dynamics

Here, we study the well-posedness of the Cauchy problem corresponding to the quasi-2D equation I (3.4)-(3.5). Using the Fourier transform of kernel U_ε^{2D} in Lemma 3.1, it is straightforward to see that the nonlinear term introduced by U_ε^{2D} behaviors like cubic term. Thus, those methods for classic cubic nonlinear Schrödinger equation would apply [43, 139, 155]. In particular, we have the following theorem concerning the Cauchy problem of (3.4)-(3.5).

Theorem 3.2 *(Well-posedness of the Cauchy problem) Suppose the real-valued trap potential satisfies $V_2(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^2$ and*

$$V_2(\mathbf{x}) \in C^\infty(\mathbb{R}^2) \text{ and } D^\alpha V_2(\mathbf{x}) \in L^\infty(\mathbb{R}^2), \qquad \text{for all } \alpha \in \mathbb{N}_0^2 \text{ with } |\alpha| \geq 2, \tag{3.46}$$

then we have

(i) For any initial data $\phi(\mathbf{x}, t = 0) = \phi_0(\mathbf{x}) \in \Xi_2$, there exists a $T_{\max} \in (0, +\infty]$ such that the problem (3.4)-(3.5) has a unique maximal solution $\phi \in C([0, T_{\max}), \Xi_2)$. It is maximal in the sense that if $T_{\max} < \infty$, then $\|\phi(\cdot, t)\|_{\Xi_2} \to \infty$ when $t \to T_{\max}^-$.

(ii) As long as the solution $\phi(\mathbf{x}, t)$ remains in the energy space Ξ_2, the L^2-norm $\|\phi(\cdot, t)\|_2$ and energy $E_{2D}(\phi(\cdot, t))$ in (3.13) are conserved for $t \in [0, T_{\max})$.

(iii) Under either condition (A1) or (A2) in Theorem 3.1, the solution of (3.4)-(3.5) is global in time, i.e., $T_{max} = \infty$.

Proof: The proof is standard. We shall use the known results for semi-linear Schrödinger equation [43]. For $\phi \in \Xi_2$, denote $\rho = |\phi|^2$ and consider the following

$$G(\phi, \bar{\phi}) := G(\rho) = \frac{1}{2}\int_{\mathbb{R}^2} |\phi|^2 \left(\partial_{\mathbf{n}_\perp \mathbf{n}_\perp} - n_3^2 \Delta\right)(U_\varepsilon^{2D} * |\phi|^2)\, d\mathbf{x},$$
$$g(\phi) = \frac{\delta G(\phi, \bar{\phi})}{\delta \bar{\phi}} = \phi \left(\partial_{\mathbf{n}_\perp \mathbf{n}_\perp} - n_3^2 \Delta\right)(U_\varepsilon^{2D} * |\phi|^2).$$

Then the equations (3.4)-(3.5) read

$$i\partial_t \phi = -[\frac{1}{2}\Delta + V_2(\mathbf{x})]\phi + \beta_0 |\phi|^2 \phi - 3\lambda g(\phi), \quad \mathbf{x} \in \mathbb{R}^2,\, t > 0, \tag{3.47}$$

where $\beta_0 = \frac{\beta - \lambda + 3n_3^2 \lambda}{\sqrt{2\pi}\varepsilon}$. Using the L^p boundedness of T_{jk} (cf. Lemma 3.1 and Remark 3.1) and Sobolev inequality, for $\|u\|_{\Xi_2} + \|v\|_{\Xi_2} \le M$, it is easy to prove the following

$$\|g(u) - g(v)\|_{4/3} \le C(M)\|u - v\|_4. \tag{3.48}$$

In view of the standard Theorems 9.2.1, 4.12.1 and 5.7.1 in [43] and [139] for the well-posedness of the nonlinear Schrödinger equation, we can obtain the results (I), (II) immediately. The global existence (III) comes from the uniform bound for $\|\phi(\cdot, t)\|_{\Xi_2}$ which can be derived from energy and L^2 norm conservation. □

When the initial data is small, there also exists global solutions [42, 43]. Otherwise, blow-up may happen in finite time, and we have the following results.

Theorem 3.3 *(Finite time blow-up) If conditions (A1) and (A2) are not satisfied and assume $V_2(\mathbf{x})$ satisfies $2V_2(\mathbf{x}) + \mathbf{x} \cdot \nabla V_2(\mathbf{x}) \ge 0$, for any initial data $\phi(\mathbf{x}, t = 0) = \phi_0(\mathbf{x}) \in \Xi_2$ with $\int_{\mathbb{R}^2} |\mathbf{x}|^2 |\phi_0(\mathbf{x})|^2\, d\mathbf{x} < \infty$ and solution $\phi(\mathbf{x}, t)$ to the problem (3.4), there exists finite time blow-up, i.e., $T_{max} < \infty$, if $\lambda = 0$, or $\lambda > 0$ and $n_3^2 \ge \frac{1}{2}$, and one of the following holds:*

(i) $E_{2D}(\phi_0) < 0$;

(ii) $E_{2D}(\phi_0) = 0$ *and* $\text{Im}\left(\int_{\mathbb{R}^2} \bar{\phi}_0(\mathbf{x})\ (\mathbf{x}\cdot\nabla\phi_0(\mathbf{x}))\,d\mathbf{x}\right) < 0$;

(iii) $E_{2D}(\phi_0) > 0$ *and* $\text{Im}\left(\int_{\mathbb{R}^2} \bar{\phi}_0(\mathbf{x})\ (\mathbf{x}\cdot\nabla\phi_0(\mathbf{x}))\,d\mathbf{x}\right) < -\sqrt{2E_{2D}(\phi_0)}\|\mathbf{x}\phi_0\|_2$.

Proof: Similar as (2.49), define the variance

$$\sigma_V(t) := \sigma_V(\phi(\cdot,t)) = \int_{\mathbb{R}^2} |\mathbf{x}|^2|\phi(\mathbf{x},t)|^2\,d\mathbf{x} = \sigma_x(t) + \sigma_y(t), \qquad t \geq 0, \tag{3.49}$$

where

$$\sigma_\alpha(t) := \sigma_\alpha(\phi(\cdot,t)) = \int_{\mathbb{R}^2} \alpha^2|\phi(\mathbf{x},t)|^2\,d\mathbf{x}, \qquad \alpha = x,\ y. \tag{3.50}$$

For $\alpha = x$, or y, differentiating (3.50) with respect to t, integrating by parts, we get

$$\frac{d}{dt}\sigma_\alpha(t) = -i\int_{\mathbb{R}^2} \left[\alpha\bar{\phi}(\mathbf{x},t)\partial_\alpha\phi(\mathbf{x},t) - \alpha\phi(\mathbf{x},t)\partial_\alpha\bar{\phi}(\mathbf{x},t)\right]\,d\mathbf{x}, \qquad t \geq 0. \tag{3.51}$$

Similarly, we have

$$\frac{d^2}{dt^2}\sigma_\alpha(t) = \int_{\mathbb{R}^2} \left[2|\partial_\alpha\phi|^2 + \beta_0|\phi|^4 + 3\lambda|\phi|^2\alpha\partial_\alpha(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi - 2\alpha|\phi|^2\partial_\alpha V_2(\mathbf{x})\right]\,d\mathbf{x}, \tag{3.52}$$

where $b_0 = \frac{\beta-\lambda+\lambda n_3^2}{\sqrt{2\pi}\,\varepsilon}$, $\varphi = U_\varepsilon^{2D} * |\phi|^2$. Writing $\rho = |\phi|^2$, $\tilde{\varphi} = (\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi$, $n_\xi = (n_1\xi_1 + n_2\xi_2)^2 - n_3^2|\xi|^2$ and noticing that ρ is real function, by Plancherel formula, we have

$$\begin{aligned}
\int_{\mathbb{R}^2} |\phi|^2\,(\mathbf{x}\cdot\nabla\tilde{\varphi})\,d\mathbf{x} &= \frac{-1}{4\pi^2}\int_{\mathbb{R}^2} \hat{\rho}(\xi)\,\nabla\cdot\left(\xi\bar{\hat{\tilde{\varphi}}}\right)\,d\xi \\
&= \frac{1}{4\pi^2}\int_{\mathbb{R}^2} \hat{\rho}(\xi)\,\nabla\cdot\left(\xi n_\xi\widehat{U_\varepsilon^{2D}}\bar{\hat{\rho}}\right)\,d\xi \\
&= \frac{1}{4\pi^2}\int_{\mathbb{R}^2} \hat{\rho}\,\left(\bar{\hat{\rho}}\nabla(\xi n_\xi\widehat{U_\varepsilon^{2D}}) + n_\xi\widehat{U_\varepsilon^{2D}}\xi\cdot\nabla\bar{\hat{\rho}}\right)\,d\xi \\
&= \frac{1}{4\pi^2}\int_{\mathbb{R}^2} \left(|\hat{\rho}|^2\nabla(\xi n_\xi\widehat{U_\varepsilon^{2D}}) + n_\xi\widehat{U_\varepsilon^{2D}}\xi\cdot\frac{1}{2}\nabla|\hat{\rho}|^2\right)\,d\xi \\
&= \frac{1}{4\pi^2}\int_{\mathbb{R}^2} (n_\xi\widehat{U_\varepsilon^{2D}} + \frac{1}{2}\xi\cdot\nabla(n_\xi\widehat{U_\varepsilon^{2D}}))|\hat{\rho}|^2\,d\xi \\
&= -\int_{\mathbb{R}^2} |\phi|^2\tilde{\varphi}\,d\mathbf{x} + \frac{1}{4\pi^3}\int_{\mathbb{R}^3} \frac{n_\xi s^2 e^{-\varepsilon^2 s^2/2}|\hat{\rho}|^2}{(|\xi|^2+s^2)^2}\,ds d\xi.
\end{aligned}$$

Denote

$$I(t) := I(\phi(\cdot,t)) = \frac{1}{4\pi^3}\int_{\mathbb{R}^3} \frac{n_\xi s^2 e^{-\varepsilon^2 s^2/2}|\hat{\rho}|^2}{(|\xi|^2+s^2)^2}\,ds d\xi, \tag{3.53}$$

using $n_\xi \in [-n_3^2|\xi|^2, (1-2n_3^2)|\xi|^2]$, we obtain

$$\frac{-\sqrt{2}n_3^2}{\sqrt{\pi}\,\varepsilon}\|\phi(t)\|_4^4 \leq I(t) \leq \frac{\sqrt{2}(1-2n_3^2)}{\sqrt{\pi}\,\varepsilon}\|\phi(t)\|_4^4. \tag{3.54}$$

If $\lambda = 0$, or $\lambda > 0$ and $n_3 \geq \frac{1}{2}$, noticing $\lambda I(t) \leq 0$ in these cases, summing (3.52) for $\alpha = x, y$, and using energy conservation, we have

$$\begin{aligned}
\frac{d^2}{dt^2}\sigma_V(t) &= 2\int_{\mathbb{R}^2}\left[|\nabla\phi|^2 + \beta_0|\phi|^4 + \frac{3}{2}\lambda|\phi|^2\left(\mathbf{x}\cdot\nabla\tilde{\varphi}\right) - |\phi|^2\mathbf{x}\cdot\nabla V_2(\mathbf{x})\right]d\mathbf{x} \\
&= 4E_{2D}(\phi(\cdot,t)) + 3\lambda I(t) - 2\int_{\mathbb{R}^2}|\phi|^2(2V_2(\mathbf{x}) + \mathbf{x}\cdot\nabla V_2(\mathbf{x}))\,d\mathbf{x} \\
&\leq 4E_{2D}(\phi(\cdot,t)) \equiv 4E_{2D}(\phi_0).
\end{aligned}$$

Thus,

$$\sigma_V(t) \leq 2E_{2D}(\phi_0)t^2 + \sigma_V'(0)t + \sigma_V(0), \qquad t \geq 0,$$

and the conclusion follows in the same manner as those in [43, 139] for the standard nonlinear Schrödinger equation. □

3.3 Results for the quasi-2D equation II

In this section, we investigate the existence, uniqueness as well as nonexistence of ground state of the quasi-2D equation II (3.8) and the well-posedness of the corresponding Cauchy problem.

3.3.1 Existence and uniqueness of ground state

Associated to the quasi-2D equation (3.8), the energy is

$$\tilde{E}_{2D}(\phi) = \int_{\mathbb{R}^2}\left[\frac{1}{2}|\nabla\phi|^2 + V_2(\mathbf{x})|\phi|^2 + \frac{\beta - \lambda + 3n_3^2\lambda}{2\sqrt{2\pi}\,\varepsilon}|\phi|^4 - \frac{3\lambda}{4}|\phi|^2\varphi\right]d\mathbf{x}, \qquad \phi \in \Xi_2, \tag{3.55}$$

where

$$\varphi(\mathbf{x}) = \left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta\right)\left((-\Delta)^{-1/2}|\phi|^2\right). \tag{3.56}$$

The ground state $\phi_g \in S_2$ of the equation (3.8) is defined as the minimizer of the nonconvex minimization problem:

$$\text{Find } \phi_g \in S_2, \quad \text{such that } \tilde{E}_{2D}(\phi_g) = \min_{\phi\in S_2}\tilde{E}_{2D}(\phi). \tag{3.57}$$

For the above ground state, we have the following results.

Theorem 3.4 *(Existence and uniqueness of ground state) Assume* $0 \leq V_2(\mathbf{x}) \in L^\infty_{loc}(\mathbb{R}^2)$ *and* $\lim_{|\mathbf{x}|\to\infty} V_2(\mathbf{x}) = \infty$*, then we have*

(i) There exists a ground state $\phi_g \in S_2$ *of the equation (3.8) if one of the following conditions holds*

(B1) $\lambda = 0$ *and* $\beta > -\sqrt{2\pi}C_b\,\varepsilon$*;*

(B2) $\lambda > 0$*,* $n_3 = 0$ *and* $\beta - \lambda > -\sqrt{2\pi}C_b\,\varepsilon$*;*

(B3) $\lambda < 0$*,* $n_3^2 \geq \frac{1}{2}$ *and* $\beta - (1 - 3n_3^2)\lambda > -\sqrt{2\pi}C_b\,\varepsilon$*.*

(ii) The positive ground state $|\phi_g|$ *is unique under one of the following conditions*

(B1′) $\lambda = 0$ *and* $\beta \geq 0$*;*

(B2′) $\lambda > 0$*,* $n_3 = 0$ *and* $\beta \geq \lambda$*;*

(B3′) $\lambda < 0$*,* $n_3^2 \geq \frac{1}{2}$ *and* $\beta - (1 - 3n_3^2)\lambda \geq 0$*.*

Moreover, any ground state $\phi_g = e^{i\theta_0}|\phi_g|$ *for some constant* $\theta_0 \in \mathbb{R}$*.*

(iii) There exists no ground state of the equation (3.8) if one of the following conditions holds

(B1″) $\lambda > 0$ *and* $n_3 \neq 0$*;*

(B2″) $\lambda < 0$ *and* $n_3^2 < \frac{1}{2}$*;*

(B3″) $\lambda = 0$ *and* $\beta < -\sqrt{2\pi}C_b\,\varepsilon$*.*

Again, in order to prove this theorem, we first analyze the nonlocal part in the equation (3.8). In fact, following the standard proof in [134], we can get

Lemma 3.3 *(Property of fractional Poisson equation (3.6)) Assume* $f(\mathbf{x})$ *is a real valued function good enough, for the fractional Poisson equation*

$$(-\Delta)^{-1/2}\varphi(\mathbf{x}) = f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2, \qquad \lim_{|\mathbf{x}|\to\infty} \varphi(\mathbf{x}) = 0,$$

we have

$$\varphi(\mathbf{x}) = \int_{\mathbb{R}^2} \frac{f(\mathbf{x}')}{2\pi|\mathbf{x}-\mathbf{x}'|}d\mathbf{x}' = \left(\frac{1}{2\pi|\mathbf{x}|}\right) * f, \qquad \mathbf{x} \in \mathbb{R}^2,$$

and the Hardy-Littlewood-Sobolev inequality implies

$$\|\varphi\|_{p^*} \leq C_p\|f\|_p, \qquad p^* = \frac{2p}{2-p}, \qquad p \in (1,2). \tag{3.58}$$

Moreover, the first order derivatives of φ are the Riesz transforms of f and satisfy

$$\|\partial_{x_j}\varphi\|_q \le C_q\|f\|_q, \qquad q\in(1,\infty), \quad j=1,2, \tag{3.59}$$

and the second order derivatives satisfy

$$\|\partial_{x_jx_k}\varphi\|_q = \|\partial_{x_j}\left((-\Delta)^{-1/2}\partial_{x_k}f\right)\|_q \le C_q\|\partial_{x_k}f\|_q, \qquad q\in(1,\infty), \quad j,k=1,2. \tag{3.60}$$

Remark 3.2 *Similar results hold for T_{jk} defined in Lemma 3.1, i.e.*

$$\|T_{jk}f\|_p \le C_p\|\nabla f\|_p, \qquad \text{for } p\in(1,\infty). \tag{3.61}$$

Since $(-\Delta)^{-1/2}$ is taken as an approximation of U_ε^{2D} (3.5), we consider the convergence regarding with the derivatives.

Lemma 3.4 *Let $U_\varepsilon^{2D}(\mathbf{x})$ ($\mathbf{x}=(x_1,x_2)$) be given in (3.5), suppose real-valued function $f\in L^p(\mathbb{R}^2)$, let*

$$T_j^\varepsilon(f) = \partial_{x_j}(U_\varepsilon^{2D} * f), \quad R_j(f) = \partial_{x_j}(-\Delta)^{-1/2}f, \quad j=1,2, \tag{3.62}$$

we have T_j^ε is bounded from L^p to L^p ($1<p<\infty$) with the bounds independent of ε. Specially, for any fixed $f\in L^p(\mathbb{R}^2)$, ($p\in(1,\infty)$),

$$\lim_{\varepsilon\to 0^+}\|T_j^\varepsilon(f) - R_j(f)\|_p = 0, \quad p\in(1,\infty). \tag{3.63}$$

Proof: We can write R_j and T_j^ε as

$$R_j(f) = K_j * f, \quad T_j^\varepsilon(f) = K_j^\varepsilon * f, \tag{3.64}$$

where R_j is Riesz transform and

$$K_j(\mathbf{x}) = \frac{x_j}{2\pi|\mathbf{x}|^3}, \quad K_j^\varepsilon(\mathbf{x}) = \frac{1}{2\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}}\frac{x_j e^{-s^2/2}}{(|\mathbf{x}|^2+\varepsilon^2 s^2)^{3/2}}\,ds, \quad j=1,2. \tag{3.65}$$

K_j^ε obviously satisfies the following condition

$$|K_j^\varepsilon(\mathbf{x})| \le B|\mathbf{x}|^{-2}, \quad |\nabla K_j^\varepsilon(\mathbf{x})| \le B|\mathbf{x}|^{-3}, \quad |\mathbf{x}|>0,$$
$$\int_{R_1<|\mathbf{x}|<R_2} K_j^\varepsilon(\mathbf{x})d\mathbf{x} = 0, \quad 0<R_1<R_2<\infty,$$

for some ε-independent constant B. Then standard theorem on singular integrals [134] implies that T_j^ε is well defined for L^p function and is bounded from L^p to L^p with ε-independent bound.

Thus, we only need to prove the convergence in L^2 , other cases can be derived by an approximation argument and interpolation. For L^2 convergence, looking at the Fourier domain, we find that

$$\begin{aligned}\|T_j^\varepsilon(f) - R_j(f)\|_2^2 &= \frac{1}{4\pi^2}\int_{\mathbb{R}^2} |\hat{f}|^2(\xi)\left[\frac{\xi_j}{|\xi|} - \frac{\xi_j}{\pi}\int_{\mathbb{R}} \frac{e^{-\varepsilon^2 s^2/2}}{|\xi|^2+s^2}ds\right]^2 d\xi \\ &\le \frac{1}{4\pi^2}\int_{\mathbb{R}^2} |\hat{f}|^2(\xi)\left[\frac{1}{\pi}\int_{\mathbb{R}} \frac{(1-e^{-\varepsilon^2 s^2/2})|\xi|}{|\xi|^2+s^2}ds\right]^2 d\xi.\end{aligned}$$

Notice that for fixed $\xi \neq 0$, dominated convergence theorem suggests that

$$\lim_{\varepsilon\to 0^+}\frac{1}{\pi}\left|\int_{\mathbb{R}} \frac{(1-e^{-\varepsilon^2 s^2/2})|\xi|}{|\xi|^2+s^2}ds\right| = 0, \tag{3.66}$$

hence, the conclusion in L^2 case is obvious by dominated convergence theorem again. Using approximation and noticing that $L^2\cap L^q$ is dense in L^p $(q\in(1,\infty))$, combined with uniform bound on $T_j^\varepsilon : L^p \to L^p$ $(p\in(1,\infty))$, we can complete the proof. □

Lemma 3.5 *For the energy $\tilde{E}_{2D}(\cdot)$ in (3.55), the following properties hold*

(i) For any $\phi \in S_2$, denote $\rho(\mathbf{x}) = |\phi(\mathbf{x})|^2$, then we have

$$\tilde{E}_{2D}(\phi) \ge \tilde{E}_{2D}(|\phi|) = \tilde{E}_{2D}\left(\sqrt{\rho}\right), \qquad \forall \phi \in S_2, \tag{3.67}$$

so the ground state ϕ_g of (3.55) is of the form $e^{i\theta_0}|\phi_g|$ for some constant $\theta_0 \in \mathbb{R}$.

(ii) If condition (B1) or (B2) or (B3) in Theorem 3.4 holds, then $\tilde{E}_{2D}$ is bounded below.

(iii) If condition (B1′) or (B2′) or (B3′) in Theorem 3.4 holds, then $\tilde{E}_{2D}(\sqrt{\rho})$ is strictly convex.

Proof: (i) It is similar to the case of Lemma 3.2.

(ii) Similar as Lemma 3.2, for $\phi \in S_2$, denote $\rho = |\phi|^2$, we only need to consider the following functional,

$$\tilde{H}(\rho) = -\lambda\int_{\mathbb{R}^2} \rho\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta\right)[(-\Delta)^{-1/2}\rho]\, d\mathbf{x}. \tag{3.68}$$

Using Plancherel formula and Cauchy inequality, we have for $\lambda < 0$ and $n_3^2 \ge \frac{1}{2}$,

$$\begin{aligned}\tilde{H}(\rho) &= \frac{\lambda}{4\pi^2}\int_{\mathbb{R}^2}\frac{(n_1\xi_1+n_2\xi_2)^2 - n_3^2|\xi_3|^2}{|\xi|}|\hat{\rho}(\xi)|^2\, d\xi \\ &\ge \frac{\lambda}{4\pi^2}\int_{\mathbb{R}^2}(1-2n_3^2)|\xi||\hat{\rho}(\xi)|^2\, d\xi \ge 0.\end{aligned} \tag{3.69}$$

For $\lambda > 0$ and $n_3 = 0$, it is easy to see $\tilde{H}(\rho) \geq 0$. Hence, assertion (ii) is proved.

(iii) Similar as Lemma 3.2, it is sufficient to prove the convexity of $\tilde{H}(\rho)$ (3.68) in ρ. For $\sqrt{\rho_1} \in S_2$, $\sqrt{\rho_2} \in S_2$ and any $\theta \in [0,1]$, denote $\rho_\theta = \theta\rho_1 + (1-\theta)\rho_2$,

$$\theta\tilde{H}(\rho_1) + (1-\theta)\tilde{H}(\rho_2) - \tilde{H}(\rho_\theta) = \theta(1-\theta)\tilde{H}(\rho_1 - \rho_2), \tag{3.70}$$

where the RHS is nonnegative with the given condition, i.e., $\tilde{H}(\rho)$ is convex. □

Proof of Theorem 3.4: (i) We only need to consider the existence since the uniqueness is a consequence of convexity of $\tilde{E}_{2D}(\sqrt{\rho})$ in Lemma 3.5. For existence, we may apply the same arguments in Theorem 3.1, where instead, we have to show that for sequence $\rho^n = (\phi^n)^2$,

$$\liminf_{n\to\infty} \tilde{H}(\rho^n) \geq \tilde{H}(\rho^\infty), \quad \text{with } \rho^\infty = (\phi^\infty)^2. \tag{3.71}$$

Denote

$$\varphi^n = \left(\partial_{\mathbf{n}_\perp \mathbf{n}_\perp} - n_3^2\Delta\right)[(-\Delta)^{-1/2}\rho^n], n = 0, 1, \dots, \text{ or } n = \infty.$$

Using $\phi^n \to \phi^\infty$ in $L^2(\mathbb{R}^2)$ and $\phi^n \rightharpoonup \phi^\infty$ in $H^1(\mathbb{R}^2)$, then $\rho^n \to \rho^\infty$ in $L^p(\mathbb{R}^2)$ $p > 1$, and Lemma 3.3 shows that $\varphi^n \to \varphi^\infty$ in $W^{-1,p}(\mathbb{R}^2)$(dual space of $W^{1,p'}$, $p' = p/(p-1)$). Thus (3.71) is true and the existence of ground state follows.

(ii) To prove the nonexistence results, we try to find the case where $\tilde{E}_{2D}$ doesn't have lower bound. For any $\phi(\mathbf{x}) \in S_2$ and $\rho(\mathbf{x}) = |\phi(\mathbf{x})|^2$, $\mathbf{x} = (x_1, x_2)$, let $\theta \in \mathbb{R}$ such that $(\cos\theta, \sin\theta) = \frac{1}{\sqrt{n_1^2+n_2^2}}(n_1, n_2)$ when $n_1^2 + n_2^2 \neq 0$ and $\theta = 0$ if $n_1 = n_2 = 0$, for any $\varepsilon_1, \varepsilon_2 > 0$, consider the following function

$$\phi_{\varepsilon_1,\varepsilon_2}(x_1,x_2) = \varepsilon_1^{-1/2}\varepsilon_2^{-1/2}\phi(\varepsilon_1^{-1}(x_1\cos\theta + x_2\sin\theta), \varepsilon_2^{-1}(-x_1\sin\theta + x_2\cos\theta)), \tag{3.72}$$

let $\rho_{\varepsilon_1,\varepsilon_2} = |\phi_{\varepsilon_1,\varepsilon_2}|^2$, then

$$\widehat{\rho_{\varepsilon_1,\varepsilon_2}}(\xi_1,\xi_2) = \hat{\rho}(\varepsilon_1(\xi_1\cos\theta + \xi_2\sin\theta), \varepsilon_2(-\xi_1\sin\theta + \xi_2\cos\theta)), \tag{3.73}$$

and by Plancherel formula, after changing variables,

$$\begin{aligned}
\tilde{H}(\rho_{\varepsilon_1,\varepsilon_2}) &= \frac{\lambda}{4\pi^2}\int_{\mathbb{R}^2} \frac{(n_1\xi_1 + n_2\xi_2)^2 - n_3^2|\xi^2|}{|\xi|}|\widehat{\rho_{\varepsilon_1,\varepsilon_2}}|^2 d\xi \\
&= \frac{\lambda}{4\pi^2}\int_{\mathbb{R}^2} \frac{(n_1^2+n_2^2)\eta_1^2 - n_3^2|\eta|^2}{|\eta|}|\widehat{\rho}|^2(\varepsilon_1\eta_1, \varepsilon_2\eta_2) d\eta \\
&= \frac{\lambda}{4\varepsilon_1^2\varepsilon_2\pi^2}\int_{\mathbb{R}^2} \frac{(n_1^2+n_2^2)\eta_1^2 - n_3^2(\eta_1^2 + \frac{\varepsilon_2^2}{\varepsilon_1^2}\eta_2^2)}{\sqrt{\eta_1^2 + \frac{\varepsilon_2^2}{\varepsilon_1^2}\eta_2^2}}|\widehat{\rho}|^2(\eta_1,\eta_2) d\eta.
\end{aligned}$$

Let $\kappa = \frac{\varepsilon_2}{\varepsilon_1}$, then the dominated convergence theorem implies

$$\tilde{H}(\rho_{\varepsilon_1,\varepsilon_2}) = \begin{cases} \frac{n_1^2+n_2^2-n_3^2+o(1)}{4\varepsilon_1^2\varepsilon_2}\lambda \int_{\mathbb{R}^2} |\eta_1||\widehat{\rho}|^2(\eta_1,\eta_2)d\eta, & \kappa \to 0^+, \\ \frac{-n_3^2+o(1)}{4\varepsilon_1^2\varepsilon_2}\lambda \int_{\mathbb{R}^2} |\eta_1||\widehat{\rho}|^2(\eta_1,\eta_2)d\eta, & \kappa \to +\infty. \end{cases} \tag{3.74}$$

For fixed κ and letting $\varepsilon_1 \to 0^+$, we have $\int_{\mathbb{R}^2} V_2(\mathbf{x})|\phi_{\varepsilon_1,\varepsilon_2}|^2\, d\mathbf{x} = O(1)$ and

$$\|\nabla\phi_{\varepsilon_1,\varepsilon_2}\|_2^2 = \frac{1}{\varepsilon_1^2}\|\partial_{x_1}\phi\|_2^2 + \frac{1}{\varepsilon_2^2}\|\partial_{x_2}\phi\|_2^2, \quad \|\phi_{\varepsilon_1,\varepsilon_2}\|_4^4 = \frac{1}{\varepsilon_1\varepsilon_2}\|\phi\|_4^4. \tag{3.75}$$

Thus under the condition (B1$''$), i.e $n_3 \neq 0$ and $\lambda > 0$, choosing κ large enough, we get

$$\tilde{E}_{2D}(\phi_{\varepsilon_1,\varepsilon_2}) = \frac{C_1}{\varepsilon_1^2} + \frac{C_2}{\kappa^2\varepsilon_1^2} + \frac{C_3}{\kappa\varepsilon_1^2} + C_4\lambda\frac{-n_3^2 + o(1)}{\kappa\varepsilon_1^3} + O(1), \tag{3.76}$$

where C_k $(k = 1, 2, 3, 4)$ are constants independent of κ, ε_1 and $C_4 > 0$. Since $n_3 \neq 0$, the last term is negative for κ large, sending $\varepsilon_1 \to 0^+$, one immediately finds that $\lim_{\varepsilon_1\to 0^+,\varepsilon_2=\kappa\varepsilon_1} \tilde{E}_{2D}(\phi_{\varepsilon_1,\varepsilon_2}) = -\infty$, which justifies the nonexistence. Under the condition (B2$''$), i.e. $n_3^2 \le \frac{1}{2}$ and $\lambda < 0$, by choosing κ small enough in (3.74), sending ε_1 to 0^+, we will have the same results. Case (B3$''$) will reduce to Theorem 3.1. □

3.3.2 Existence results for dynamics

Let us consider the Cauchy problem of equation (3.8), noticing the nonlinearity $\phi(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)((-\Delta)^{-1/2}|\phi|^2)$ is actually a derivative nonlinearity, and it would bring significant difficulty in analyzing the dynamical behavior. The common approach to solve the Schrödinger equation is trying to solve the corresponding integral equation by fixed point theorem. However, the loss of order 1 derivative due to the nonlocal term will cause trouble. This can be overcome by the smoothing effect of inhomogeneous problem $iu_t + \Delta u = g(x,t)$, which provides a gain of one derivative [35,90]. To implement the idea in our case, it is convenient to consider the case $V_2(\mathbf{x}) = 0$. By configuring that $(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)((-\Delta)^{-1/2}|\phi|^2)$ is almost a first order derivative, we are able to discuss the well-posedness of (3.8) with above technical tool.

Cauchy problem of Schrödinger equation with derivative nonlinearity has been investigated extensively [80, 91] in the literature. Here, we present an existence results in the energy space with the special structure of our nonlinearity, which will show that the approximation (3.8) of (3.4) is reasonable in suitable sense.

Theorem 3.5 *(Existence for Cauchy problem) Suppose the real potential* $V_2(\mathbf{x}) = \frac{1}{2}|\mathbf{x}|^2$*, and initial value* $\phi_0(\mathbf{x}) \in \Xi_2$*, one of the condition (1′), (2′) (3′) in Theorem 3.4 holds, then there exists a solution* $\phi \in L^\infty([0,\infty);\Xi_2) \cap W^{1,\infty}([0,\infty);\Xi_2^*)$ *for the Cauchy problem of (3.8). Moreover, there holds for* L^2 *norm and energy* $\tilde{E}_{2D}$ *(3.55),*

$$\|\phi(\cdot,t)\|_{L^2(\mathbb{R}^2)} = \|\phi_0\|_{L^2(\mathbb{R}^2)}, \quad \tilde{E}_{2D}(\phi(t)) \le \tilde{E}_{2D}(\phi_0), \quad \forall t \ge 0. \tag{3.77}$$

Proof: We first consider the Cauchy problem for the following equation,

$$i\partial_t \phi^\delta = \mathbf{H_x}\phi^\delta + g_1(\phi^\delta) + g_2(\phi^\delta), \tag{3.78}$$

with initial value ϕ_0, where $\beta_0 = \frac{\beta - \lambda + \lambda n_3^2}{\varepsilon\sqrt{2\pi}}$, $\varphi^\delta = U_\delta^{2D} * |\phi^\delta|^2$ (3.5) and

$$\mathbf{H_x} = -\frac{1}{2}\Delta + V_2(\mathbf{x}), \quad g_1(\phi^\delta) = \beta_0|\phi^\delta|^2\phi^\delta, \quad g_2(\phi^\delta) = -\frac{3\lambda}{2}\phi^\delta(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi^\delta. \tag{3.79}$$

Then our quasi-2D equation II (3.4) can be written as

$$i\partial_t \phi = \mathbf{H_x}\phi + g_1(\phi) + \tilde{g}_2(\phi), \tag{3.80}$$

where

$$\tilde{g}_2(\phi) = -\frac{3\lambda}{2}\phi(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)(-\Delta)^{-1/2}(|\phi|^2). \tag{3.81}$$

We denote the pairing of Ξ_2 and its dual Ξ_2^* by $\langle,\rangle_{\Xi_2,\Xi_2^*}$ as

$$\langle f_1, f_2\rangle_{\Xi_2,\Xi_2^*} = \mathrm{Re}\int_{\mathbb{R}^2} f_1(\mathbf{x})\bar{f}_2(\mathbf{x})\,d\mathbf{x}. \tag{3.82}$$

Using the results in [43] and Theorem 3.2, we see there exists a unique maximal solution $\varphi^\delta \in C([-T_{min}^\delta, T_{max}^\delta], \Xi_2) \cap C^1([-T_{min}^\delta, T_{max}^\delta], \Xi_2^*)$. Maximal means that if either $t \uparrow T_{max}^\delta$ or $t \downarrow -T_{min}^\delta$, $\|\phi^\delta(t)\|_{\Xi_2} \to \infty$. We want to show that as $\delta \to 0^+$, ϕ^δ will converge to a solution of equation (3.8).

Existence. First, we show that $T_{min}^\delta = -\infty$, $T_{max}^\delta = +\infty$. The energy conservation for (3.78) is

$$E_\delta(t) := \frac{1}{2}\|\nabla\phi^\delta\|_2^2 + \frac{1}{2}\beta_0\|\phi^\delta\|_4^4 + \int_{\mathbb{R}^2} V_2(\mathbf{x})|\phi^\delta|^2 d\mathbf{x} + E_{dip}^\delta(t) = E_\delta(0), \tag{3.83}$$

where

$$E_{dip}^\delta(t) = -\frac{3\lambda}{4}\int_{\mathbb{R}^2} |\phi^\delta|^2(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi^\delta d\mathbf{x}. \tag{3.84}$$

Similar computation as in Lemma 3.5 confirms that $E^\delta_{dip} \geq 0$, $\beta_0 \geq 0$. Hence energy conservation will imply that $\|\phi^\delta(t)\|_{\Xi_2} < \infty$ for all t, i.e. $T^\delta_{max} = T^\delta_{min} = \infty$.

We notice that

$$\Xi_2 \hookrightarrow H^1 \hookrightarrow L^2 \hookrightarrow H^{-1} \hookrightarrow \Xi_2^*, \tag{3.85}$$

where H^{-1} is viewed as the dual of H^1. Consider a bounded time interval $I = [-T, T]$. It follows from energy conservation that there exists a constant $C_1(\phi_0) > 0$ such that

$$\|\phi^\delta\|_{C([-T,T];\Xi_2)} \leq C_1(\phi_0). \tag{3.86}$$

Moreover, Lemma 3.1 and Remark 3.2 would imply

$$\|\phi^\delta(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi^\delta\|_q \leq C\|\phi^\delta\|_{q^*}\|\nabla|\phi^\delta|^2\|_p \leq C\|\phi^\delta\|_{q^*}\|\phi^\delta\|_{2p/(2-p)}\|\nabla\phi^\delta\|_2, \tag{3.87}$$

for $q, p \in (1,2)$, $\frac{1}{q^*} + \frac{1}{p} = \frac{1}{q}$. Then we have

$$\|\phi^\delta\|_{C^1([-T,T];\Xi_2^*)} \leq C_2(\phi_0). \tag{3.88}$$

Thus, from (3.86) and (3.88), there exist a sequence $\delta_n \to 0^+$ $(n = 1, 2, \ldots,)$ and a function $\phi \in L^\infty([-T,T];\Xi_2) \cap W^{1,\infty}([-T,T];\Xi_2^*)$, such that

$$\phi^{\delta_n}(t) \rightharpoonup \phi(t) \quad \text{in } \Xi_2, \text{ for all } t \in [-T,T]. \tag{3.89}$$

For each $t \in [-T,T]$, due to the mass conservation of equation (3.78), we know $\|\phi^{\delta_n}(t)\|_2 = \|\phi_0\|_2$, by a similar proof in Theorem 3.1, the weak convergence of $\phi^{\delta_n}(t)$ in Ξ_2 would imply that $\phi^{\delta_n}(t)$ converges strongly in L^2, which is a consequence of the fact that $V_2(\mathbf{x}) = \frac{1}{2}|\mathbf{x}|^2$ is a confining potential. So, $\lim_{n\to\infty} \|\phi^{\delta_n}(t)\|_2 = \|\phi(t)\|_2$, and it turns out that [43]

$$\phi^{\delta_n} \to \phi, \qquad \text{in } C([-T,T];L^2(\mathbb{R}^2)). \tag{3.90}$$

In view of (3.89), (3.90) and Gagliardo-Nirenberg's inequality, we obtain

$$\phi^{\delta_n} \to \phi, \qquad \text{in } C([-T,T];L^p(\mathbb{R}^2)), \qquad \text{for all } p \in [2,\infty). \tag{3.91}$$

We now try to say that ϕ actually solves equation (3.8). For any function $\psi(\mathbf{x}) \in \Xi_2$ and $f(t) \in C_c^\infty([-T,T])$, from equation (3.78), we have

$$\int_{-T}^{T} \left[\langle i\phi^{\delta_n}, \psi\rangle_{\Xi_2,\Xi_2^*} f'(t) + \langle \mathbf{H_x}\phi^{\delta_n} + g_1(\phi^{\delta_n}) + g_2(\phi^{\delta_n}), \psi\rangle_{\Xi_2,\Xi_2^*} f(t)\right] dt = 0. \tag{3.92}$$

Recalling $|g_1(u) - g_1(v)| \leq C(|u|^2 + |v|^2)|u - v|$, (3.91) implies that [43] for all $t \in [-T, T]$

$$g_1(\phi^{\delta_n}(t)) \to g_1(\phi(t)), \quad \text{in } L^\rho(\mathbb{R}^2) \text{ for some } \rho \in [1, \infty), \tag{3.93}$$

$$\langle g_1(\phi^{\delta_n}(t)), \psi(t)\rangle_{\Xi_2, \Xi_2^*} \to \langle g_1(\phi(t)), \psi(t)\rangle_{\Xi_2, \Xi_2^*}. \tag{3.94}$$

For $g_2(\phi^{\delta_n})$, consider $\varphi^{\delta_n}(\mathbf{x}, t)$, $\mathbf{x} = (x_1, x_2)$, noticing the $\partial_{x_j}\varphi^{\delta_n} = T_j^{\delta_n}(|\phi^{\delta_n}|^2)$ $(j = 1, 2)$ (defined in Lemma 3.4), we have proven in Lemma 3.4 $T_j^{\delta_n}$ is uniformly bounded from L^p to L^p and as $\delta_n \to 0^+$,

$$T_j^{\delta_n}(|\phi(t)|^2) \to R_j(|\phi(t)|^2) = \partial_{x_j}(-\Delta)^{-1/2}(|\phi(t)|^2) \text{ in } L^p(\mathbb{R}^2), p \in (1, \infty), \tag{3.95}$$

thus by rewriting

$$T_j^{\delta_n}(|\phi^{\delta_n}(t)|^2) = T_j^{\delta_n}(|\phi^{\delta_n}(t)|^2 - |\phi(t)|^2) + T_j^{\delta_n}(|\phi(t)|^2), \tag{3.96}$$

recalling the fact (3.91), we immediately have

$$T_j^{\delta_n}(|\phi^{\delta_n}(t)|^2) \to R_j(|\phi(t)|^2) \text{ in } L^p(\mathbb{R}^2), \text{ for some } p \in (1, \infty), \tag{3.97}$$

which is actually

$$\partial_{x_j}\varphi^{\delta_n}(t) \to \partial_{x_j}(-\Delta)^{-1/2}(|\phi(t)|^2), \text{ in } L^p(\mathbb{R}^2), \text{ for some } p \in (1, \infty). \tag{3.98}$$

Hence, integration by parts,

$$\begin{aligned}\langle \phi^{\delta_n}(t)\partial_{x_j x_k}\varphi^{\delta_n}(t), \psi(t)\rangle_{\Xi_2, \Xi_2^*} &= \mathrm{Re}\int_{\mathbb{R}^2} \phi^{\delta_n}(t)\partial_{x_j x_k}\varphi^{\delta_n}(t)\bar{\psi}(t)d\mathbf{x} \\ &= -\mathrm{Re}\int_{\mathbb{R}^2} \partial_{x_j}\varphi^{\delta_n}(t)(\partial_{x_k}\phi^{\delta_n}(t)\bar{\psi}(t) + \phi^{\delta_n}(t)\overline{\partial_{x_k}\psi}(t))d\mathbf{x},\end{aligned}$$

passing to the limit as $n \to \infty$,

$$\begin{aligned}\lim_{n\to\infty}\langle \phi^{\delta_n}(t)\partial_{x_j x_k}\varphi^{\delta_n}(t), \psi(t)\rangle_{\Xi_2, \Xi_2^*} &= -\mathrm{Re}\int_{\mathbb{R}^2} R_j(|\phi(t)|^2)(\partial_{x_k}\phi(t)\bar{\psi}(t) + \phi(t)\overline{\partial_{x_k}\psi}(t))d\mathbf{x} \\ &= \langle \phi(t)\partial_{x_j x_k}(-\Delta)^{-1/2}(|\phi(t)|^2), \psi(t)\rangle_{\Xi_2, \Xi_2^*},\end{aligned}$$

in view of (3.98) and (3.89), we obtain

$$\lim_{n\to\infty}\langle g_2(\varphi^{\delta_n}(t)), \psi(t)\rangle_{\Xi_2, \Xi_2^*} = \langle \tilde{g}_2(\phi(t)), \psi(t)\rangle_{\Xi_2, \Xi_2^*}. \tag{3.99}$$

Combining the above results and (3.94) together, sending $n \to \infty$, dominated convergence theorem will yield

$$\int_{-T}^{T} \left[\langle i\phi, \psi\rangle_{\Xi_2, \Xi_2^*} f'(t) + \langle \mathbf{H_x}\phi + g_1(\phi) + \tilde{g}_2(\phi), \psi\rangle_{\Xi_2, \Xi_2^*} f(t)\right] dt = 0,$$

which proves that

$$i\partial_t\phi = \mathbf{H}_{\mathbf{x}}\phi + g_1(\phi) + \tilde{g}_2(\phi), \text{ in } \Xi_2^*, \quad \text{a.a. } t \in [-T,T], \tag{3.100}$$

with $\phi(t=0) = \phi_0$, and $\phi \in L^\infty([-T,T];\Xi_2) \cap W^{1,\infty}([-T,T];\Xi_2^*)$. Moreover, by lower semi-continuity of Ξ_2 norm, (3.93) and (3.99), the energy $\tilde{E}_{2D}$ (3.55) satisfies

$$\tilde{E}_{2D}(\phi(t)) \le \tilde{E}_{2D}(\phi_0). \tag{3.101}$$

It is easy to see that we can choose $T = \infty$. □

If the uniqueness of the $L^\infty([-T,T];\Xi_2) \cap W^{1,\infty}([-T,T];\Xi_2^*)$ solution to the quasi-2D equation II (3.8) is known, we can prove that the solution constructed above in the Theorem 3.5 is actually $C([-T,T];\Xi_2) \cap C^1([-T,T];\Xi_2^*)$ and conserves the energy.

Next, we discuss possible blow-up for continuous solutions of the quasi-2D equation II (3.8). To this purpose, the following assumptions are introduced:

(A) Assumption on the trap and coefficient of the cubic term, i.e. $V_2(\mathbf{x})$ satisfies $3V_2(\mathbf{x}) + \mathbf{x}\cdot\nabla V_2(\mathbf{x}) \ge 0$, $\frac{\beta-\lambda+\lambda n_3^2}{\sqrt{2\pi}\,\varepsilon} \ge -\frac{C_b}{\|\psi_0\|_2^2}$, with ψ_0 being the initial data of equation (3.8);

(B) Assumption on the trap and coefficient of the nonlocal term, i.e. $V_2(\mathbf{x})$ satisfies $2V_2(\mathbf{x}) + \mathbf{x}\cdot\nabla V_2(\mathbf{x}) \ge 0$, $\lambda = 0$ or $\lambda > 0$ and $n_3^2 \ge \frac{1}{2}$.

Theorem 3.6 *(Finite time blow-up) If conditions (B1), (B2) and (B3) are not satisfied, for any initial data* $\phi(\mathbf{x},t=0) = \phi_0(\mathbf{x}) \in \Xi_2$ *with* $\int_{\mathbb{R}^2} |\mathbf{x}|^2|\phi_0(\mathbf{x})|^2\,d\mathbf{x} < \infty$ *and* $C([0,T_{max}),\Xi_2)$ *solution* $\phi(\mathbf{x},t)$ *to the problem (3.8) with* L^2 *norm and energy conservation, there exists finite time blow-up, i.e.,* $T_{max} < \infty$*, if one of the following condition holds:*

(i) $\tilde{E}_{2D}(\phi_0) < 0$*, and either assumption (A) or (B) holds;*

(ii) $\tilde{E}_{2D}(\phi_0) = 0$ *and* $\mathrm{Im}\left(\int_{\mathbb{R}^2} \bar{\phi}_0(\mathbf{x})\ (\mathbf{x}\cdot\nabla\phi_0(\mathbf{x}))\,d\mathbf{x}\right) < 0$*, and either assumption (A) or (B) holds;*

(iii) $\tilde{E}_{2D}(\phi_0) > 0$*, and* $\mathrm{Im}\left(\int_{\mathbb{R}^2} \bar{\phi}_0(\mathbf{x})\ (\mathbf{x}\cdot\nabla\phi_0(\mathbf{x}))\,d\mathbf{x}\right) < -\sqrt{3\tilde{E}_{2D}(\phi_0)}\|\mathbf{x}\phi_0\|_2$ *if assumption (A) holds, or* $\mathrm{Im}\left(\int_{\mathbb{R}^2} \bar{\phi}_0(\mathbf{x})\ (\mathbf{x}\cdot\nabla\phi_0(\mathbf{x}))\,d\mathbf{x}\right) < -\sqrt{2\tilde{E}_{2D}(\phi_0)}\|\mathbf{x}\phi_0\|_2$ *if assumption (B) holds.*

Proof: Calculating the derivative of variance defined in (3.49), for $\alpha = x, y$, we have

$$\frac{d}{dt}\sigma_\alpha(t) = 2\,\mathrm{Im}\left(\int_{\mathbb{R}^2} \bar{\phi}(\mathbf{x},t)\ \alpha\partial_\alpha\phi(\mathbf{x},t)\,d\mathbf{x}\right), \tag{3.102}$$

and

$$\frac{d^2}{dt^2}\sigma_\alpha(t) = \int_{\mathbb{R}^2}\left[2|\partial_\alpha\phi|^2 + \beta_0|\phi|^4 + 3\lambda|\phi|^2\alpha\partial_\alpha(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi - 2\alpha|\phi|^2\partial_\alpha V_2(\mathbf{x})\right]\,d\mathbf{x}, \tag{3.103}$$

where $\beta_0 = \frac{\beta-\lambda+\lambda n_3^2}{\sqrt{2\pi\varepsilon}}$, $(-\Delta)^{1/2}\varphi = |\phi|^2$. Writing $\rho = |\phi|^2$, $\tilde{\varphi} = (\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi$ and noticing that ρ is real function, by Plancherel formula, similarly as Theorem 3.3, we get

$$\int_{\mathbb{R}^2}|\phi|^2\left(\mathbf{x}\cdot\nabla\tilde{\varphi}\right)\,d\mathbf{x} = -\frac{3}{2}\int_{\mathbb{R}^2}|\phi|^2\tilde{\varphi}\,d\mathbf{x}. \tag{3.104}$$

Hence, summing (3.103) for $\alpha = x$, y, and using energy conservation, if assumption (A) holds, we have

$$\begin{aligned}\frac{d^2}{dt^2}\sigma_V(t) &= 2\int_{\mathbb{R}^2}\left(|\nabla\phi|^2 + \beta_0|\phi|^4 - \frac{9}{4}\lambda|\phi|^2\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta\right)\varphi - |\phi|^2(\mathbf{x}\cdot\nabla V_2(\mathbf{x}))\right)\,d\mathbf{x}\\ &= 6E(\phi) - \int_{\mathbb{R}^2}(|\nabla\phi|^2 + \beta_0|\phi|^4)\,d\mathbf{x} - 2\int_{\mathbb{R}^2}|\phi(\mathbf{x},t)|^2\left(3V_2(\mathbf{x}) + \mathbf{x}\cdot\nabla V_2(\mathbf{x})\right)\,d\mathbf{x}\\ &\le 6E(\phi(\cdot,t)) \equiv 6E(\phi_0), \qquad t\ge 0. \end{aligned}\tag{3.105}$$

Thus,

$$\sigma_V(t) \le 3E(\phi_0)t^2 + \sigma_V'(0)t + \sigma_V(0), \qquad t \ge 0,$$

and the conclusion follows as in Theorem 3.3. If assumption (B) holds, the energy contribution of the nonlocal part is non-positive and we have

$$\begin{aligned}\frac{d^2}{dt^2}\sigma_V(t) &= 2\int_{\mathbb{R}^2}\left(|\nabla\phi|^2 + \beta_0|\phi|^4 - \frac{9}{4}\lambda|\phi|^2\left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta\right)\varphi - |\phi|^2(\mathbf{x}\cdot\nabla V_2(\mathbf{x}))\right)\,d\mathbf{x}\\ &= 4E(\phi) - \frac{3\lambda}{2}\int_{\mathbb{R}^2}|\phi|^2\tilde{\varphi}\,d\mathbf{x} - 2\int_{\mathbb{R}^2}|\phi(\mathbf{x},t)|^2\left(2V_2(\mathbf{x}) + \mathbf{x}\cdot\nabla V_2(\mathbf{x})\right)\,d\mathbf{x}\\ &\le 4E(\phi(\cdot,t)) \equiv 4E(\phi_0), \qquad t\ge 0, \end{aligned}\tag{3.106}$$

and the conclusion follows in a similar way as the assumption (A) case. □

3.4 Results for the quasi-1D equation

In this section, we prove the existence and uniqueness of the ground state for the quasi-1D equation (3.10) and establish the well-posedness for dynamics.

3.4.1 Existence and uniqueness of ground state

Associated to the quasi-1D equation (3.10), the energy is

$$E_{1D}(\phi) = \frac{1}{2}\int_{\mathbb{R}} \left[|\partial_x \phi|^2 + 2V_1(x)|\phi|^2 + \beta_{1D}|\phi|^4 + \frac{3\lambda(1-3n_3^2)}{8\sqrt{2\varepsilon^2\pi}}|\phi|^2\varphi \right] dx, \tag{3.107}$$

where $\beta_{1D} = \frac{\beta+\lambda(1-3n_3^2)/2}{2\varepsilon^2\pi}$ and

$$\varphi(x) = \partial_{xx}(U_\varepsilon^{1D} * |\phi|^2), \quad U_\varepsilon^{1D}(x) = \frac{2e^{\frac{x^2}{2\varepsilon^2}}}{\sqrt{\pi}} \int_{|x|}^{\infty} e^{-\frac{s^2}{2\varepsilon^2}}\, ds. \tag{3.108}$$

Theorem 3.7 *(Existence and uniqueness of ground state)Assume $0 \le V_1(x) \in L^\infty_{loc}(\mathbb{R})$ and $\lim_{|x|\to\infty} V_1(x) = \infty$, for any parameter β, λ and ε, there exists a ground state $\phi_g \in S_1$ of the quasi-1D equation (3.10)-(3.11), and the positive ground state $|\phi_g|$ is unique under one of the following condition:*

(C1) $\lambda(1-3n_3^2) \ge 0$, $\beta - (1-3n_3^2)\lambda \ge 0$;

(C2) $\lambda(1-3n_3^2) < 0$, $\beta + \frac{\lambda}{2}(1-3n_3^2) \ge 0$.

Moreover, $\phi_g = e^{i\theta_0}|\phi_g|$ for some constant $\theta_0 \in \mathbb{R}$.

To complete the proof, we first study the property of the convolution kernel U_ε^{1D} (3.11).

Lemma 3.6 *(Kernel U_ε^{1D}(3.11)) For any $f(x)$ in the Schwartz space $\mathcal{S}(\mathbb{R})$, we have*

$$\widehat{U_\varepsilon^{1D} * f}(\xi) = \hat{f}(\xi)\widehat{U_\varepsilon^{1D}}(\xi) = \frac{\sqrt{2}\,\varepsilon \hat{f}(\xi)}{\sqrt{\pi}} \int_0^\infty \frac{e^{-\varepsilon^2 s/2}}{|\xi|^2 + s} ds. \tag{3.109}$$

Hence

$$\|\partial_{xx}(U_\varepsilon^{1D} * f)\|_2 \le \frac{2\sqrt{2}}{\sqrt{\pi}\,\varepsilon}\|f\|_2. \tag{3.110}$$

Proof: For any $f(x) \in \mathcal{S}$, rewrite the kernel

$$U_\varepsilon^{1D}(x) = \frac{\sqrt{2}\,\varepsilon}{\sqrt{\pi}} \int_{\mathbb{R}^4} \varepsilon^{-4} \frac{w^2(y'/\varepsilon, z'/\varepsilon)w^2(y/\varepsilon, z/\varepsilon)}{\sqrt{x^2 + (y-y')^2 + (z-z')^2}}\, dydzdy'dz',$$

where $w(y,z) = \frac{1}{\pi^{1/2}} e^{-(y^2+z^2)/2}$, applying Fourier transform to both sides and using Plancherel formula as in Lemma 3.1,

$$\widehat{U_\varepsilon^{1D}}(\xi) = \frac{\sqrt{2}\,\varepsilon}{\pi^{3/2}} \int_{\mathbb{R}^2} \frac{|\widehat{w^2}(\varepsilon\xi_1, \varepsilon\xi_2)|^2}{\xi^2 + \xi_1^2 + \xi_2^2}\, d\xi_1\, d\xi_2, \tag{3.111}$$

direct computation would yield the conclusion. □

Lemma 3.7 *For the energy $E_{1D}(\cdot)$ in (3.107), we have*

(i) For any $\phi \in S_1$, denote $\rho(x) = |\phi(x)|^2$ for $x \in \mathbb{R}$, then we have

$$E_{1D}(\phi) \geq E_{1D}(|\phi|) = E_{1D}\left(\sqrt{\rho}\right), \qquad \forall \phi \in S_1, \tag{3.112}$$

so the ground state ϕ_g of (3.107) is of the form $e^{i\theta_0}|\phi_g|$ for some constant $\theta_0 \in \mathbb{R}$.

(ii) E_{1D} is bounded below.

(iii) If condition (C1) or (C2) in Theorem 3.7 holds, $E_{1D}(\sqrt{\rho})$ is strictly convex in ρ.

Proof: Part (i) is similar to that in Lemma 3.1. Part (ii) is well-known, once we notice the property of kernel U_ε^{1D} (Lemma 3.6) and the Sobolev inequality in one dimension,

$$\|f\|_\infty^2 \leq \|f\|_2 \|f'\|_2. \tag{3.113}$$

(iii) We come to the convexity of $E_{1D}(\sqrt{\rho})$. Following Lemma 3.2, we only need to consider the functional

$$H_{1D}(\rho) = \int_{\mathbb{R}} \left[\frac{\beta + \lambda(1-3n_3^2)/2}{2\varepsilon^2\pi}\rho^2 + \frac{3\lambda(1-3n_3^2)}{8\sqrt{2\varepsilon^2\pi}}\rho(\partial_{xx}(U_\varepsilon^{1D} * \rho))\right] dx. \tag{3.114}$$

Then under condition (C1) or (C2), using Plancherel formula and Lemma 3.6, after similar computation as in Lemma 3.1, we would have $H_{1D}(\rho) \geq 0$. For arbitrary $\sqrt{\rho_1}, \sqrt{\rho_2} \in S_1$ and $\theta \in [0,1]$, denote $\rho_\theta = \theta\rho_1 + (1-\theta)\rho_2$, then $\sqrt{\rho_\theta} \in S_1$ and

$$\theta H_{1D}(\rho_1) + (1-\theta)H_{1D}(\rho_2) - H_{1D}(\rho_\theta) = \theta(1-\theta)H_{1D}(\rho_1 - \rho_2) \geq 0, \tag{3.115}$$

which proves the convexity. $\square$

Proof of Theorem 3.7: The uniqueness follows from the strict convexity in Lemma 3.7. The existence part is similar as Theorem 3.1 and we omit it here for brevity. . $\square$

3.4.2 Well-posedness for dynamics

Concerning the Cauchy problem, Lemma 3.6 shows that the nonlinearity in the quasi-1D equation (3.10) is almost like a cubic nonlinearity, while the same property has been observed in the quasi-2D equation (3.4)-(3.5). Hence similar results as Theorem 3.2 can be obtained for equation (3.10) and we omit the proof here.

Theorem 3.8 *(Well-posedness for Cauchy problem) Suppose the real-valued trap potential $V_1(x) \in C^\infty(\mathbb{R})$ such that $V_1(x) \geq 0$ for $x \in \mathbb{R}$ and $D^\alpha V_1(x) \in L^\infty(\mathbb{R})$ for all integers $\alpha \geq 2$. For any initial data $\phi(x, t=0) = \phi_0(x) \in \Xi_1$, there exists a unique solution $\phi \in C([0,\infty), \Xi_1) \cap C^1([0,\infty), \Xi_1^*)$ to the Cauchy problem of equation (3.10).*

3.5 Convergence rate of dimension reduction

In this section, we discuss the dimension reduction of 3D GPPS to lower dimensions. Inspired by the formal work of Ben Abdallah et al. [29, 30] for GPE without the dipolar term (i.e. $\lambda = 0$), we are going to find a limiting ε-independent equation as $\varepsilon \to 0^+$. Thus in the quasi-2D equation I (3.4), II (3.8) and the quasi-1D equation (3.10), we have to consider the coefficients to be $O(1)$. [10, 42] have shown that the global solution exists for the full 3D system (2.19)-(2.20) for $\lambda \in [-\frac{1}{2}\beta, \beta]$ with $\beta \geq 0$, hence we would expect the limiting equation in lower dimensions valid in a similar regime. Thus in lower dimensions, we require that in the quasi-2D case, $\beta = O(\varepsilon)$, $\lambda = O(\varepsilon)$, and in the quasi-1D case, $\beta = O(\varepsilon^2)$, $\lambda = O(\varepsilon^2)$, i.e., we are considering the weak interaction regime, then we would get an ε-independent limiting equation. In this regime, we will see that GPPS will reduce to regular GPE in lower dimensions.

3.5.1 Reduction to 2D

We consider the weak regime, i.e., $\beta \to \beta/\varepsilon$, $\lambda \to \lambda/\varepsilon$. In **Case I** (3.1), for full 3D GPPS (2.19)-(2.20), introducing the scaling $z \to z/\varepsilon$, $\psi \to \varepsilon^{1/2}\psi^\varepsilon$ which preserves the normalization, then

$$i\partial_t \psi^\varepsilon(\mathbf{x}, t) = \left[\mathbf{H}_\perp + \frac{1}{\varepsilon^2}\mathbf{H}_z + (\beta - \lambda)|\psi^\varepsilon|^2 - 3\varepsilon\lambda\partial_{\mathbf{n}_\varepsilon\mathbf{n}_\varepsilon}\varphi^\varepsilon\right]\psi^\varepsilon, \; \mathbf{x} = (x, y, z)^T \in \mathbb{R}^3, \tag{3.116}$$

where

$$\mathbf{H}_\perp = -\frac{1}{2}(\partial_{xx} + \partial_{yy}) + V_2(x, y), \quad \mathbf{H}_z = -\frac{1}{2}\partial_{zz} + \frac{z^2}{2}, \tag{3.117}$$

$$\mathbf{n}_\varepsilon = (n_1, n_2, n_3/\varepsilon), \quad \partial_{\mathbf{n}_\varepsilon} = \mathbf{n}_\varepsilon \cdot \nabla, \quad \partial_{\mathbf{n}_\varepsilon\mathbf{n}_\varepsilon} = \partial_{\mathbf{n}_\varepsilon}(\partial_{\mathbf{n}_\varepsilon}), \tag{3.118}$$

$$(-\partial_{xx} - \partial_{yy} - \frac{1}{\varepsilon^2}\partial_{zz})\varphi^\varepsilon = \frac{1}{\varepsilon}|\psi^\varepsilon|^2, \; \lim_{|\mathbf{x}|\to\infty} \varphi^\varepsilon(\mathbf{x}) = 0. \tag{3.119}$$

It is well-known that $\mathbf{H}_z$ has eigenvalues $\mu_k = k + 1/2$ with corresponding eigenfunction $w_k(z)$ $(k = 0, 1, \ldots,)$, where $\{w_k\}_{k=0}^{\infty}$ forms an orthornormal basis of $L^2(\mathbb{R})$ [65, 140], specially, $w_0(z) = \frac{1}{\pi^{1/4}} e^{-z^2/2}$. Following [29], it is convenient to consider the initial data polarized on the ground state mode of $\mathbf{H}_z$, i.e.,

$$\psi^\varepsilon(\mathbf{x}, 0) = \phi_0(x, y) w_0(z), \quad \phi_0 \in \Xi_2 \text{ and } \|\phi_0\|_{L^2(\mathbb{R}^2)} = 1. \tag{3.120}$$

In **Case I** (3.1), when $\varepsilon \to 0^+$, quasi-2D equation I (3.4), II (3.8) will yield an ε-independent equation in the weak regime,

$$i\partial_t \phi(x, y, t) = \mathbf{H}_\perp \phi + \frac{\beta - (1 - 3n_3^2)\lambda}{\sqrt{2\pi}} |\phi|^2 \phi, \quad (x, y) \in \mathbb{R}^2, \tag{3.121}$$

with initial condition $\phi(x, y, 0) = \phi_0(x, y)$. We will show the convergence from the full 3D model to 2D. We follow the ideas in [29, 30] to show the convergence from the 3D GPPS to the 2D approximation. First, let us state the main result.

Theorem 3.9 *(Dimension reduction) Suppose V_2 satisfies condition (3.46), and $-\frac{\beta}{2} \le \lambda \le \beta$, $\beta \ge 0$, let $\psi^\varepsilon \in C([0, \infty); \Xi_3)$, $\phi \in C([0, \infty); \Xi_2)$ be the unique solution of equation (3.116)-(3.120) and (3.121) respectively, then for any $T > 0$, there exists $C_T > 0$ such that*

$$\|\psi^\varepsilon(x, y, z, t) - e^{-i\frac{\mu_0 t}{\varepsilon^2}} \phi(x, y, t) w_0(z)\|_2 \le C_T \varepsilon, \quad \forall t \in [0, T]. \tag{3.122}$$

Under the assumption, we have the global existence of ψ^ε [10, 42] as well as ϕ [29, 43]. Define the projection operator onto the ground state mode of $\mathbf{H}_z$ by

$$\Pi\psi^\varepsilon(\mathbf{x}, t) = e^{-i\mu_0 t/\varepsilon^2} \phi^\varepsilon(x, y, t) w_0(z), \tag{3.123}$$

where

$$\phi^\varepsilon(x, y, t) = e^{i\mu_0 t/\varepsilon^2} \int_{\mathbb{R}} \psi^\varepsilon(\mathbf{x}, t) w_0(z) dz. \tag{3.124}$$

Since the space (x, y, z) is anisotropic, we introduce the $L_z^p L_{x,y}^q$ space by the norm

$$\|f\|_{(p,q)} := \|f\|_{L_z^p L_{x,y}^q} = \| \, \|f(\cdot, z)\|_{L_{x,y}^q} \|_{L_z^p}, \quad p, q \in [1, \infty]. \tag{3.125}$$

The corresponding anisotropic Sobolev inequalities are available [29].

Lemma 3.8 *(Uniform bound) Let ψ^ε, ϕ be the solution of (3.116) and (3.121) respectively, $\lambda \in [-\frac{\beta}{2}, \beta]$, $\beta \geq 0$, we have*

$$\psi^\varepsilon \in L^\infty((0,\infty), H^1(\mathbb{R}^3)), \quad \phi, \phi^\varepsilon \in L^\infty((0,T), H^1(\mathbb{R}^2)), \tag{3.126}$$

with uniform bound in ε. Moreover, for $p \in [2,\infty]$,

$$\|\psi^\varepsilon - \Pi\psi^\varepsilon\|^2_{L^2(\mathbb{R}^3)} + \|\partial_z(\psi^\varepsilon - \Pi\psi^\varepsilon)\|^2_{L^2(\mathbb{R}^3)} \leq C\varepsilon^2, \quad \|\psi^\varepsilon - \Pi\psi^\varepsilon\|_{(p,2)} \leq C\varepsilon, \tag{3.127}$$

with C depending on $\|\phi_0\|_{\Xi_2}$, uniform in time t.

Proof: From energy conservation for equation (3.116), we have

$$E(t) := (\mathbf{H}_\perp\psi^\varepsilon(t), \psi^\varepsilon(t)) + \frac{1}{\varepsilon^2}(\mathbf{H}_z\psi^\varepsilon(t), \psi^\varepsilon(t)) + \frac{\beta-\lambda}{2}\|\psi^\varepsilon\|_4^4 + \frac{3\varepsilon^2\lambda}{2}\|\partial_{\mathbf{n}_\varepsilon}\nabla\varphi^\varepsilon(t)\|_2^2 = E(0),$$

where $(\cdot,\cdot)$ denotes the standard L^2 inner product. Using estimates for rescaled Poisson equation (3.119), we have $\|\partial_{\mathbf{n}_\varepsilon}\nabla\varphi^\varepsilon(t)\|_2 \leq \frac{1}{\varepsilon}\|\psi^\varepsilon(t)\|_4^2$, which follows

$$\frac{\beta-\lambda}{2}\|\psi^\varepsilon\|_4^4 + \frac{3\varepsilon^2\lambda}{2}\|\partial_{\mathbf{n}_\varepsilon}\nabla\varphi^\varepsilon(t)\|_2^2 \geq 0, \quad \text{and } E(0) = \frac{\mu_0}{\varepsilon^2} + C_0, \tag{3.128}$$

where C_0 depends on $\|\phi_0\|_{\Xi_2}$. Writing $\psi^\varepsilon(t) = \sum_{k=0}^{\infty}\phi_k(x,y,t)w_k(z)$, and using the L^2 conservation $\sum_{k=0}^{\infty}\|\phi_k(t)\|^2_{L^2(\mathbb{R}^2)} = 1$, we can deduce from energy conservation that

$$\begin{aligned}
\frac{\mu_0}{\varepsilon^2} + C_0 &\geq (\mathbf{H}_\perp\psi^\varepsilon(t), \psi^\varepsilon(t)) + \frac{1}{\varepsilon^2}(\mathbf{H}_z\psi^\varepsilon(t), \psi^\varepsilon(t)) \\
&= (\mathbf{H}_\perp\psi^\varepsilon(t), \psi^\varepsilon(t)) + \frac{1}{\varepsilon^2}\sum_{k=0}^{\infty}\mu_k\|\phi_k(t)\|^2_{L^2(\mathbb{R}^2)} \\
&= (\mathbf{H}_\perp\psi^\varepsilon(t), \psi^\varepsilon(t)) + \frac{1}{\varepsilon^2}\sum_{k=1}^{\infty}(\mu_k-\mu_0)\|\phi_k(t)\|^2_{L^2(\mathbb{R}^2)} + \frac{\mu_0}{\varepsilon^2}.
\end{aligned}$$

Hence,

$$\|\partial_x\psi^\varepsilon\|^2_{L^2(\mathbb{R}^3)} + \|\partial_y\psi^\varepsilon\|^2_{L^2(\mathbb{R}^3)} \leq (\mathbf{H}_\perp\psi^\varepsilon(t), \psi^\varepsilon(t)) \leq C_0, \tag{3.129}$$

$$\|\partial_z\psi^\varepsilon\|^2_{L^2(\mathbb{R}^3)} \leq (\mathbf{H}_z\psi^\varepsilon, \psi^\varepsilon) \leq \mu_0 + C_0\varepsilon^2, \tag{3.130}$$

$$\|\psi^\varepsilon - \Pi\psi^\varepsilon\|^2_{L^2(\mathbb{R}^3)} \leq \frac{1}{\mu_1-\mu_0}\sum_{k=1}^{\infty}(\mu_k-\mu_0)\|\phi_k(t)\|^2_{L^2(\mathbb{R}^2)} \leq 2C_0\varepsilon^2, \tag{3.131}$$

$$\|\partial_z(\psi^\varepsilon - \Pi\psi^\varepsilon)\|^2_{L^2(\mathbb{R}^3)} \leq \sum_{k=1}^{\infty}\frac{\mu_k}{\mu_k-\mu_0}(\mu_k-\mu_0)\|\phi_k(t)\|^2_{L^2(\mathbb{R}^2)} \leq \frac{3}{2}C_0\varepsilon^2. \tag{3.132}$$

Estimates on $\|\psi^\varepsilon - \Pi\psi^\varepsilon\|_{(p,2)}$ follows from Sobolev embedding. □

We also need the following Strichartz estimates for the unitary group $e^{it\mathbf{H}_\perp}$, which is valid when V_2 satisfies condition (3.46) [43].

Definition. In two dimensions, let q', r' be the conjugate index of q and r ($1 \le q, r \le \infty$) respectively, i.e. $1 = 1/q' + 1/q = 1/r' + 1/r$, we call the pair (q, r) admissible and (q', r') conjugate admissible if

$$\frac{2}{q} = 2(\frac{1}{2} - \frac{1}{r}), \quad 2 \le r < \infty. \tag{3.133}$$

Following [42, 43, 136], the following estimates can be established.

Lemma 3.9 *(Strichartz's estimates) Let (q, r) be an admissible pair and (γ, ρ) be a conjugate admissible pair, I be a bounded interval of $\mathbb{R}$, and $0 \in I$.*

(i) There exists constant a C depending on I and q such that

$$\|e^{-it\mathbf{H}_\perp}\varphi\|_{L^q(I,L^r(\mathbb{R}^2))} \le C(I, q)\|\varphi\|_{L^2(\mathbb{R}^2)}. \tag{3.134}$$

(ii) If $f \in L^\gamma(I, L^\rho(\mathbb{R}^2))$, there exists C depending on I, q, ρ, such that

$$\|\int_{I\bigcap s\le t} e^{i(t-s)\mathbf{H}_\perp} f(s)\, ds\|_{L^q(I,L^r(\mathbb{R}^2))} \le C(I, q, \rho)\|f\|_{L^\gamma(I,L^\rho(\mathbb{R}^2))}. \tag{3.135}$$

Now, we are able to prove the theorem.

Proof of Theorem 3.9: In view of Lemma 3.8, we can derive

$$\begin{aligned} \|\psi^\varepsilon - e^{-i\frac{t\mu_0}{\varepsilon^2}}\phi w_0(z)\|_{L^2(\mathbb{R}^3)} &\le \|\psi^\varepsilon - \Pi\psi^\varepsilon\|_{L^2(\mathbb{R}^3)} + \|\Pi\psi^\varepsilon - e^{-i\frac{t\mu_0}{\varepsilon^2}}\phi w_0(z)\|_{L^2(\mathbb{R}^3)} \\ &\le C\varepsilon + \|\phi^\varepsilon(t) - \phi(t)\|_{L^2(\mathbb{R}^2)}. \end{aligned} \tag{3.136}$$

Hence, we need to estimate the difference between ϕ^ε and ϕ. By (3.116) and (3.119), we know $\phi^\varepsilon(x, y, t)$ (3.124) solves the following equation

$$\begin{aligned} & i\partial_t\phi^\varepsilon = \mathbf{H}_\perp\phi^\varepsilon + (\beta - \lambda + 3n_3^3\lambda)e^{i\mu_0 t/\varepsilon^2}\int_{\mathbb{R}} |\psi^\varepsilon|^2\psi^\varepsilon w_0(z)dz + \varepsilon g^\varepsilon, \\ & g^\varepsilon = e^{i\mu_0 t\varepsilon^2}\int_{\mathbb{R}} P_\varepsilon(\varphi^\varepsilon)\psi^\varepsilon w_0(z)dz, \\ \text{with} \quad & P_\varepsilon(\varphi^\varepsilon) = -3\lambda((n_1^2 - n_3^2)\partial_{xx} + (n_2^2 - n_3^2)\partial_{yy} + 2n_1n_2\partial_{xy} + \frac{2}{\varepsilon}(\partial_{xz} + \partial_{yz}))\varphi^\varepsilon. \end{aligned}$$

Denote $\chi^\varepsilon(x,y,t) = \phi^\varepsilon - \phi$, noticing that $\|w_0\|_4^4 = 1/\sqrt{2\pi}$, χ^ε satisfies the following equation

$$\begin{aligned}
&i\partial_t\chi^\varepsilon = \mathbf{H}_\perp\chi^\varepsilon + f_1^\varepsilon + f_2^\varepsilon + \varepsilon g^\varepsilon, \quad \chi^\varepsilon(t=0) = 0,\\
&f_1^\varepsilon = \frac{\beta - \lambda + 3n_3^3\lambda}{\sqrt{2\pi}}(|\phi^\varepsilon|^2\phi^\varepsilon - |\phi|^2\phi),\\
&f_2^\varepsilon = (\beta - \lambda + 3n_3^3\lambda)e^{i\mu_0 t/\varepsilon^2}\int_{\mathbb{R}}\left(|\psi^\varepsilon|^2\psi^\varepsilon - e^{-i\mu_0 t/\varepsilon^2}|\phi^\varepsilon w_0|^2\phi^\varepsilon w_0\right)w_0(z)dz.
\end{aligned}$$

Applying Strichartz estimates on bounded interval $[0,T]$ and recalling that $(\infty,2)$ is an admissible pair, we can obtain

$$\|\chi^\varepsilon\|_{L^\infty([0,T];L^2(\mathbb{R}^2))} \le C(\|f_1^\varepsilon\|_{L^{\rho^*}([0,T];L^\rho(\mathbb{R}^2))} + \|f_2^\varepsilon\|_{L^{\gamma^*}([0,T];L^\gamma(\mathbb{R}^2))} + \varepsilon\|g^\varepsilon\|_{L^{q^*}([0,T];L^q(\mathbb{R}^2))}),$$

where (ρ^*,ρ), (γ^*,γ) and (q^*,q) are some conjugate admissible pairs. By a similar argument in [29], we have the estimates for f_1^ε and f_2^ε which comes from the cubic nonlinearity, for appropriate $\rho \in (1,2)$ and $\gamma \in (1,2)$,

$$\|f_1^\varepsilon\|_{L^{\rho^*}([0,T];L^\rho(\mathbb{R}^2))} \le C\|\chi^\varepsilon\|_{L^{\rho^*}([0,T];L^2(\mathbb{R}^2))}, \quad \|f_2^\varepsilon\|_{L^{\gamma^*}([0,T];L^\gamma(\mathbb{R}^2))} \le C\varepsilon. \tag{3.137}$$

The basic tools involved are Hölder's inequality, Sobolev inequalities and the estimates in Lemma 3.9, and we omit the proof of this part here for brevity. So,

$$\|\chi^\varepsilon\|_{L^\infty([0,T];L^2(\mathbb{R}^2))} \le C(\|\chi^\varepsilon\|_{L^{\rho^*}([0,T];L^\rho(\mathbb{R}^2))} + \varepsilon\|g^\varepsilon\|_{L^{q^*}([0,T];L^q(\mathbb{R}^2))} + \varepsilon), \tag{3.138}$$

Next, we shall estimate g^ε. Let φ_1^ε, φ_2^ε to be the solution of rescaled Poisson equation (3.119) with $|\psi^\varepsilon|^2$ replaced by $|\Pi\psi^\varepsilon|^2$ and $|\psi^\varepsilon|^2 - |\Pi\psi^\varepsilon|^2$ respectively, then rewrite

$$g^\varepsilon = J_1^\varepsilon + J_2^\varepsilon + J_3^\varepsilon, \tag{3.139}$$

where

$$J_1^\varepsilon = \int_{\mathbb{R}} P_\varepsilon(\varphi_1^\varepsilon)\phi^\varepsilon w_0^2 dz,\ J_2^\varepsilon = e^{\frac{i\mu_0 t}{\varepsilon^2}}\int_{\mathbb{R}} P_\varepsilon(\varphi^\varepsilon)(\psi^\varepsilon - \Pi\psi^\varepsilon)w_0 dz,\ J_3^\varepsilon = e^{\frac{i\mu_0 t}{\varepsilon^2}}\int_{\mathbb{R}} P_\varepsilon(\varphi_2^\varepsilon)\Pi\psi^\varepsilon w_0 dz.$$

For J_1^ε, this one reduces to the quasi-2D equation I (3.4), where we have that

$$J_1^\varepsilon = -3\lambda(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta_\perp)\varphi_{2D}^\varepsilon\phi^\varepsilon, \text{ and } \varphi_{2D}^\varepsilon = U_\varepsilon^{2D} * |\phi^\varepsilon|^2, \tag{3.140}$$

with U_ε^{2D} given in (3.5). In view of the property of U_ε^{2D} in Lemma 3.1 and Remark 3.2, recalling $\phi^\varepsilon \in L^\infty([0,\infty);H^1(\mathbb{R}^2))$, using Hölder's inequality and Sobolev inequality, we obtain

$$\|J_1^\varepsilon\|_p \le \|P_\varepsilon(\varphi_{2D}^\varepsilon)\|_{p_1}\|\phi^\varepsilon\|_{p_2} \le C\|\nabla|\phi^\varepsilon|^2\|_{p_1}\|\phi^\varepsilon\|_{p_2} \le C, \tag{3.141}$$

where $1 < p < p_1 < 2$, $\frac{1}{p} = \frac{1}{p_1} + \frac{1}{p_2}$.

For J_2^ε, applying Minkowski inequality, Hölder's inequality and Sobolev inequality, as well as estimates for Poisson equation, noticing $\psi^\varepsilon \in L^\infty([0,\infty); H^1(\mathbb{R}^3))$ and Lemma 3.8, we estimate

$$\begin{aligned}
\|J_2^\varepsilon\|_p &\leq \|P_\varepsilon(\varphi^\varepsilon)(\psi^\varepsilon - \Pi\psi^\varepsilon)w_0\|_{(1,p)} \leq C\|P_\varepsilon(\varphi^\varepsilon)\|_{L^{p^*}(\mathbb{R}^3)}\|\psi^\varepsilon - \Pi\psi^\varepsilon\|_{(\infty,2)} \\
&\leq C\varepsilon \left\| \frac{|\psi^\varepsilon|^2}{\varepsilon} \right\|_{L^{p^*}(\mathbb{R}^3)} \leq C,
\end{aligned}$$

where $p^* = 2p/(2-p) \leq 3$.

For J_3^ε, similar as J_ε^1, J_ε^2, we have

$$\begin{aligned}
\|J_3^\varepsilon\|_p &\leq \|P_\varepsilon(\varphi_2^\varepsilon)\Pi\psi^\varepsilon w_0\|_{(1,p)} \leq C\|P_\varepsilon(\varphi_2^\varepsilon)\|_{L^{p_1}(\mathbb{R}^3)}\|\phi^\varepsilon\|_{L^{p_2}(\mathbb{R}^2)} \\
&\leq \frac{C}{\varepsilon}\||\psi^\varepsilon|^2 - |\Pi\psi^\varepsilon|^2\|_{L^{p_1}(\mathbb{R}^3)} \\
&\leq \frac{C}{\varepsilon}\|\psi^\varepsilon - \Pi\psi^\varepsilon\|_{L^2(\mathbb{R}^3)}(\|\psi^\varepsilon\|_{L^{p_3}(\mathbb{R}^3)} + \|\Pi\psi^\varepsilon\|_{L^{p_3}(\mathbb{R}^3)}) \leq C,
\end{aligned}$$

where $p_3 = 2p_1^2/(2-p_1) \leq 6$. Hence, by choosing $p = 6/5$, and $p_1 = 4/3$ would satisfy all the conditions for J_k^ε (k=1,2,3), where we shall derive that uniformly in t,

$$\|g^\varepsilon\|_{L^p(\mathbb{R}^2)} \leq \|J_1^\varepsilon\|_{L^p(\mathbb{R}^2)} + \|J_2^\varepsilon\|_{L^p(\mathbb{R}^2)} + \|J_3^\varepsilon\|_{L^p(\mathbb{R}^2)} \leq C. \tag{3.142}$$

Then choose $q = p$ in (3.138), we have

$$\|\chi^\varepsilon\|_{L^\infty([0,T];L^2(\mathbb{R}^2))} \leq C(\|\chi^\varepsilon\|_{L^{\rho^*}([0,T];L^2(\mathbb{R}^2))} + \varepsilon). \tag{3.143}$$

Applying the results for all $t \in [0,T]$, we find

$$\|\chi^\varepsilon(t)\|_2^{\rho^*} \leq C\left(\int_0^t \|\chi^\varepsilon(s)\|_2^{\rho^*}\, ds + \varepsilon^{\rho^*}\right), \quad t \in [0,T], \tag{3.144}$$

and Gronwal's inequality will give that $\|\chi^\varepsilon(t)\|_2 \leq C\varepsilon$ for all $t \in [0,T]$. Combined with (3.136), we can draw the desired conclusion. □

3.5.2 Reduction to 1D

In this case, we also consider the weak regime $\beta \to \varepsilon^{-2}\beta$, $\lambda \to \varepsilon^{-2}\lambda$. In **Case II** (3.2), for full 3D GPPS (2.19)-(2.20), introducing the scaling $x \to x/\varepsilon$, $y \to y/\varepsilon$, $\psi \to \varepsilon\psi^\varepsilon$ which preserves the normalization, then for $\mathbf{x} = (x,y,z)^T \in \mathbb{R}^3$,

$$i\partial_t\psi^\varepsilon(\mathbf{x},t) = \left[\mathbf{H}_z + \frac{1}{\varepsilon^2}\mathbf{H}_{x,y} + (\beta-\lambda)|\psi^\varepsilon|^2 - 3\varepsilon\lambda\partial_{\tilde{\mathbf{n}}_\varepsilon\tilde{\mathbf{n}}_\varepsilon}\varphi^\varepsilon\right]\psi^\varepsilon, \tag{3.145}$$

where

$$\mathbf{H}_z = -\frac{1}{2}\partial_{zz} + V_1(z), \quad \mathbf{H}_{x,y} = -\frac{1}{2}(\partial_{xx} + \partial_{yy} + x^2 + y^2), \tag{3.146}$$

$$\tilde{\mathbf{n}}_\varepsilon = (n_1/\varepsilon, n_2/\varepsilon, n_3), \quad \partial_{\tilde{\mathbf{n}}_\varepsilon} = \tilde{\mathbf{n}}_\varepsilon \cdot \nabla, \quad \partial_{\tilde{\mathbf{n}}_\varepsilon\tilde{\mathbf{n}}_\varepsilon} = \partial_{\tilde{\mathbf{n}}_\varepsilon}(\partial_{\tilde{\mathbf{n}}_\varepsilon}), \tag{3.147}$$

$$(-\frac{1}{\varepsilon^2}\partial_{xx} - \frac{1}{\varepsilon^2}\partial_{yy} - \partial_{zz})\varphi^\varepsilon = \frac{1}{\varepsilon^2}|\psi^\varepsilon|^2, \ \lim_{|\mathbf{x}|\to\infty} \varphi^\varepsilon(\mathbf{x}) = 0. \tag{3.148}$$

Note that the ground mode of $\mathbf{H}_{x,y}$ would be given by $w_0(x)w_0(y)$ with eigenvalue 1, and the initial data is then assumed to be

$$\psi^\varepsilon(\mathbf{x}, 0) = \phi_0(z)w_0(x)w_0(y), \quad \phi_0 \in \Xi_1 \text{ and } \|\phi_0\|_{L^2(\mathbb{R})} = 1. \tag{3.149}$$

In **Case II** (3.2), when $\varepsilon \to 0^+$, quasi-1D equation (3.10) will lead to an ε-independent equation in the weak regime,

$$i\partial_t\phi(z,t) = \mathbf{H}_z\phi + \frac{\beta + \frac{1}{2}\lambda(1-3n_3^2)}{2\pi}|\phi|^2\phi, \quad z \in \mathbb{R}, \tag{3.150}$$

with initial condition $\phi(z, 0) = \phi_0(z)$.

Following the steps in the last subsection, we can prove the following results.

Theorem 3.10 *(Dimension reduction) Suppose the real-valued trap potential $V_1(z) \in C^\infty(\mathbb{R})$ such that $V_1(z) \geq 0$ for $z \in \mathbb{R}$ and $D^\alpha V_1(z) \in L^\infty(\mathbb{R})$ for all $\alpha \geq 2$. Assume $-\frac{\beta}{2} \leq \lambda \leq \beta$, $\beta \geq 0$, let $\psi^\varepsilon \in C([0,\infty); \Xi_3)$, $\phi \in C([0,\infty); \Xi_1)$ be the unique solution of equation (3.145)-(3.149) and (3.150) respectively, then for any $T > 0$, there exists $C_T > 0$ such that*

$$\|\psi^\varepsilon(x,y,z,t) - e^{-it/\varepsilon^2}\phi(z,t)w_0(x)w_0(y)\|_2 \leq C_T\varepsilon, \quad \forall t \in [0,T]. \tag{3.151}$$

3.6 Numerical methods

In this section, we consider the numerical methods for computing ground states of the reduced models. In physical experiments, ε is usually not sufficiently close to 0. In such cases, quasi 2D equation II would not be a good approximation of the quasi-2D equation I (3.4)-(3.5). Hence, we will only consider the quasi-2D equation I (3.4)-(3.5) and the quasi-1D equation (3.10). In practical computation, the problem is usually truncated on a bounded interval $[a, b]$ in 1D or a bounded rectangle $[a, b] \times [c, d]$ in 2D, with zero Dirichlet boundary conditions. We adopt the method of gradient flow with discrete normalization, widely used in the literature: choose a time step $\Delta t > 0$ and set $t_n = n\,\Delta t$ for $n = 0, 1, \ldots$. Applying the steepest decent method to the energy functional $E_{2D}(\phi)$ (3.13) or $E_{1D}(\phi)$ (3.107) without the constraint $\phi \in S_d$, and then projecting the solution back to the unit sphere S_d at the end of each time interval $[t_n, t_{n+1}]$ in order to satisfy the constraint $\phi \in S_d$.

3.6.1 Numerical method for the quasi-2D equation I

After truncation, the gradient flow with discrete normalization for the quasi-2D equation I (3.4)-(3.5) for $\phi := \phi(x, y, t)$ reads as

$$\partial_t\phi = \left[\frac{1}{2}\Delta - V_2 - \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi|^2 + \frac{3\lambda}{2}(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi\right]\phi, \tag{3.152}$$

$$\varphi(x, y, t) = U_\varepsilon^{2D} * |\phi|^2, \qquad (x, y) \in U = [a, b] \times [c, d], \quad t_n \le t < t_{n+1}, \tag{3.153}$$

$$\phi(x, y, t_{n+1}) := \phi(x, y, t_{n+1}^+) = \frac{\phi(x, y, t_{n+1}^-)}{\|\phi(\cdot, t_{n+1}^-)\|_2}, \qquad (x, y) \in U, \quad n \ge 0, \tag{3.154}$$

$$\phi(x, y, t)|_{\partial U} = \varphi(x, y, t)|_{\partial U} = 0, \qquad t \ge 0, \tag{3.155}$$

$$\phi(x, y, 0) = \phi_0(x, y), \qquad \text{with} \quad \|\phi_0\|_2 = 1, \tag{3.156}$$

where $\phi(x, y, t_n^\pm) = \lim\limits_{t \to t_n^\pm} \phi(x, y, t)$.

Let J and K be two even positive integers, choose the mesh size $\Delta x = \frac{b-a}{J}$ and $\Delta y = \frac{d-c}{K}$, define the grid points $x_j = a + j\Delta x$, $y_k = c + k\Delta y$ for $0 \le j \le J$ and $0 \le k \le K$, let ϕ_{jk}^n be the numerical approximation of $\phi(x_j, y_k, t_n)$ and denote

$$\lambda_p^x = \frac{2p\pi}{b - a}, \quad \lambda_q^y = \frac{2q\pi}{d - c}, \quad p = -J/2, \ldots, J/2 - 1,\ q = -K/2, \ldots, K/2 - 1. \tag{3.157}$$

Then a backward Euler Fourier pseudospectral (BEFP) discretization for (3.152) read as

$$\begin{aligned} \frac{\phi_{jk}^* - \phi_{jk}^n}{\Delta t} =& \frac{1}{2}\left(\Delta^s\phi^*\right)\Big|_{jk} - \left[V_2(x_j, y_k) + \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi_{jk}^n|^2\right. \\ &\left. - \frac{3\lambda}{2}\left((\partial_{\mathbf{n}_\perp\mathbf{n}_\perp}^s\varphi^n)\Big|_{jk} - n_3^2(\Delta^s\varphi^n)\Big|_{jk}\right)\right]\phi_{jk}^n, \end{aligned} \tag{3.158}$$

$$\varphi_{jk}^n = \frac{1}{JK}\sum_{p=-J/2}^{J/2-1}\sum_{q=-K/2}^{K/2-1}\left(\widehat{\varphi^n}\right)_{pq} e^{i\frac{2jp\pi}{J}} e^{i\frac{2kq\pi}{K}}, \tag{3.159}$$

$$\widehat{\varphi^n}_{pq} = \left(\widehat{|\phi^n|^2}\right)_{pq}\widehat{U_\varepsilon^{2D}}(\lambda_p^x, \lambda_q^y), \quad -J/2 \le p \le J/2 - 1,\ -K/2 \le q \le K/2 - 1,$$

$$\phi_{jk}^{n+1} = \frac{\phi_{jk}^*}{\|\phi_{jk}^*\|}, \quad \phi_{jk}^0 = \phi_0(x_j, y_k), \quad 0 \le j \le J,\ 0 \le k \le K, \tag{3.160}$$

where $\widehat{U_\varepsilon^{2D}}$ is given by (3.16), $\hat{\phi}_{pq}$ denotes the Fourier coefficients of ϕ_{jk} defined by

$$\hat{\phi}_{pq} = \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} \phi_{jk} e^{-i\frac{2jp\pi}{J}} e^{-i\frac{2kq\pi}{K}} = \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} \phi_{jk} e^{-i\lambda_p^x(x_j-a)} e^{-i\lambda_q^y(y_k-c)}, \tag{3.161}$$

$\|\phi^*\|$ denotes the discrete l^2 norm of ϕ^* defined as

$$\|\phi^*\| := \sqrt{\Delta x \Delta y \sum_{j=0}^{J-1}\sum_{k=0}^{K-1} |\phi^*_{jk}|^2}\ , \tag{3.162}$$

and Δ^s and $\partial^s_{\mathbf{n}_\perp \mathbf{n}_\perp}$ are pseudospectral approximations of Δ and $\partial_{\mathbf{n}_\perp \mathbf{n}_\perp}$ respectively, defined as follows:

$$(\Delta^s \phi)_{jk} = \frac{-1}{JK} \sum_{p=-J/2}^{J/2-1} \sum_{q=-K/2}^{K/2-1} \left[(\lambda_p^x)^2 + (\lambda_q^y)^2\right] \widehat{\phi}_{pq} e^{i\lambda_p^x(x_j-a)} e^{i\lambda_q^y(y_k-c)} \tag{3.163}$$

$$\left(\partial^s_{\mathbf{n}_\perp \mathbf{n}_\perp}\phi\right)_{jk} = \frac{-1}{JK} \sum_{p=-J/2}^{J/2-1} \sum_{q=-K/2}^{K/2-1} \left(n_1\lambda_p^x + n_2\lambda_q^y\right)^2 \widehat{\phi}_{pq} e^{i\lambda_p^x(x_j-a)} e^{i\lambda_q^y(y_k-c)}, \tag{3.164}$$

for $-J/2 \le p \le J/2-1$, $-K/2 \le q \le K/2-1$. Similar as [12, 21], one can introduce stabilization parameter to the BEFP discretization. Above method is implicit and can be solved explicitly via Fast Fourier Transform (FFT). Actually, taking discrete Fourier transform of (3.158), we have

$$\left(1 + \frac{\Delta t}{2}(\lambda_p^x)^2 + \frac{\Delta t}{2}(\lambda_q^y)^2\right)\left(\widehat{\phi^*}\right)_{pq} = \left(\widehat{\phi^n}\right)_{pq} + \Delta t\left(\widehat{S^n}\right)_{pq}, \tag{3.165}$$

with the mesh function S^n for $0 \le j \le J$ and $0 \le k \le K$ given by

$$S^n_{jk} = -\left[V_2(x_j, y_k) + \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi^n_{jk}|^2 - \frac{3\lambda}{2}\left((\partial^s_{\mathbf{n}_\perp \mathbf{n}_\perp}\varphi^n)\Big|_{jk} - n_3^2(\Delta^s\varphi^n)\Big|_{jk}\right)\right]\phi^n_{jk}.$$

Equation (3.165) can be solved explicitly and then BEFP (3.158) is solved.

3.6.2 Numerical method for the quasi-1D equation

Similar as the quasi-2D equation I case, we have the gradient flow with discrete normalization associated to the quasi-1D equation (3.10)-(3.11) for $\phi := \phi(z,t)$ as

$$\partial_t\phi = \left[\frac{1}{2}\partial_{zz} - V_1 - \left(\beta + \frac{\lambda}{2}(1-3n_3^2)\right)\frac{1}{2\pi\varepsilon^2}|\phi|^2 + \frac{3\lambda}{8\sqrt{2\varepsilon^2\pi}}(3n_3^2-1)\partial_{zz}\varphi\right]\phi, \tag{3.166}$$

$$\varphi(z,t) = U_\varepsilon^{1D} * |\phi|^2, \qquad z\in U=[a,b], \quad t_n \le t < t_{n+1}, \tag{3.167}$$

$$\phi(z,t_{n+1}) := \phi(z,t_{n+1}^+) = \frac{\phi(z,t_{n+1}^-)}{\|\phi(\cdot,t_{n+1}^-)\|_2}, \qquad z\in U, \quad n\ge 0, \tag{3.168}$$

$$\phi(z,t)|_{\partial U} = \varphi(z,t)|_{\partial U} = 0, \qquad t\ge 0, \tag{3.169}$$

$$\phi(z,0) = \phi_0(z), \qquad \text{with} \quad \|\phi_0\|_2 = 1, \tag{3.170}$$

where $\phi(z,t_n^\pm) = \lim_{t\to t_n^\pm}\phi(z,t)$. Let L be an even positive integer, choose the mesh size $\Delta z = \frac{b-a}{L}$, define the grid points $z_l = a + l\Delta z$ for $0\le l\le L$, let ϕ_l^n be the numerical approximation of $\phi(z_l,t_n)$ and denote

$$\lambda_r^z = \frac{2r\pi}{b-a}, \qquad r = -L/2, -L/2+1, \ldots, L/2-1. \tag{3.171}$$

Then a backward Euler Fourier pseudospectral (BEFP) discretization for (3.166) reads as

$$\begin{aligned}\frac{\phi_l^*-\phi_l^n}{\Delta t} =& \frac{1}{2}\left(\partial_{zz}^s\phi^*\right)\Big|_l - \left[V_1(z_l) + \left(\beta+\frac{\lambda}{2}(1-3n_3^2)\right)\frac{1}{2\pi\varepsilon^2}|\phi_l^n|^2\right.\\ &\left. - \frac{3\lambda}{8\sqrt{2\varepsilon^2\pi}}(3n_3^2-1)\left(\partial_{zz}^s\varphi^n\right)\Big|_l\right]\phi_l^n, \end{aligned}\tag{3.172}$$

$$\varphi_r^n = \frac{1}{L}\sum_{r=-L/2}^{L/2-1}\left(\widehat{\varphi^n}\right)_r e^{i\frac{2lr\pi}{L}}, \quad \widehat{\varphi^n}_l = \left(\widehat{|\phi^n|^2}\right)_r \widehat{U_\varepsilon^{1D}}(\lambda_r^z), \quad -L/2\le r\le L/2-1,$$

$$\phi_l^{n+1} = \frac{\phi_l^*}{\|\phi_l^*\|}, \quad \phi_l^0 = \phi_0(z_l), \quad 0\le l\le L, \tag{3.173}$$

where $\widehat{U_\varepsilon^{1D}}$ is given by (3.109), $\hat{\phi}_r$ denotes the Fourier coefficients of ϕ_l defined by

$$\hat{\phi}_r = \sum_{l=0}^{L-1}\phi_l e^{-i\frac{2lp\pi}{L}} = \sum_{l=0}^{L-1}\phi_l e^{-i\lambda_r^z(z_l-a)}, \tag{3.174}$$

$\|\phi^*\|$ denotes the discrete l^2 norm of ϕ^* defined as

$$\|\phi^*\| := \sqrt{\Delta z\sum_{l=0}^{L-1}|\phi_l^*|^2}\;, \tag{3.175}$$

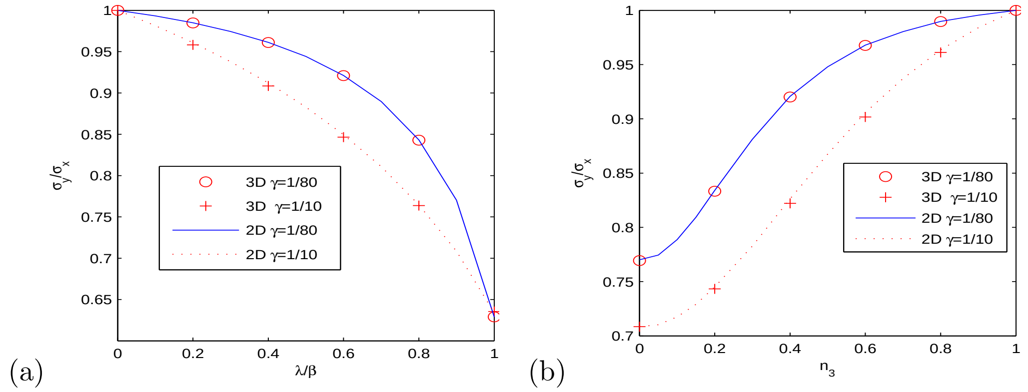

Figure 3.1: Comparison between the aspect ratios calculated by 3D and 2D models for different $\gamma = 1/10, 1/80$, β and $V(x, y, z)$ are chosen as **Example 1**. (a) λ/β increase from 0 to 1 with $\mathbf{n} = (1, 0, 0)^T$; (b) $\lambda = 90$, $\mathbf{n} = (\sqrt{1 - n_3^2}, 0, n_3)$, n_3 increase from 0 to 1.

and ∂_{zz}^s is the pseudospectral approximation of ∂_{zz} defined as

$$(\partial_{zz}^s \phi)_l = \frac{-1}{L} \sum_{r=-L/2}^{L/2-1} (\lambda_r^z)^2 \left(\widehat{\phi}\right)_r e^{i\lambda_r^z (z_l - a)}, \quad -L/2 \le r \le L/2 - 1. \tag{3.176}$$

Taking discrete Fourier transform of (3.172), we have

$$\left(1 + \frac{\Delta t}{2} (\lambda_r^z)^2\right) \left(\widehat{\phi^*}\right)_r = \left(\widehat{\phi^n}\right)_r + \Delta t \left(\widehat{F^n}\right)_r, \tag{3.177}$$

with the mesh function F^n for $0 \le l \le L$ given by

$$F_l^n = -\left[V_1(z_l) + \left(\beta + \frac{\lambda}{2}(1 - 3n_3^2)\right) \frac{1}{2\pi\varepsilon^2} |\phi_l^n|^2 - \frac{3\lambda}{8\sqrt{2\varepsilon^2 \pi}} (3n_3^2 - 1) \left(\partial_{zz}^s \varphi^n\right)\Big|_l \right] \phi_l^n.$$

Thus BEFP discretization (3.172) can be solved explicitly.

3.7 Numerical results

In this section, we report numerical results for ground states of the quasi-2D equation I (3.4) and the quasi-1D equation (3.10). We compare the ground states of the reduced models with the ground states of the 3D model. Let $\phi^{3D}(x, y, z)$ be the ground states of 3D GPPS (2.19)-(2.20), define the projection of ϕ^{3D} over the 2D $x - y$ plane as

$$\left(\Pi_\perp \phi^{3D}\right)(x, y) = \sqrt{\int_{\mathbb{R}} |\phi^{3D}(x, y, z)|^2 \, dz}, \tag{3.178}$$

and the projection of ϕ^{3D} over the 1D z direction as

$$\left(\Pi_z \phi^{3D}\right)(z) = \sqrt{\int_{\mathbb{R}} |\phi^{3D}(x, y, z)|^2 \, dxdy}, \tag{3.179}$$

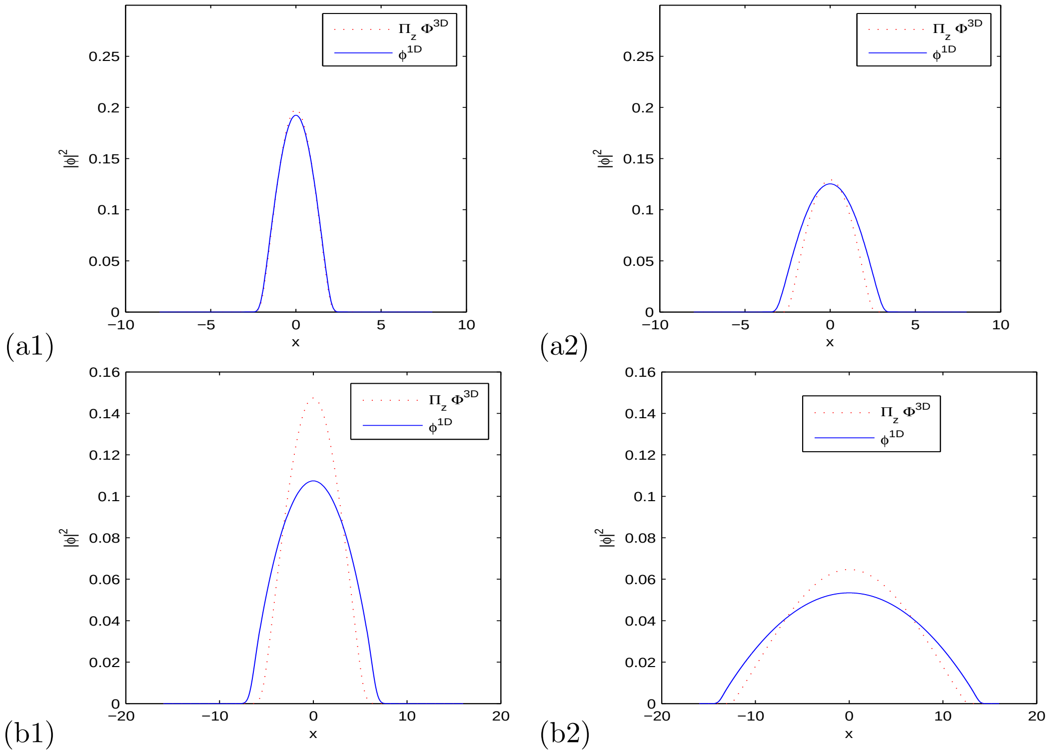

Figure 3.2: Comparison between the density $|\phi(z)|^2$, calculated by 3D and 1 D models for different $\gamma = 1/10, 1/80$, with $\lambda = 90$, β and $V(x,y,z)$ are chosen as **Example 2**. $\gamma = 1/10$ on the left ((a1) and (b1)); $\gamma = 1/80$ on the right ((a2) and (b2)); $\mathbf{n} = (0,0,1)^T$ for (a1) and (a2); $\mathbf{n} = (1,0,0)^T$ for (b1) and (b2).

and let $\phi^{2D}(x,y)$ and $\phi^{1D}(z)$ be the ground states of the quasi-2D equation I (3.4) and the quasi-1D equation (3.10) respectively. We measure the difference between $\Pi_\perp \phi^{3D}$ and ϕ^{2D} for the quasi-2D approximation, and the difference between $\Pi_z \phi^{3D}$ and ϕ^{1D} for the quasi-1D approximation. In order to investigate the anisotropic properties of the ground states in x, y directions, induced by the dipolar interaction, we use the aspect ratio given by

$$\frac{\sigma_x}{\sigma_y} = \frac{\sqrt{\int_{\mathbb{R}^3} x^2 |\phi^{3D}(x,y,z)|^2 \, dxdydz}}{\sqrt{\int_{\mathbb{R}^3} y^2 |\phi^{3D}(x,y,z)|^2 \, dxdydz}}, \tag{3.180}$$

and we can define the aspect ratio for the quasi-2D model as

$$\frac{\sigma_x}{\sigma_y} = \frac{\sqrt{\int_{\mathbb{R}^2} x^2 |\phi^{2D}(x,y)|^2 \, dxdy}}{\sqrt{\int_{\mathbb{R}^2} y^2 |\phi^{2D}(x,y)|^2 \, dxdy}}. \tag{3.181}$$

We will also compare the aspect ratios calculated by the full model and the reduced model.

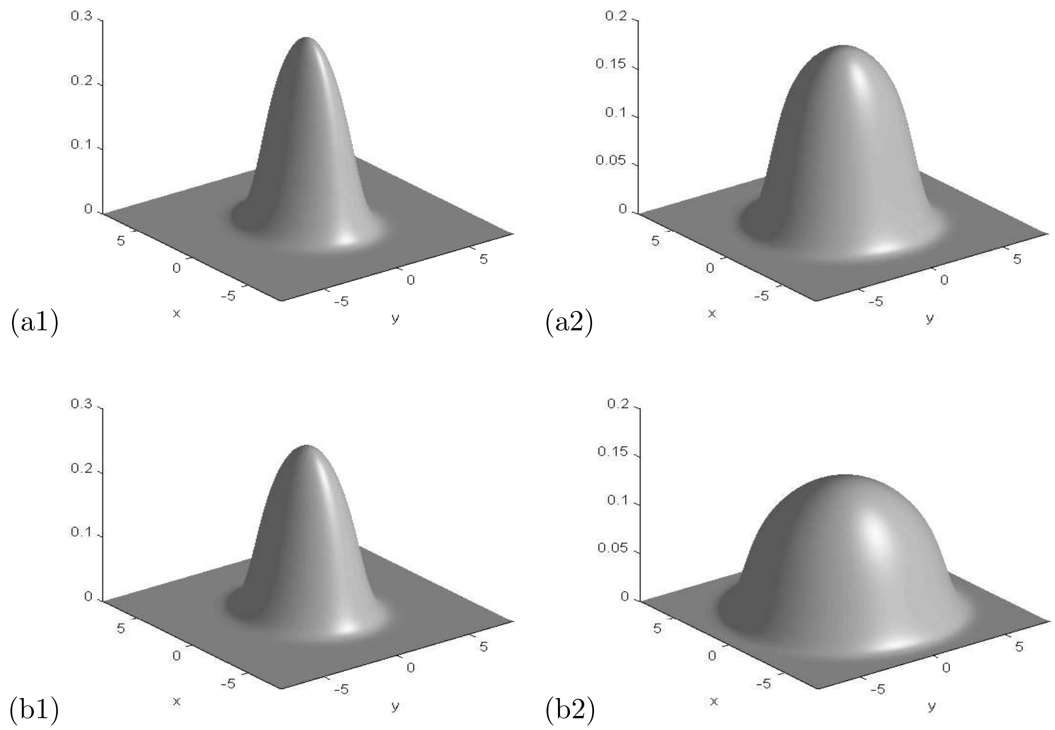

Figure 3.3: Surface plots for ground states $\phi(x,y)$ computed by the quasi-2D equation I, $V(x,y,z)$ and $\beta = 100$ are given in **Example 1**, $\lambda = 90$; $\gamma = 10$ for (a1) and (a2); $\gamma = 80$ (b1) and (b2); $\mathbf{n} = (1,0,0)^T$ for (a1) and (b1); $\mathbf{n} = (0,0,1)^T$ for (a2) and (b2).

Example 1. (Quasi-2D case) For GPPS (2.19)-(2.20) and corresponding quasi-2D I equation, chooses $\beta = 100$, $\lambda = 90$ and

$$V(x,y,z) = \frac{1}{2}(x^2+y^2) + \frac{1}{2\gamma^2}z^2, \quad \gamma = \varepsilon^2, \quad \gamma = 1/10 \text{ or} 1/80. \tag{3.182}$$

Example 2. (Quasi-1D case) For GPPS (2.19)-(2.20) and corresponding quasi-1D equation, chooses $\beta = 100$, $\lambda = 90$ and

$$V(x,y,z) = \frac{1}{2\gamma^2}(x^2+y^2) + \frac{1}{2}z^2, \quad \gamma = \varepsilon^2, \quad \gamma = 1/10 \text{ or} 1/80. \tag{3.183}$$

Fig. 3.2 implies that the quasi 1D approximation (3.10) is fairly good. From Figs. 3.5 & 3.1, we see that the quasi 2D I approximation (3.4) is a quite good approximation. Figs. 3.3 & 3.4 show the rich phenomenon behind the dipolar BEC. Our extensive numerical results confirm that our numerical methods can compute the ground states accurately and efficiently. The results also confirm that our approximate equations: the quasi 2D equation I and the quasi 1D equation are accurate.

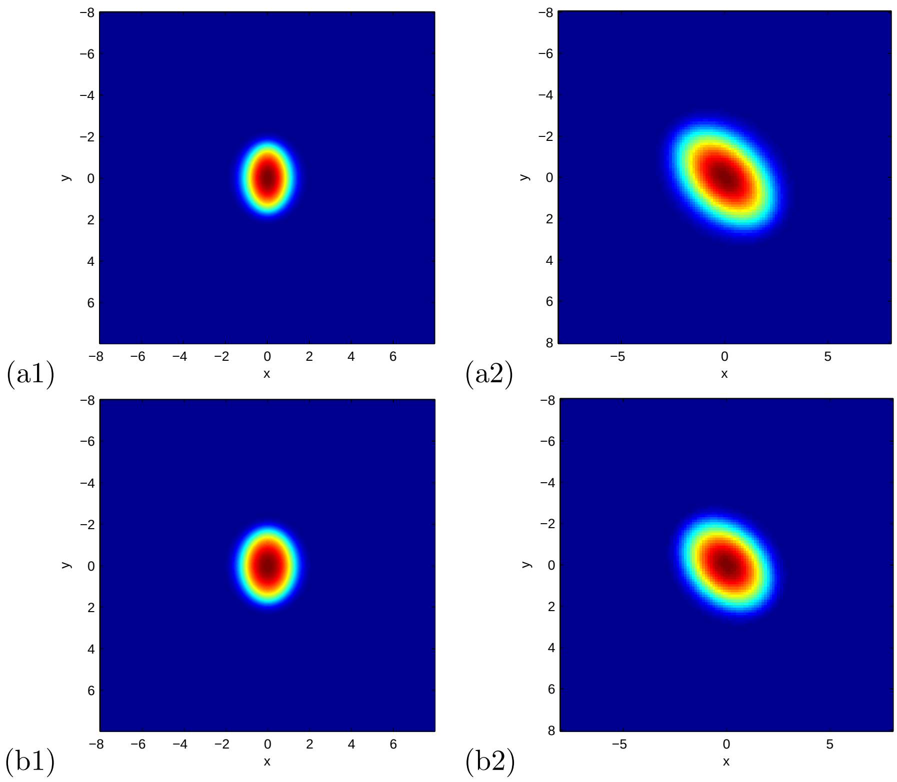

Figure 3.4: Contour plots for density $\rho(x, y) := |\phi(x, y)|^2$ of ground state computed by the quasi-2D equation I , $V(x, y, z)$ and $\beta = 100$ are given in **Example 1**, $\lambda = 90$; $\gamma = 10$ for (a1) and (a2); $\gamma = 80$ (b1) and (b2); $\mathbf{n} = (1, 0, 0)^T$ for (a1) and (b1); $\mathbf{n} = (1/\sqrt{2}, 1/\sqrt{2}, 0)^T$ for (a2) and (b2).

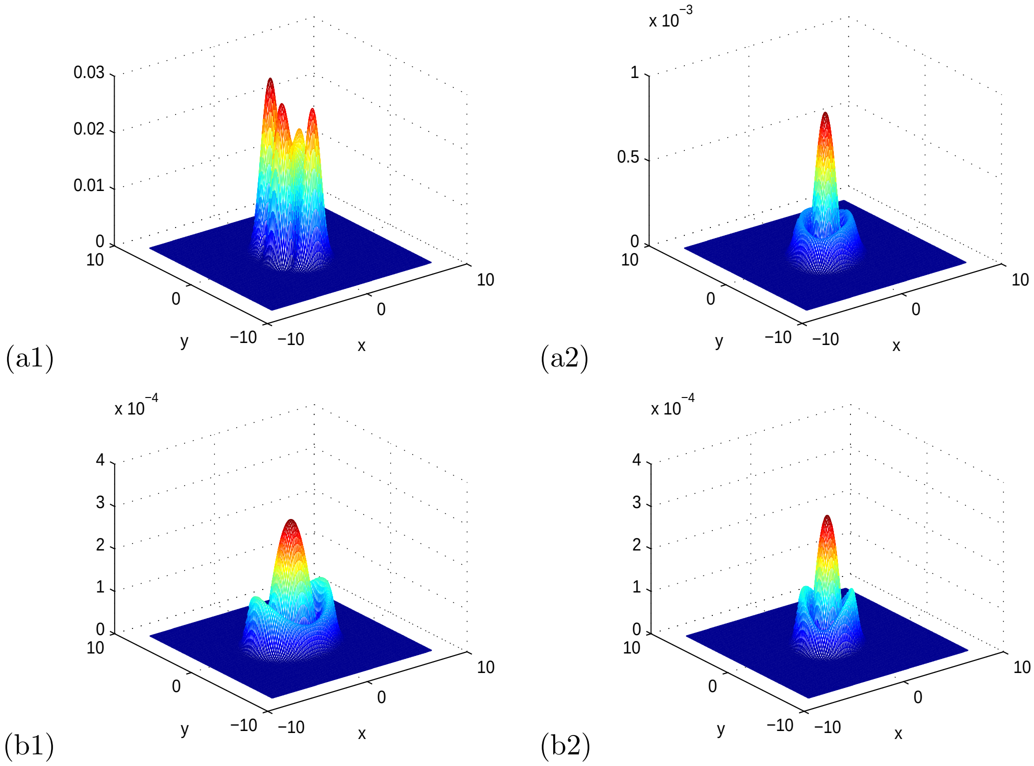

Figure 3.5: Difference between the density $\rho(x, y) := |\phi(x, y)|^2$ of ground state computed by the 3D GPPS and that computed by the quasi-2D equation I , $V(x, y, z)$ and $\beta = 100$ are given in **Example 1**, $\lambda = 90$; $\gamma = 10$ for (a1) and (a2); $\gamma = 80$ (b1) and (b2); $\mathbf{n} = (1, 0, 0)^T$ for (a1) and (b1); $\mathbf{n} = (1/\sqrt{2}, 1/\sqrt{2}, 0)^T$ for (a2) and (b2).

Chapter 4

Dipolar Gross-Pitaevskii equation with rotational frame

In this chapter, we discuss the 3D dipolar GPE with rotational frame and its reduced 2D model.

4.1 Introduction

At temperature T much smaller than the critical temperature T_c, a dipolar BEC in a rotating frame can be well described by the following dipolar GPE [92,113,161]:

$$i\hbar\partial_t\psi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + U_0|\psi|^2 + \left(V_{\text{dip}} * |\psi|^2\right) - \Omega L_z\right]\psi,\ \mathbf{x}\in\mathbb{R}^3,\ t>0, \quad (4.1)$$

where $\mathbf{x} = (x,y,z)^T \in \mathbb{R}^3$ is the Cartesian coordinates, Ω is the angular velocity of the laser beam, $V(\mathbf{x})$ is the harmonic trap described in (2.2), L_z is the z-component of angular momentum (1.13) and other terms can be found in equation (2.1). Again the wave function ψ satisfies the normalization condition (2.4).

Introducing the dimensionless variables as in Chapter 2, $t \to \frac{t}{\omega_0}$, $\Omega \to \Omega/\omega_0$ with $\omega_0 = \min\{\omega_x,\omega_y,\omega_z\}$, $\mathbf{x} \to a_0\mathbf{x}$ with $a_0 = \sqrt{\frac{\hbar}{m\omega_0}}$, $\psi \to \frac{\sqrt{N}\psi}{a_0^{3/2}}$, we obtain the dimensionless rotational dipolar GPE as

$$i\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) - \Omega L_z + \beta|\psi|^2 + \lambda\left(U_{\text{dip}} * |\psi|^2\right)\right]\psi, \quad \mathbf{x}\in\mathbb{R}^3, \quad t>0. \quad (4.2)$$

where $\beta = \frac{NU_0}{\hbar\omega_0 a_0^3} = \frac{4\pi a_s N}{a_0}$, $\lambda = \frac{mN\mu_0\mu_{\text{dip}}^2}{3\hbar^2 a_0}$, $V(\mathbf{x}) = \frac{1}{2}(\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2)$ is the dimensionless harmonic trapping potential with $\gamma_x = \frac{\omega_x}{\omega_0}$, $\gamma_y = \frac{\omega_y}{\omega_0}$ and $\gamma_z = \frac{\omega_z}{\omega_0}$, and the dimensionless long-range dipolar interaction potential $U_{\text{dip}}(\mathbf{x})$ is given by (2.6).

Similar to the non-rotational case (2.1), (4.2) conserves the *mass*

$$N(\psi(\cdot,t)) = \int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|\, d\mathbf{x} \equiv N(\psi(\cdot,0)) = 1 \tag{4.3}$$

and the *energy* per particle

$$\begin{aligned} E_{\text{rot}}(\psi(\cdot,t)) :=& \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta}{2}|\psi|^4 - \Omega \text{Re}(\overline{\psi} L_z \psi) + \frac{\lambda}{2}\left(U_{\text{dip}} * |\psi|^2\right)|\psi|^2\right] d\mathbf{x} \\ \equiv& E_{\text{rot}}(\psi(\cdot,0)), \qquad t \geq 0. \end{aligned} \tag{4.4}$$

Quantized vortices have been observed in BEC experiments [2, 41] when a rotating laser beam is applied to rotate the condensate. Quantized vortices are quite related to the superfluidity. Hence, it is important to understand the vortex properties. In addition, the current experiments of rotating BEC are performed at ultra-cold temperature and the system is on its ground state. As a result, ground state of rotational dipolar GPE (4.2) plays an important role in understanding quantized vortices in dipolar BEC. So, for the rotational dipolar GPE (4.2), we are more interested in the ground states. In Chapter 6, we will consider Cauchy problem of rotational GPE (4.2) with $\lambda = 0$, i.e. without dipolar interaction term. Here, we focus on the ground states. Again, the ground state is defined as the solution of the following minimization problem:

Find $\phi_g \in S_3$ such that

$$E_{\text{rot}}^g := E_{\text{rot}}(\phi_g) = \min_{\phi \in S_3} E_{\text{rot}}(\phi). \tag{4.5}$$

In view of the identity (2.17), we can reformulate the above rotational dipolar GPE into the following rotational Gross-Pitaevskii-Poisson system (see Chapter 2):

$$i\partial_t \psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) - \Omega L_z + (\beta - \lambda)|\psi(\mathbf{x},t)|^2 - 3\lambda \partial_{\mathbf{nn}}\varphi(\mathbf{x},t)\right]\psi(\mathbf{x},t), \tag{4.6}$$

$$\nabla^2 \varphi(\mathbf{x},t) = -|\psi(\mathbf{x},t)|^2, \qquad \lim_{|\mathbf{x}|\to\infty} \varphi(\mathbf{x},t) = 0 \qquad \mathbf{x} \in \mathbb{R}^3, \quad t > 0, \tag{4.7}$$

and the energy can be rewritten as

$$E_{\text{rot}}(\psi) = \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta - \lambda}{2}|\psi|^4 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla\varphi|^2 - \Omega\, \text{Re}(\bar{\psi} L_z \psi)\right] d\mathbf{x}\,, \tag{4.8}$$

where φ is defined through (4.7).

Two dimensional model. With the same setup of the anisotropic external trap $V(\mathbf{x})$ as Chapter 3, effective lower dimensional equations can be derived. In particular, consider the **Case I** in Chapter 3 where

$$V(\mathbf{x}) = V_2(x,y) + \frac{z^2}{2\varepsilon^4}, \tag{4.9}$$

then for small ε, evolution of the solution $\psi(\mathbf{x},t)$ of rotational GPPS (4.6)-(4.7) would be confined in the ground mode of $-\frac{1}{2}\partial_{zz} + \frac{z^2}{2\varepsilon^4}$, which is spanned by $\varepsilon^{-1/2}\pi^{-1/4}e^{-\frac{z^2}{2\varepsilon^2}}$. Thus the three dimensional (3D) rotational GPPS (4.6)-(4.7) will reduce to a quasi two-dimensional (2D) equation. Due to the normalization condition $\|\psi\|_2 = 1$, taking ansatz

$$\psi(\mathbf{x},t) = e^{-i\mu_0 t/\varepsilon^2}\varepsilon^{-1/2}\phi(x,y,t)w_0(z/\varepsilon), \text{where } \mu_0 = \frac{1}{2}, \quad w_0(z) = \frac{1}{\pi^{1/4}}e^{-\frac{z^2}{2}}, \tag{4.10}$$

we have the **quasi-2D rotational dipolar GPE** for rotational GPPS (4.6)-(4.7) as (see Chapter 3)

$$i\partial_t\phi = \left[-\frac{1}{2}\Delta + V_2 + \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi|^2 - \frac{3\lambda}{2}(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta)\varphi^{2D} - \Omega L_z\right]\phi, \tag{4.11}$$

where

$$\mathbf{n}_\perp = (n_1,n_2)^T, \quad \partial_{\mathbf{n}_\perp} = \mathbf{n}_\perp\cdot(\partial_x,\partial_y)^T, \quad \partial_{\mathbf{n}_\perp\mathbf{n}_\perp} = \partial_{\mathbf{n}_\perp}(\partial_{\mathbf{n}_\perp}), \quad \Delta = \partial_{xx} + \partial_{yy},$$

and

$$\varphi^{2D}(x,y,t) = U_\varepsilon^{2D} * |\phi|^2, \quad U_\varepsilon^{2D}(x,y) = \frac{1}{2\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}} \frac{e^{-s^2/2}}{\sqrt{x^2+y^2+\varepsilon^2 s^2}}\,ds. \tag{4.12}$$

The energy of quasi-2D rotational dipolar GPE (4.11) is

$$E_{2D}(\phi) = \int_{\mathbb{R}^2}\left(\frac{1}{2}|\nabla\phi|^2 + V_2|\phi|^2 + \frac{\beta-\lambda+3n_3^2\lambda}{2\varepsilon\sqrt{2\pi}}|\phi|^4 - \frac{3}{4}\lambda|\phi|^2\widetilde{\varphi^{2D}} - \Omega\,\mathrm{Re}(\bar{\phi}L_z\phi)\right)d\mathbf{x}, \tag{4.13}$$

where

$$\widetilde{\varphi^{2D}} = \left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\Delta\right)\varphi^{2D}. \tag{4.14}$$

The ground state of equation (4.11) is defined as the solution to the following minimization problem:

Find $\phi_g \in S_2$ such that

$$E_{2D}^g := E_{2D}(\phi_g) = \min_{\phi\in S_2} E_{2D}(\phi). \tag{4.15}$$

4.2 Analytical results for ground states

In this section, we report some fundamental results concerning the ground states of the 3D rotational GPPS and the quasi-2D rotational dipolar GPE (4.11).

In the model case where the external trap $V(\mathbf{x})$ is harmonic

$$V(x,y,z) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), \quad \gamma_x, \gamma_y, \gamma_z > 0, \tag{4.16}$$

from physical intuition, when rotational speed $0 \le \Omega < \min\{\gamma_x, \gamma_y\}$, there exists ground state of rotational GPPS (4.6)-(4.7); when $\Omega > \min\{\gamma_x, \gamma_y\}$, there exists no ground state of rotational GPPS (4.6)-(4.7). Actually, we can justify this intuition and obtain the following results.

Theorem 4.1 *(Three dimensional case) Assume the trap $V(x,y,z)$ is given by (4.16), then there exists ground state of 3D rotational GPPS (4.6)-(4.7) , if $\beta \ge 0$, $-\frac{\beta}{2} \le \lambda \le \beta$ and $|\Omega| < \min\{\gamma_x, \gamma_y\}$. In contrast, there exists no ground state of (4.6)-(4.7) if one of the following condition holds:*

(1) $\beta < 0$;

(2) $\beta \ge 0$ and $\lambda < -\frac{\beta}{2}$ or $\lambda > \beta$;

(3) $\Omega > \min\{\gamma_x, \gamma_y\}$.

Proof: Under the condition $|\Omega| < \min\{\gamma_x, \gamma_y\}$, Cauchy inequality implies for any $\phi \in \Xi_3$

$$\left|\Omega \int_{\mathbb{R}^3} \bar{\phi} L_z \phi \, d\mathbf{x}\right| \le \frac{1}{2}\left(|\partial_x \psi|^2 + |\partial_y \psi|^2 + \Omega^2(x^2+y^2)|\psi|^2\right). \tag{4.17}$$

Hence, in the case $|\Omega| < \min\{\gamma_x, \gamma_y\}$, $\beta \ge 0$ and$-\frac{\beta}{2} \le \lambda \le \beta$, energy $E_{\rm rot}$ is bounded below in $S_3 \subset \Xi_3$. Similar arguments as those in Theorem 2.1 will yield the existence for the minimizer of the energy $E_{\rm rot}$ (4.8) in S_3, i.e. the ground state.

Next, we show the nonexistence if the conditions are not satisfied. First, let us notice that for real-valued function $\phi \in \Xi_3$, $\int_{\mathbb{R}^3} \bar{\phi} L_z \phi \, d\mathbf{x} = 0$. Hence, if either $\beta < 0$ or $\beta \ge 0$ and $\lambda < -\frac{\beta}{2}$ or $\lambda > \beta$, choose the same test functions as in Theorem 2.1, then it is easy to obtain $\inf\limits_{\phi \in S_3} E_{\rm rot}(\phi) = -\infty$, i.e. there is no ground state. In order to prove the assertion, we only need to check the case $|\Omega| > \min\{\gamma_x, \gamma_y\}$.

Without loss of generality, we assume that $\gamma_x \le \gamma_y$ and $\Omega > \gamma_x$. Choose a nonnegative $C_0^\infty(\mathbb{R}^2; [0,\infty))$ function $\rho(x,y)$ satisfying

$$\int_{\mathbb{R}^2} \rho^2(x,y) dxdy = 1, \quad \text{supp}(\rho) \subset \{(x,y) \in \mathbb{R}^2 \big| 1 \le \sqrt{x^2+y^2} \le 2\} \tag{4.18}$$

and

$$\int_{\mathbb{R}^2} V_2(x,y)\rho^2(x,y)\,dxdy = \frac{(\gamma_x+\epsilon)^2}{2}, \qquad 0<\epsilon<\frac{\Omega-\gamma_x}{2}, \tag{4.19}$$

then introduce the cylindric coordinate (r,θ,z) $(r\geq 0,\ \theta\in[0,2\pi))$ with $x=r\cos\theta, y=r\sin\theta$, and denote

$$f_n(r,\theta,z)=e^{-in\theta}\rho(x,y)w_0(z), \quad w_0(z)=\pi^{-1/4}e^{-z^2/2}, \quad n\in\mathbb{Z}^+. \tag{4.20}$$

Such ρ exists as we can take ρ^2 to be a Dirac distribution concentrated on point $(1,0)^T$ in the limit sense. Then, using the property $\rho=0$ for $r\leq 1$, we have

$$\begin{aligned}&\int_{\mathbb{R}^3}\frac{1}{2}\left(|\partial_x f_n|^2+|\partial_y f_n|^2\right)\,d\mathbf{x}=\pi\int_0^\infty|\partial_r\rho|^2 r\,dr+n^2\pi\int_0^\infty\frac{|\rho|^2}{r^2}r\,dr\\&\leq C_1+n^2\pi\int_0^\infty|\rho|^2 r\,dr=C_1+\frac{n^2}{2}.\end{aligned}$$

Furthermore, noticing the proof in Theorem 2.1 and the property of ρ, we get

$$\begin{aligned}&-\Omega\int_{\mathbb{R}^3}\overline{f_n}L_z(f_n)\,d\mathbf{x}=-\Omega\int_{\mathbb{R}^3}i\overline{f_n}\partial_\theta(f_n)\,d\mathbf{x}=-n\Omega,\\&\int_{\mathbb{R}^3}V_2(x,y)|f_n|^2\,d\mathbf{x}=\frac{(\gamma_x+\epsilon)^2}{2},\\&\int_{\mathbb{R}^3}\left((\beta-\lambda)|f_n|^4+\frac{3\lambda}{2}\right)|\partial_{\mathbf{n}}\nabla(-\nabla^2)^{-1}|f_n|^2|^2\,d\mathbf{x}\leq 2\beta\|\rho\|^2_{L^4(\mathbb{R}^2)}.\end{aligned}$$

Set $f_n^\delta=\delta^{-1}f_n(r/\delta,\theta,z)=\delta^{-1}f_n(x/\delta,y/\delta,z)$ for $\delta>0$, then the energy $E_{\rm rot}(f_n^\delta)$ (4.8) satisfies

$$E_{\rm rot}(f_n^\delta)\leq(C_1+\frac{n^2}{2})\delta^{-2}+\delta^2\frac{(\gamma_x+\epsilon)^2}{2}+C_3\delta^{-2}-n\Omega+C_4, \quad C_1,C_3\geq 0. \tag{4.21}$$

Choose

$$\delta_n^2=\sqrt{\frac{2C_1+n^2}{(\gamma_x+\epsilon)^2}}, \tag{4.22}$$

then

$$\delta_n\geq n/\Omega, \quad \text{for sufficient large } n, \tag{4.23}$$

and we have

$$E_{\rm rot}(f_n^{\delta_n})\leq(\gamma_x+\epsilon)(\sqrt{2C_1+n^2})-n\Omega+C_4+\Omega C_3/n\leq(\gamma_x+\epsilon)\frac{2C_1}{\sqrt{2C_1+n^2}}-n\epsilon+C_4+\Omega C_3/n.$$

Let $n\to+\infty$, it is obvious that $E_{\rm rot}(f_n^{\delta_n})\to-\infty$, i.e. there exists no ground state. □

Similarly, we can obtain the following results for two dimensional equation (4.11).

Theorem 4.2 *(Two dimensional results) Assume* $V_2(x,y)=\frac{1}{2}(\gamma_x^2x^2+\gamma_y^2y^2)$ $(\gamma_x,\gamma_y>0)$*.*
(i) If $|\Omega|<\min\{\gamma_x,\gamma_y\}$ *and one of the following condition holds,*

(1) $\lambda\geq 0$, $\beta-\lambda>-\varepsilon\sqrt{2\pi}C_b$*;*

(2) $\lambda<0$, $\beta+(\frac{1}{2}+3|n_3^2-\frac{1}{2}|)\lambda>-\varepsilon\sqrt{2\pi}C_b$*;*

where C_b *is given by (3.12), there exists a ground state* $\phi_g\in S_2$ *of equation (4.11).*
(ii) If $\beta+\frac{1}{2}\lambda(1-3n_3^2)<-\varepsilon\sqrt{2\pi}C_b$ *or* $|\Omega|>\min\{\gamma_x,\gamma_y\}$*, there exists no ground state of equation (4.11).*

Proof: The proof combines Theorem 3.1 and Theorem 4.1. It is quite straightforward and we omit it here for brevity. □

4.3 A numerical method for computing ground states of (4.11)

In the study of the quantized vortices in rotating BEC, two dimensional model is a starting point, because vortex structure in two dimensions is relative simpler compared to the three dimensions case. In this section, we study the quasi-2D equation (4.11). To compute the ground states, we use a backward Euler Fourier pseudospectral method, which has been used for computing rotating GPE without dipolar term in literature [166]. The idea is to use the gradient flow with discrete normalization as the non-rotating case (Chapter 3). After truncation, the gradient flow method with discrete normalization for quasi-2D equation(4.11) for $\phi:=\phi(x,y,t)$ reads as

$$\partial_t\phi=\left[\frac{1}{2}\Delta-V_2+\Omega L_z-\frac{\beta-\lambda+3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi|^2+\frac{3\lambda}{2}(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp}-n_3^2\Delta)\varphi\right]\phi, \quad (4.24)$$

$$\varphi(x,y,t)=U_\varepsilon^{2D}*|\phi|^2, \qquad (x,y)\in U=[a,b]\times[c,d], \quad t_n\leq t<t_{n+1}, \quad (4.25)$$

$$\phi(x,y,t_{n+1}):=\phi(x,y,t_{n+1}^+)=\frac{\phi(x,y,t_{n+1}^-)}{\|\phi(\cdot,t_{n+1}^-)\|_2}, \qquad (x,y)\in U, \quad n\geq 0, \quad (4.26)$$

$$\phi(x,y,t)|_{\partial U}=\varphi(x,y,t)|_{\partial U}=0, \qquad t\geq 0, \quad (4.27)$$

$$\phi(x,y,0)=\phi_0(x,y), \qquad \text{with} \quad \|\phi_0\|_2=1, \quad (4.28)$$

where $\phi(x,y,t_n^\pm)=\lim\limits_{t\to t_n^\pm}\phi(x,y,t)$.

Hereafter, we use the same notations as in subsection 3.6.1. Then a backward Euler Fourier pseudospectral (BEFP) discretization for (3.152) read as

$$\frac{\phi^*_{jk}-\phi^n_{jk}}{\Delta t} =\frac{1}{2}\left(\Delta^s\phi^*\right)\Big|_{jk} + i\Omega\left(y_k\left(\partial^s_x\phi^n\right)\Big|_{jk} - x_j\left(\partial^s_y\phi^n\right)\Big|_{jk}\right) - \left[\frac{\beta-\lambda+3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi^n_{jk}|^2 + V_2(x_j,y_k) - \frac{3\lambda}{2}\left((\partial^s_{\mathbf{n}_\perp\mathbf{n}_\perp}\varphi^n)\Big|_{jk} - n_3^2(\Delta^s\varphi^n)\Big|_{jk}\right)\right]\phi^n_{jk}, \tag{4.29}$$

$$\varphi^n_{jk} =\frac{1}{JK}\sum_{p=-J/2}^{J/2-1}\sum_{q=-K/2}^{K/2-1}\left(\widehat{\varphi^n}\right)_{pq} e^{i\frac{2jp\pi}{J}}e^{i\frac{2kq\pi}{K}}, \tag{4.30}$$

$$\widehat{\varphi^n}_{pq} = \left(\widehat{|\phi^n|^2}\right)_{pq}\widehat{U^{2D}_\varepsilon}(\lambda^x_p,\lambda^y_q), \quad -J/2\le p\le J/2-1,\ -K/2\le q\le K/2-1,$$

$$\phi^{n+1}_{jk} =\frac{\phi^*_{jk}}{\|\phi^*_{jk}\|}, \quad \phi^0_{jk}=\phi_0(x_j,y_k), \quad 0\le j\le J,\ 0\le k\le K, \tag{4.31}$$

where $\widehat{U^{2D}_\varepsilon}$ is given by (3.16), $\hat{\phi}_{pq}$ denotes the Fourier coefficients of ϕ_{jk}, $\|\phi^*\|$ denotes the discrete l^2 norm of ϕ^* and Δ^s and $\partial^s_{\mathbf{n}_\perp\mathbf{n}_\perp}$ are pseudospectral approximations of Δ and $\partial_{\mathbf{n}_\perp\mathbf{n}_\perp}$ respectively (see subsection 3.6.1). ∂^s_x and ∂^s_y are pseudospectral approximations of ∂_x and ∂_y respectively, defined as

$$(\partial^s_x\phi)_{jk} = \frac{i}{JK}\sum_{p=-J/2}^{J/2-1}\sum_{q=-K/2}^{K/2-1}\lambda^x_p\widehat{\phi}_{pq}e^{i\lambda^x_p(x_j-a)}e^{i\lambda^y_q(y_k-c)} \tag{4.32}$$

$$\left(\partial^s_y\phi\right)_{jk} = \frac{i}{JK}\sum_{p=-J/2}^{J/2-1}\sum_{q=-K/2}^{K/2-1}\lambda^y_q\widehat{\phi}_{pq}e^{i\lambda^x_p(x_j-a)}e^{i\lambda^y_q(y_k-c)}, \tag{4.33}$$

for $-J/2\le p\le J/2-1$, $-K/2\le q\le K/2-1$. Again, we can introduce stabilization parameter to the BEFP discretization [12, 21]. The above numerical method is implicit and can be solved explicitly via Fast Fourier transform (FFT). Actually, taking discrete Fourier transform of (4.29), we have

$$\left(1+\frac{\Delta t}{2}(\lambda^x_p)^2+\frac{\Delta t}{2}(\lambda^y_q)^2\right)\left(\widehat{\phi^*}\right)_{pq} = \left(\widehat{\phi^n}\right)_{pq} + \Delta t\left(\widehat{S^n}\right)_{pq}, \tag{4.34}$$

with the mesh function S^n for $0\le j\le J$ and $0\le k\le K$ given by

$$S^n_{jk} =-\left[V_2(x_j,y_k)+\frac{\beta-\lambda+3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\phi^n_{jk}|^2 - \frac{3\lambda}{2}\left((\partial^s_{\mathbf{n}_\perp\mathbf{n}_\perp}\varphi^n)\Big|_{jk} - n_3^2(\Delta^s\varphi^n)\Big|_{jk}\right)\right]\phi^n_{jk} + i\Omega\left(y_k\left(\partial^s_x\phi^n\right)\Big|_{jk} - x_j\left(\partial^s_y\phi^n\right)\Big|_{jk}\right).$$

Equation (4.34) can be solved explicitly and then BEFP (4.29) is solved.

4.4 Numerical results

To test the BEFP method for computing the ground states of the quasi-2D equation (4.11), we report some numerical results in this section.

Example 1. In quasi-2D equation (4.11), we choose $V_2(x,y) = \frac{1}{2}(x^2+y^2)$, $\varepsilon = 1/\sqrt{10}$, $(n_1, n_2) = (0.58, 0)$, $\beta = 135$, $\lambda = 125$.

Example 2. In quasi-2D equation (4.11), we choose $V_2(x,y) = \frac{1}{2}(x^2+y^2)$, $\varepsilon = 1/\sqrt{10}$, $(n_1, n_2) = (\sqrt{0.5}, \sqrt{0.5})$, $\beta = 135$, $\lambda = 90$.

We choose the computational domain as $[-8, 8] \times [-8, 8]$ with 257 grid points in each direction, time step $\Delta t = 0.005$. Ground state is numerically achieved if $\max_{jk} |\phi_{jk}^{n+1} - \phi_{jk}^n| < 10^{-6}$. To find the ground state, we test different initial data. In the current study, we choose the ground state of equation (4.11) with $\lambda = 0$ and same β, ε, or the central vortex state of it with single vortex, or a linear combination of them.

From Figs. 4.1 & 4.2, we can see that when the rotational speed Ω is small, there is no vortex. When Ω becomes larger and larger above a critical value, there are vortices in the ground state. The critical value of Ω for the existence of vortex depends on the trap V_2, parameter β and λ. There are also critical values for n vortices appearing in the ground state. In the case of 2D equation (4.11) with $\lambda = 0$ and a radial trap V_2, there have been estimates [130] for such critical value. For our case with $\lambda \neq 0$, it is also interesting to estimate the critical value of Ω. Further mathematical analysis and numerical investigation will be carried out in future.

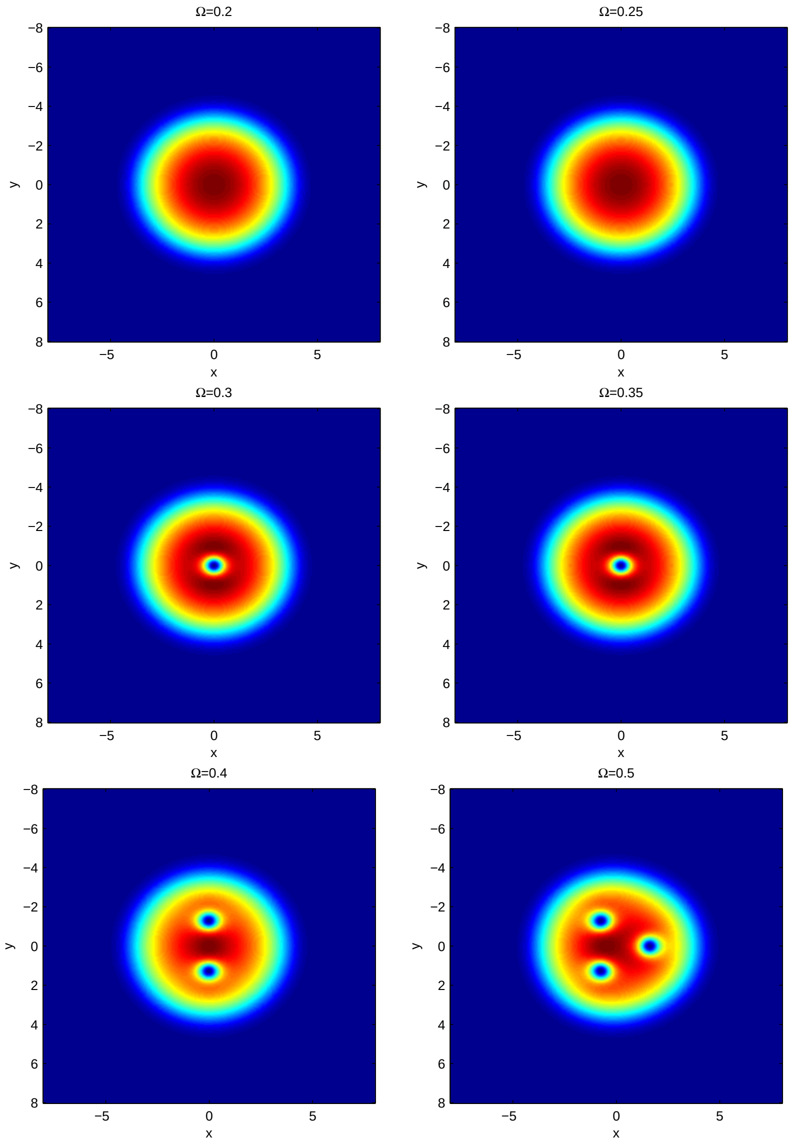

Figure 4.1: Contour plots for ground states in **Example 1**, for different Ω.

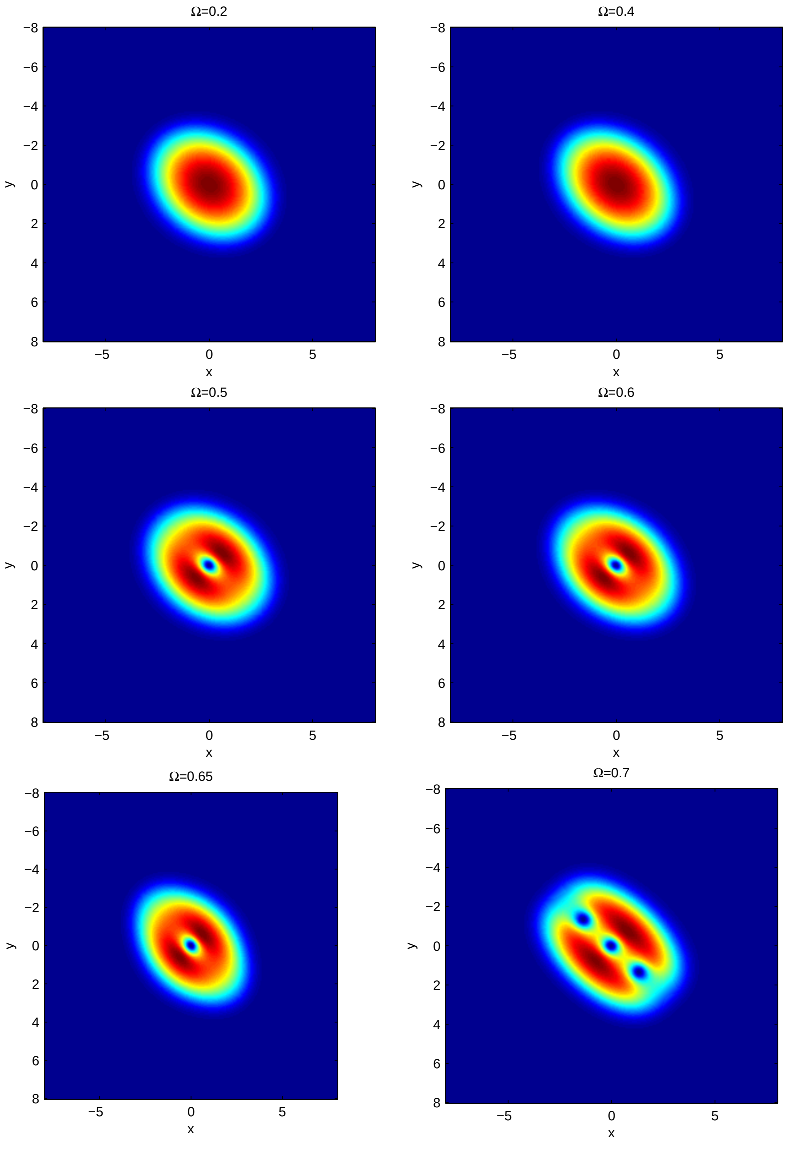

Figure 4.2: Contour plots for ground states in **Example 2**, for different Ω.

Chapter 5

Ground states of coupled Gross-Pitaevskii equations

In this chapter, we investigate ground state properties of the coupled GPEs modeling a two component BEC in optical resonators. We analyze the existence, uniqueness as well as non-uniqueness of the ground states. Efficient and accurate numerical methods are presented to compute the ground states of the coupled GPEs modeling a two component BEC with Josephson junction.

5.1 The model

At temperature T much smaller than the critical temperature T_c and after proper nondimensionalization and dimension reduction [117,167], we recall that a two-component BEC with an internal atomic Josephson junction in optical resonators can be well described by the coupled Gross-Pitaevskii equations (CGPE) (1.15) in d ($d = 1, 2, 3$) dimensions:

$$\begin{aligned} i\partial_t\psi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + (\beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2)\right]\psi_1 + (\lambda + \gamma P(t))\psi_2, \\ i\partial_t\psi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_{12}|\psi_1|^2 + \beta_{22}|\psi_2|^2)\right]\psi_2 + (\lambda + \gamma \bar{P}(t))\psi_1, \\ i\partial_t P(t) &= \int_{\mathbb{R}^d} \gamma\bar{\psi}_2(\mathbf{x}, t)\psi_1(\mathbf{x}, t)\, d\mathbf{x} + \nu P(t), \qquad \mathbf{x} \in \mathbb{R}^d. \end{aligned} \tag{5.1}$$

It is necessary to ensure that the wave function is properly normalized. Especially, we require

$$\|\Psi\|^2 := \|\Psi\|_2^2 = \int_{\mathbb{R}^d} \left[|\psi_1(\mathbf{x},t)|^2 + |\psi_2(\mathbf{x},t)|^2\right] d\mathbf{x} = 1. \tag{5.2}$$

The dimensionless CGPEs (5.1) conserve the total mass or normalization, i.e.

$$N(t) := \|\Psi(\cdot,t)\|^2 = N_1(t) + N_2(t) \equiv \|\Psi(\cdot,0)\|^2 = 1, \qquad t \geq 0, \tag{5.3}$$

with

$$N_j(t) = \|\psi_j(\mathbf{x},t)\|^2 := \|\psi_j(\mathbf{x},t)\|_2^2 = \int_{\mathbb{R}^d} |\psi_j(\mathbf{x},t)|^2\, d\mathbf{x}, \qquad t \geq 0, \qquad j = 1,2, \tag{5.4}$$

and the energy

$$\begin{aligned} E(\Psi) = \int_{\mathbb{R}^d} \Bigg[& \frac{1}{2}\left(|\nabla\psi_1|^2 + |\nabla\psi_2|^2\right) + V(\mathbf{x})(|\psi_1|^2 + |\psi_2|^2) + \delta|\psi_1|^2 + \beta_{12}|\psi_1|^2|\psi_2|^2 \\ & + \frac{\beta_{11}}{2}|\psi_1|^4 + \frac{\beta_{22}}{2}|\psi_2|^4 + 2\lambda\,\mathrm{Re}(\psi_1\bar{\psi}_2) + 2\nu\,\mathrm{Re}(\psi_1\overline{P(t)\psi_2})\Bigg] d\mathbf{x} + \nu\,|P(t)|^2. \end{aligned} \tag{5.5}$$

In addition, if there is no internal atomic Josephson junction and no photons in (5.1) , i.e. $\lambda = \nu = 0$, the mass of each component is also conserved, i.e.

$$N_1(t) \equiv \int_{\mathbb{R}^d} |\psi_1(\mathbf{x},0)|^2\, d\mathbf{x} := \alpha, \quad N_2(t) \equiv \int_{\mathbb{R}^d} |\psi_2(\mathbf{x},0)|^2\, d\mathbf{x} := 1-\alpha, \quad t \geq 0, \tag{5.6}$$

with $0 \leq \alpha \leq 1$ a given constant.

In order to study the ground states (stationary states) of (5.1), we substitute the following ansatz into CGPE (5.1)

$$\psi_1(\mathbf{x},t) = e^{-i\mu t}\phi_1(\mathbf{x}), \quad \psi_2(\mathbf{x},t) = e^{-i\mu t}\phi_2(\mathbf{x}), \quad P(t) = p_0 \in \mathbb{C}. \tag{5.7}$$

Then we obtain the time independent CGPE as

$$\begin{aligned} \mu\,\phi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\right]\phi_1 + (\lambda + \gamma p_0)\phi_2, \\ \mu\,\phi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\right]\phi_2 + (\lambda + \gamma\bar{p}_0)\phi_1, \\ \nu p_0 &= -\gamma\int_{\mathbb{R}^d} \bar{\phi}_2(\mathbf{x})\phi_1(\mathbf{x})\, d\mathbf{x}, \qquad \mathbf{x} \in \mathbb{R}^d, \end{aligned} \tag{5.8}$$

under the constraint

$$\|\Phi\|^2 := \|\Phi\|_2^2 = \int_{\mathbb{R}^d} \left[|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2\right] d\mathbf{x} = 1, \tag{5.9}$$

with the eigenvalue μ being the Lagrange multiplier or chemical potential corresponding to the constraint (5.9), which can be computed as

$$\begin{aligned}\mu &= \mu(\Phi) = \int_{\mathbb{R}^d} \Big[\frac{1}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) + V(\mathbf{x})(|\phi_1|^2 + |\phi_2|^2) + \delta|\phi_1|^2 + \beta_{11}|\phi_1|^4 \\ &\quad +\beta_{22}|\phi_2|^4 + 2\beta_{12}|\phi_1|^2|\phi_2|^2 + (\lambda + \gamma p_0)\bar{\phi}_1\phi_2 + (\lambda + \gamma\bar{p}_0)\phi_1\bar{\phi}_2\Big] d\mathbf{x}. \quad (5.10)\end{aligned}$$

The eigenfunctions of the nonlinear eigenvalue problem (5.8) under the normalization (5.9) are usually called as stationary states of the two-component BEC (5.1). Among them, the eigenfunction with minimum energy is the ground state and those whose energy are larger than that of the ground state are usually called as excited states.

Similar as dipolar GPE in Chapter 2 and 3, we will formulate the ground state as a minimization problem. From the nonlinear eigenvalue problem (5.8), in convenience of studying the ground state, we introduce the energy for stationary states $\Phi = (\phi_1, \phi_2)^T$ of CGPE (5.1) as

$$\begin{aligned}E_s(\Phi) &= \int_{\mathbb{R}^d} \Big[\frac{1}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) + V(\mathbf{x})(|\phi_1|^2 + |\phi_2|^2) + \delta|\phi_1|^2 + \beta_{12}|\phi_1|^2|\phi_2|^2 \\ &\quad + \frac{\beta_{11}}{2}|\phi_1|^4 + \frac{\beta_{22}}{2}|\phi_2|^4 + 2\lambda\cdot\mathrm{Re}(\phi_1\bar{\phi}_2)\Big] d\mathbf{x} - \sigma\left|\int_{\mathbb{R}^d}\phi_1(\mathbf{x})\overline{\phi}_2(\mathbf{x})\,d\mathbf{x}\right|^2, \quad (5.11)\end{aligned}$$

where we denote $\sigma = \gamma^2/\nu$ (when $\nu = 0$, $\gamma = 0$ and $\sigma = 0$). In the case of CGPE (5.1) without optical resonator, E_s collapses to E.

Hence, the ground state $\Phi_g(\mathbf{x}) = (\phi_1^g(\mathbf{x}), \phi_2^g(\mathbf{x}))^T$ of the two-component BEC with an internal atomic Josephson junction in optical resonators (5.1) is defined as the minimizer of the following nonconvex minimization problem:

Find $(\Phi_g \in S)$, such that

$$E_g := E_s(\Phi_g) = \min_{\Phi\in S} E_s(\Phi), \quad (5.12)$$

where S is a nonconvex set defined as

$$S := \left\{\Phi = (\phi_1, \phi_2)^T \mid \|\Phi\|^2 = 1,\ E_s(\Phi) < \infty\right\}. \quad (5.13)$$

If there is no internal atomic Josephson junction and optical resonator in (5.1), i.e. $\lambda = \gamma = \nu = 0$, for any given $\alpha \in [0,1]$, another type ground state $\Phi_g^\alpha(\mathbf{x}) = (\phi_1^\alpha(\mathbf{x}), \phi_2^\alpha(\mathbf{x}))^T$ of the two-component BEC is defined as the minimizer of the following nonconvex minimization problem:

Find $\left(\Phi_g^\alpha \in S_\alpha\right)$, such that

$$E_g^\alpha := E_0\left(\Phi_g^\alpha\right) = \min_{\Phi \in S_\alpha} E_0\left(\Phi\right), \tag{5.14}$$

where S_α is a nonconvex set defined as

$$S_\alpha := \left\{\Phi = (\phi_1, \phi_2)^T \mid \|\phi_1\|^2 = \alpha,\ \|\phi_2\|^2 = 1-\alpha,\ E_0(\Phi) < \infty\right\}, \tag{5.15}$$

and the energy functional $E_0(\Phi)$ is defined as

$$\begin{aligned} E_0(\Phi) \quad = \quad & \int_{\mathbb{R}^d} \left[\frac{1}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) + V(\mathbf{x})(|\phi_1|^2 + |\phi_2|^2) + \delta|\phi_1|^2 + \frac{1}{2}\beta_{11}|\phi_1|^4 \right. \\ & \left. + \frac{1}{2}\beta_{22}|\phi_2|^4 + \beta_{12}|\phi_1|^2|\phi_2|^2\right] d\mathbf{x}. \end{aligned} \tag{5.16}$$

Again, it is easy to see that the ground state Φ_g^α satisfies the following Euler-Lagrange equations,

$$\begin{aligned} \mu_1\,\phi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\right]\phi_1, \\ \mu_2\,\phi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\right]\phi_2, \qquad \mathbf{x} \in \mathbb{R}^d, \end{aligned} \tag{5.17}$$

under the two constraints

$$\|\phi_1\|^2 := \int_{\mathbb{R}^d} |\phi_1(\mathbf{x})|^2\, d\mathbf{x} = \alpha, \qquad \|\phi_2\|^2 := \int_{\mathbb{R}^d} |\phi_2(\mathbf{x})|^2\, d\mathbf{x} = 1-\alpha, \tag{5.18}$$

with μ_1 and μ_2 being the Lagrange multipliers or chemical potentials corresponding to the two constraints (5.18). Again, the above time-independent CGPEs (5.17) can also be obtained from the CGPEs (5.1) with $\lambda = 0$ by substituting the ansatz

$$\psi_1(\mathbf{x}, t) = e^{-i\mu_1 t}\phi_1(\mathbf{x}), \qquad \psi_2(\mathbf{x}, t) = e^{-i\mu_2 t}\phi_2(\mathbf{x}). \tag{5.19}$$

It is easy to see that the ground state Φ_g defined in (5.12) is equivalent to the following minimization problem

Find $(\Phi_g \in S)$, such that

$$E_s\left(\Phi_g\right) = \min_{\Phi \in S} E_s\left(\Phi\right) = \min_{\alpha \in [0,1]} E_s(\alpha), \qquad E_s(\alpha) = \min_{\Phi \in S_\alpha} E_s(\Phi). \tag{5.20}$$

There are some analytical and numerical studies for the ground states of two-component BEC without internal atomic Josephson junction or optical resonator, i.e. based on the definition of (5.14), in the literatures [9, 48, 49, 99]. To the author's knowledge, there are no analytical results for the ground states of two-component BEC with an internal atomic Josephson junction, i.e. based on the definition of (5.12). We are going to establish existence and uniqueness results for the ground states of two-component BEC with an internal atomic Josephson junction and optical resonator and to propose efficient and accurate numerical methods for computing these ground states.

5.2 Existence and uniqueness results for the ground states

In this section, we will establish existence and uniqueness results for the ground states of two-component BEC with and without an internal atomic Josephson junction and optical resonator, i.e. the nonconvex minimization problems (5.12) and (5.14), respectively. Let

$$B = \begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{pmatrix}, \tag{5.21}$$

we say B is positive semi-definite iff $\beta_{11} \geq 0$ and $\beta_{11}\beta_{22} - \beta_{12}^2 \geq 0$; and B is nonnegative iff $\beta_{11} \geq 0$, $\beta_{12} \geq 0$ and $\beta_{22} \geq 0$. Without loss of generality, throughout the paper, we assume $\beta_{11} \geq \beta_{22}$. In two dimensions (2D), i.e. $d = 2$, let C_b be the best constant defined in (3.12). The best constant C_b can be attained at some H^1 function [155] and it is crucial in considering the existence of ground states in 2D.

5.2.1 For the case with optical resonator, i.e. problem (5.12)

Denote

$$\mathcal{D} = \left\{ \Phi = (\phi_1, \phi_2)^T \mid V\,|\phi_j|^2 \in L^1(\mathbb{R}^d),\ \phi_j \in H^1(\mathbb{R}^d) \cap L^4(\mathbb{R}^d),\ j = 1, 2 \right\}, \tag{5.22}$$

then the ground state Φ_g of (5.12) is also given by

Find ($\Phi_g \in \mathcal{D}_1$), such that

$$E_g := E_s\left(\Phi_g\right) = \min_{\Phi \in \mathcal{D}_1} E_s\left(\Phi\right), \tag{5.23}$$

where

$$\mathcal{D}_1 = \mathcal{D} \cap \left\{ \Phi = (\phi_1, \phi_2)^T \mid \|\Phi\|_2^2 = \int_{\mathbb{R}^d} (|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2)\, d\mathbf{x} = 1 \right\}. \tag{5.24}$$

In addition, we introduce the auxiliary energy functional

$$\widetilde{E}(\Phi) = \int_{\mathbb{R}^d} \left\{ \frac{1}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) + \left[V(\mathbf{x})\left(|\phi_1|^2 + |\phi_2|^2\right) + \delta|\phi_1|^2\right] + \beta_{12}|\phi_1|^2|\phi_2|^2 \right.$$
$$\left. + \frac{\beta_{11}}{2}|\phi_1|^4 + \frac{\beta_{22}}{2}|\phi_2|^4 - 2|\lambda|\cdot|\phi_1|\cdot|\phi_2| \right\} d\mathbf{x} - \sigma\left(\int_{\mathbb{R}^d} |\phi_1|\,|\phi_2|\,d\mathbf{x}\right)^2, \qquad (5.25)$$

and the auxiliary nonconvex minimization problem

Find $(\Phi_g \in \mathcal{D}_1)$, such that

$$\widetilde{E}\left(\Phi_g\right) = \min_{\Phi\in\mathcal{D}_1} \widetilde{E}\left(\Phi\right). \qquad (5.26)$$

For $\Phi = (\phi_1, \phi_2)^T$, we write $E_s(\phi_1, \phi_2) = E_s(\Phi)$ and $\widetilde{E}(\phi_1, \phi_2) = \widetilde{E}(\Phi)$. Then we have the following lemmas:

Lemma 5.1 *For the minimizers $\Phi_g(\mathbf{x}) = (\phi_1^g(\mathbf{x}), \phi_2^g(\mathbf{x}))^T$ of the nonconvex minimization problems (5.23) and (5.26), if $-2|\lambda| \le \sigma$, we have*

(i) If Φ_g is a minimizer of (5.23), then $\phi_1^g(\mathbf{x}) = e^{i\theta_1}|\phi_1^g(\mathbf{x})|$ and $\phi_2^g(\mathbf{x}) = e^{i\theta_2}|\phi_2^g(\mathbf{x})|$ with θ_1 and θ_2 two constants satisfying $\theta_1 = \theta_2$ if $\lambda < 0$; and $\theta_1 = \theta_2 \pm \pi$ if $\lambda > 0$. In addition, $\widetilde{\Phi}_g = \left(e^{i\theta_3}\phi_1^g, e^{i\theta_4}\phi_2^g\right)^T$ with θ_3 and θ_4 two constants satisfying $\theta_3 = \theta_4$ if $\lambda < 0$; and $\theta_3 = \theta_4 \pm \pi$ if $\lambda > 0$ is also a minimizer of (5.23).

(ii) If Φ_g is a minimizer of (5.26), then $\phi_1^g(\mathbf{x}) = e^{i\theta_1}|\phi_1^g(\mathbf{x})|$ and $\phi_2^g(\mathbf{x}) = e^{i\theta_2}|\phi_2^g(\mathbf{x})|$ with θ_1 and θ_2 two constants. In addition, $\widetilde{\Phi}_g = \left(e^{i\theta_3}\phi_1^g, e^{i\theta_4}\phi_2^g\right)^T$ with θ_3 and θ_4 two constants is also a minimizer of (5.26).

(iii) If Φ_g is a minimizer of (5.23), then Φ_g is also a minimizer of (5.26).

(iv) If Φ_g is a minimizer of (5.26), then $\widetilde{\Phi}_g = (|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ is a minimizer of (5.23).

Proof: For any $\Phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}))^T \in \mathcal{D}_1$, we write it as

$$\phi_1(\mathbf{x}) = e^{i\theta_1(\mathbf{x})}|\phi_1(\mathbf{x})|, \qquad \phi_2(\mathbf{x}) = e^{i\theta_2(\mathbf{x})}|\phi_2(\mathbf{x})|, \qquad \mathbf{x} \in \mathbb{R}^d. \qquad (5.27)$$

Then we have

$$\nabla\phi_1(\mathbf{x}) = e^{i\theta_1(\mathbf{x})}\left[\nabla|\phi_1(\mathbf{x})| + i|\phi_1(\mathbf{x})|\nabla\theta_1(\mathbf{x})\right],$$
$$\nabla\phi_2(\mathbf{x}) = e^{i\theta_2(\mathbf{x})}\left[\nabla|\phi_2(\mathbf{x})| + i|\phi_2(\mathbf{x})|\nabla\theta_2(\mathbf{x})\right]. \qquad (5.28)$$

Noticing in the case of $\sigma \geq -2|\lambda|$, function $h(s) = -2|\lambda|s - \sigma s^2$ ($s \in [0, s_0]$, $0 \leq s_0 \leq 1/2$) reaches its minimal at s_0, in view of $\int_{\mathbb{R}} |\phi_1|\,|\phi_2|\,d\mathbf{x} \leq 1/2$, we have

$$2\lambda \int_{\mathbb{R}^d} \mathrm{Re}(\phi_1\bar{\phi}_2)\,d\mathbf{x} - \sigma \left|\int_{\mathbb{R}} \phi_1\bar{\phi}_2\,d\mathbf{x}\right|^2 \geq -2|\lambda| \int_{\mathbb{R}^d} |\phi_1|\,|\phi_2|\,d\mathbf{x} - \sigma \left(\int_{\mathbb{R}} |\phi_1|\,|\phi_2|\,d\mathbf{x}\right)^2,$$

where the equality can be attained. Plugging (5.28) into (5.11) with Φ and (5.25), we obtain

$$E_s(\phi_1,\phi_2) = E_s(|\phi_1|, -\mathrm{sign}(\lambda)|\phi_2|) + \int_{\mathbb{R}^d} \frac{1}{2}\Big[|\phi_1|^2|\nabla\theta_1|^2 + |\phi_2|^2|\nabla\theta_2|^2 + 4|\lambda|\,[1+\mathrm{sign}(\lambda)\cos(\theta_1-\theta_2)]\,|\phi_1||\phi_2|\Big]d\mathbf{x}, \tag{5.29}$$

$$\widetilde{E}(\phi_1,\phi_2) = \widetilde{E}(|\phi_1|,|\phi_2|) + \int_{\mathbb{R}^d} \frac{1}{2}\Big[|\phi_1|^2|\nabla\theta_1|^2 + |\phi_2|^2|\nabla\theta_2|^2\Big]d\mathbf{x}, \tag{5.30}$$

$$E_s(|\phi_1|, -\mathrm{sign}(\lambda)|\phi_2|) = \widetilde{E}(|\phi_1|,|\phi_2|) \leq \widetilde{E}(\phi_1,\phi_2), \tag{5.31}$$

$$\widetilde{E}(\phi_1,\phi_2) \leq E_s(\phi_1,\phi_2), \qquad \Phi \in \mathcal{D}_1. \tag{5.32}$$

(i) If Φ_g is a minimizer of (5.23), then we have

$$E_s(\phi_1^g,\phi_2^g) \leq E_s(|\phi_1^g|, -\mathrm{sign}(\lambda)|\phi_2^g|). \tag{5.33}$$

Plugging (5.33) into (5.29) with $\Phi = \Phi_g$, we get

$$\int_{\mathbb{R}^d} \frac{1}{2}\Big[|\phi_1^g|^2|\nabla\theta_1^g|^2 + |\phi_2^g|^2|\nabla\theta_2^g|^2 + 4|\lambda|\,[1+\mathrm{sign}(\lambda)\cos(\theta_1^g-\theta_2^g)]\,|\phi_1^g||\phi_2^g|\Big]d\mathbf{x} = 0.$$

This immediately implies that

$$\nabla\theta_1^g = 0, \qquad \nabla\theta_2^g = 0, \qquad 1+\mathrm{sign}(\lambda)\cos(\theta_1^g-\theta_2^g) = 0, \tag{5.34}$$

and thus

$$\theta_1^g(\mathbf{x}) \equiv \theta_1, \qquad \theta_2^g(\mathbf{x}) \equiv \theta_2, \qquad \theta_1 = \begin{cases} \theta_2 & \lambda < 0, \\ \theta_2 \pm \pi & \lambda > 0. \end{cases} \tag{5.35}$$

In addition, we have

$$E_s(\Phi_g) = E_s(|\phi_1^g|, -\mathrm{sign}(\lambda)|\phi_2^g|) = E_s(\widetilde{\Phi}_g), \tag{5.36}$$

which immediately implies that $\widetilde{\Phi}_g$ is also a minimizer of (5.23).

(ii) Follows the analogue proof as those in part i) and we omitted the details here.

(iii) If Φ_g is a minimizer of (5.23), noticing (5.29)-(5.31), we have

$$\begin{aligned}\widetilde{E}(\phi_1^g,\phi_2^g) &= \widetilde{E}(|\phi_1^g|,|\phi_2^g|) = E_s(|\phi_1^g|,-\mathrm{sign}(\lambda)|\phi_2^g|) = E_s(\phi_1^g,\phi_2^g)\\ &\le E_s(|\phi_1|,-\mathrm{sign}(\lambda)|\phi_2|) \le \widetilde{E}(\phi_1,\phi_2) = \widetilde{E}(\Phi), \qquad \Phi\in\mathcal{D}_1, \end{aligned}\tag{5.37}$$

which immediately implies that Φ_g is a minimizer of (5.26).

(iv) If Φ_g is a minimizer of (5.26), noticing (5.30) and (5.32), we have

$$\begin{aligned}E_s(\widetilde{\Phi}_g) &= E_s(|\phi_1^g|,-\mathrm{sign}(\lambda)|\phi_2^g|) = \widetilde{E}(|\phi_1^g|,|\phi_2^g|) = \widetilde{E}(\phi_1^g,\phi_2^g)\\ &\le \widetilde{E}(\phi_1,\phi_2) \le E_s(\phi_1,\phi_2) = E_s(\Phi), \qquad \Phi\in\mathcal{D}_1, \end{aligned}\tag{5.38}$$

which immediately implies that $\widetilde{\Phi}_g$ is a minimizer of (5.23). □

Lemma 5.2 *(strict convexity of $\widetilde{E}$) Assume that the matrix B is positive semi-definite and at least one of the parameters λ, $\gamma_1 := \beta_{11}-\beta_{22}$ and $\gamma_2 := \beta_{11}-\beta_{12}$ is nonzero, $-2|\lambda| \le \sigma \le 0$, for $(\rho_1,\rho_2)^T$ with $\rho_1,\rho_2\ge 0$, $\sqrt{\rho_1}$, $\sqrt{\rho_2}\in\mathcal{D}_1$, then $\widetilde{E}[\sqrt{\rho_1},\sqrt{\rho_2}]$ is strictly convex in (ρ_1,ρ_2).*

Proof: Similar to [98] for single-component BEC, the first term in $\widetilde{E}$ is convex. The second and third terms in $\widetilde{E}$ are linear and quadratic forms, respectively, since we assume that B is positive semi-definite, thus these two terms are convex. Now we just need to verify the convexity of remaining terms. Let $\Phi_1 = (\sqrt{\rho_1},\sqrt{\rho_2})^T\in\mathcal{D}_1$ and $\Phi_2 = (\sqrt{\rho_1'},\sqrt{\rho_2'})^T\in\mathcal{D}_1$, for $\alpha\in(0,1)$, then $\Phi(\alpha) = ([\alpha\rho_1+(1-\alpha)\rho_1']^{1/2},[\alpha\rho_2+(1-\alpha)\rho_2']^{1/2})^T\in\mathcal{D}_1$. Denote

$$g(\alpha) = \int_{\mathbb{R}^d}[\alpha\rho_1+(1-\alpha)\rho_1']^{1/2}\times[\alpha\rho_2+(1-\alpha)\rho_2']^{1/2}\,d\mathbf{x},\tag{5.39}$$

then consider the remaining terms in $\widetilde{E}$ as

$$R(\alpha) = -2|\lambda|g(\alpha) - \sigma\,(g(\alpha))^2.\tag{5.40}$$

By Cauchy inequality, we have

$$\alpha\sqrt{\rho_1}\sqrt{\rho_2}+(1-\alpha)\sqrt{\rho_1'}\sqrt{\rho_2'} \le \sqrt{\alpha\rho_1+(1-\alpha)\rho_1'}\times\sqrt{\alpha\rho_2+(1-\alpha)\rho_2'}.\tag{5.41}$$

Thus $g(\alpha)$ is concave, i.e. $g''\le 0$. Hence, we get

$$R''(\alpha) = -2\sigma\left(g'(\alpha)\right)^2 - \left(2\sigma g(\alpha)+2|\lambda|\right)g''(\alpha).\tag{5.42}$$

Noticing that $g(\alpha) \in [0, 1/2]$, under the condition that $\sigma \le 0$ and $|\lambda| + \frac{\sigma}{2} \ge 0$, we have

$$R''(\alpha) \ge 0, \quad \alpha \in [0,1], \tag{5.43}$$

which shows the remaining terms in $\widetilde{E}$ is convex. The proof is complete. □

Theorem 5.1 *(Existence and uniqueness of (5.26)) Suppose $V(\mathbf{x}) \ge 0$ satisfying $\lim\limits_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, then there exists a minimizer $\Phi^\infty = (\phi_1^\infty, \phi_2^\infty)^T \in \mathcal{D}_1$ of (5.26) if one of the following conditions holds,*

(i) $d = 1$;

(ii) $d = 2$ *and* $\beta_{11} \ge -C_b, \beta_{22} \ge -C_b$, $\beta_{12} \ge -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$;

(iii) $d = 3$ *and B is either positive semi-definite or nonnegative.*

In addition, if the matrix B is positive semi-definite and at least one of the parameters δ, λ, γ_1 and γ_2 is nonzero, $-2|\lambda| \le \sigma \le 0$, then the minimizer $(|\phi_1^\infty|, |\phi_2^\infty|)^T$ is unique.

Proof: First, we claim that $\widetilde{E}$ is bounded below under the assumption. Case (iii) is clear. For case (i), using the constraint $\|\Phi\|_2^2 = 1$ and Sobolev inequality, for any $\varepsilon > 0$, there exists $C_\varepsilon > 0$ such that

$$\|\phi_j\|_4^4 \le \|\phi_j\|_\infty^2 \|\phi_j\|_2^2 \le \|\phi_j\|_\infty^2 \le \|\nabla\phi_j\|_2 \|\phi_j\|_2 \le \varepsilon \|\nabla \phi_j\|_2^2 + C_\varepsilon, \quad j = 1, 2,$$

which yields the claim. For case (ii), using Cauchy inequality and Gagliardo-Nirenberg inequality, we have

$$\begin{aligned}
&\int_{\mathbb{R}^2} \left(\beta_{11}|\phi_1|^4 + \beta_{22}|\phi_2|^4 + 2\beta_{12}|\phi_1|^2|\phi_2|^2\right) d\mathbf{x} \ge -C_b \int_{\mathbb{R}^2} \left(\sqrt{|\phi_1|^2 + |\phi_2|^2}\right)^4 d\mathbf{x} \\
&\ge -\int_{\mathbb{R}^2} \left(\sqrt{|\phi_1|^2 + |\phi_2|^2}\right)^2 d\mathbf{x} \int_{\mathbb{R}^2} \left(\nabla\sqrt{|\phi_1|^2 + |\phi_2|^2}\right)^2 d\mathbf{x} \\
&\ge -\int_{\mathbb{R}^2} \left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) dx,
\end{aligned}$$

which also leads to the claim. Thus, in all the cases, we can take a minimizing sequence $\Phi^n = (\phi_1^n, \phi_2^n)^T$ in $\mathcal{D}_1$. Then there exists a constant C such that $\|\nabla\phi_1^n\| + \|\nabla\phi_2^n\| < C$, $\|\phi_1^n\|_4 + \|\phi_2^n\|_4 < C$ and $\int_{\mathbb{R}^d} V(\mathbf{x})(|\phi_1^n(\mathbf{x})|^2 + |\phi_2^n(\mathbf{x})|^2)d\mathbf{x} < C$ for all $n \ge 0$. Therefore ϕ_1^n and ϕ_2^n belong to a weakly compact set in L^4, $H^1 = \{\phi \mid \|\phi\|^2 + \|\nabla\phi\|^2 < \infty\}$, and $L_V^2 = \{\phi \mid \int_{\mathbb{R}^d} V(\mathbf{x})|\phi(\mathbf{x})|^2 \; d\mathbf{x} < \infty\}$ with a weighted L^2-norm given by $\|\phi\|_V = [\int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 V(\mathbf{x}) d\mathbf{x}]^{1/2}$. Thus, there exists a $\Phi^\infty = (\phi_1^\infty, \phi_2^\infty)^T \in \mathcal{D}$ and a subsequence (which we denote as the original sequence for simplicity), such that

$$\begin{aligned} &\phi_1^n \rightharpoonup \phi_1^\infty, \qquad \phi_2^n \rightharpoonup \phi_2^\infty, \qquad \text{in } L^2 \cap L^4 \cap L_V^2, \\ &\nabla\phi_1^n \rightharpoonup \nabla\phi_1^\infty, \qquad \nabla\phi_2^n \rightharpoonup \nabla\phi_2^\infty, \qquad \text{in } L^2. \end{aligned} \tag{5.44}$$

Also, we can suppose that ϕ_1^n and ϕ_2^n are nonnegative, since we can replace them with $|\phi_1^n|$ and $|\phi_2^n|$, which also minimize the functional $\widetilde{E}$. To show that $\widetilde{E}$ attains its minimal at Φ^∞, we recall the constraint $\|\Phi^n\|^2 = 1$, then the functional $\widetilde{E}$ can be re-written as

$$\begin{aligned} \widetilde{E}(\phi_1^n, \phi_2^n) = \int_{\mathbb{R}^d} &\left[\frac{1}{2}\left(|\nabla\phi_1^n|^2 + |\nabla\phi_2^n|^2\right) + V(\mathbf{x})\left(|\phi_1^n|^2 + |\phi_2^n|^2\right) + \delta|\phi_1^n|^2 + \beta_{12}|\phi_1^n|^2|\phi_2^n|^2 \right. \\ &\left. + \frac{\beta_{11}}{2}|\phi_1^n|^4 + \frac{\beta_{22}}{2}|\phi_2^n|^4 + |\lambda|\,|\phi_1^n - \phi_2^n|^2\right] d\mathbf{x} - |\lambda| - \sigma\left(\int_{\mathbb{R}^d} \phi_1^n\phi_2^n \, d\mathbf{x}\right)^2. \end{aligned}$$

First, we show that for any given $\varepsilon > 0$,

$$\int_{\mathbb{R}^d} \beta_{12}\, |\phi_1^\infty|^2|\phi_2^\infty|^2 d\mathbf{x} \le \liminf_{n\to\infty} \int_{\mathbb{R}^d} \beta_{12}\, |\phi_1^n|^2|\phi_2^n|^2 d\mathbf{x} + \varepsilon. \tag{5.45}$$

When $\beta_{12} \ge 0$, this is obviously true. For general β_{12}, we decompose $\mathbb{R}^d$ into two parts, a bounded region $B_R = \{|\mathbf{x}| \le R\}$ and $B_R^c := \mathbb{R}^d \setminus B$, such that $V(\mathbf{x}) \ge 1/\eta$ on B_R^c, where $\eta > 0$ sufficiently small, using the assumption $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$. Then $\int_{B_R^c}(|\phi_1^n|^2 + |\phi_2^n|^2)d\mathbf{x} \le C\eta$. In B_R^c, using the Sobolev-Gagliardo inequality, for $d = 3$ and $2^* = 6$, we have

$$\int_{B_R^c} |\phi_1^n|^4 d\mathbf{x} \le \|\phi_1^n\|_{2^*}^{12} \left(\int_{B_R^c} |\phi_1^n|^2 d\mathbf{x}\right)^2 \le MC\eta^2\|\nabla\phi_1^n\|_2^{12} \le MC^{13}\eta^2, \tag{5.46}$$

where M is a constant. Thus, by choosing R sufficiently large, we have

$$\int_{B_R^c} |\phi_1^n|^4 d\mathbf{x} \le \frac{\varepsilon}{2(1+|\beta_{12}|)}, \qquad \text{for all } n. \tag{5.47}$$

In the case of $d = 1$, using the Sobolev inequality

$$\|f\|_\infty \le \|f'\|_2\, \|f\|_2, \qquad \text{for all } f \in H^1(\mathbb{R}^1), \tag{5.48}$$

and in the case of $d = 2$, using the Sobolev type inequality

$$\|f\|_6^2 \le C(\|\nabla f\|_2^2 + \|f\|_2^2), \qquad \text{for all } f \in H^1(\mathbb{R}^2), \tag{5.49}$$

we can get the same result.

The same conclusion holds for ϕ_2^n. Notice that for ϕ_1^∞ and ϕ_2^∞, by the weak lower semicontinuous property of $L^4(\mathbb{R}^d)$-norm, $H^1(\mathbb{R}^d)$-norm and $L_V^2(\mathbb{R}^d)$-norm, we can have $\|\nabla\phi_1^\infty\|_2 + \|\nabla\phi_2^\infty\|_2 < C$, $\|\phi_1^\infty\|_4 + \|\phi_2^\infty\|_4 < C$ and $\int_{\mathbb{R}^d} V(\mathbf{x})(|\phi_1^\infty|^2 + |\phi_2^\infty|^2)d\mathbf{x} < C$. Following the above arguments, the same conclusion holds for ϕ_1^∞ and ϕ_2^∞, i.e., we have

$$\int_{B_R^c} |\phi_j^n|^4 \, d\mathbf{x} \le \frac{\varepsilon}{2(1+|\beta_{12}|)}, \quad \int_{B_R^c} |\phi_j^\infty|^4 \, d\mathbf{x} \le \frac{\varepsilon}{2(1+|\beta_{12}|)}, \quad j=1,2, \quad n \ge 0. \tag{5.50}$$

Then, by the Cauchy-Schwartz inequality, we have

$$\begin{aligned} \left|\int_{B_R^c} \beta_{12}|\phi_1^n|^2|\phi_2^n|^2 \, d\mathbf{x}\right| &\le |\beta_{12}| \left(\int_{B_R^c} |\phi_1^n|^4 \, d\mathbf{x}\right)^{1/2} \left(\int_{B_R^c} |\phi_2^n|^4 \, d\mathbf{x}\right)^{1/2} \\ &\le \frac{\varepsilon}{2}, \qquad n \ge 0, \end{aligned} \tag{5.51}$$

and

$$\left|\int_{B_R^c} \beta_{12} \, |\phi_1^\infty|^2 \, |\phi_2^\infty|^2 \, d\mathbf{x}\right| \le \frac{\varepsilon}{2}. \tag{5.52}$$

Next, in the ball B_R, applying the Sobolev embedding theorem, the strong convergence holds,

$$\phi_1^n \longrightarrow \phi_1^\infty, \quad \phi_2^n \longrightarrow \phi_2^\infty, \qquad \text{in } L^2(B_R) \cap L^4(B_R). \tag{5.53}$$

By writing

$$\begin{aligned} &\left|\int_{B_R} \beta_{12}|\phi_1^n|^2|\phi_2^n|^2 \, d\mathbf{x} - \int_{B_R} \beta_{12}|\phi_1^\infty|^2|\phi_2^\infty|^2 \, d\mathbf{x}\right| \\ &\quad \le |\beta_{12}| \left[\left|\int_{B_R} \left(|\phi_1^n|^2 - |\phi_1^\infty|^2\right) |\phi_2^n|^2 \, d\mathbf{x}\right| + \left|\int_{B_R} \left(|\phi_2^n|^2 - |\phi_2^\infty|^2\right) |\phi_1^\infty|^2 \, d\mathbf{x}\right|\right] \\ &\quad \le C \left(\|\phi_1^n - \phi_1^\infty\|_{L^4(B_R)} + \|\phi_2^n - \phi_2^\infty\|_{L^4(B_R)}\right), \end{aligned} \tag{5.54}$$

we have

$$\int_{B_R} \beta_{12} \, |\phi_1^\infty(\mathbf{x})|^2 \, |\phi_2^\infty(\mathbf{x})|^2 \, d\mathbf{x} = \lim_{n\to\infty} \int_{B_R} \beta_{12}|\phi_1^n(\mathbf{x})|^2|\phi_2^n(\mathbf{x})|^2 \, d\mathbf{x}. \tag{5.55}$$

Hence, the inequality (5.45) holds by combining the above results.

By a similar argument, we can prove that $\phi_j^n \to \phi_j^\infty$ in $L^2 \bigcap L^4$ $(j=1,2)$,

$$\limsup_{n\to\infty} \left|\int_{\mathbb{R}^d} (|\phi_1^n|^2 + |\phi_2^n|^2) d\mathbf{x} - \int_{\mathbb{R}^d} (|\phi_1^\infty|^2 + |\phi_2^\infty|^2) d\mathbf{x}\right| \le \varepsilon. \tag{5.56}$$

Since $L^4(\mathbb{R}^d)$-norm, $H^1(\mathbb{R}^d)$-norm and $L_V^2(\mathbb{R}^d)$-norm are all weakly lower semicontinuous, we have

$$\widetilde{E}(\phi_1^\infty, \phi_2^\infty) \le \liminf_{n\to\infty} \widetilde{E}(\phi_1^n, \phi_2^n) + \varepsilon, \qquad \varepsilon > 0, \tag{5.57}$$

which immediately implies that $\widetilde{E}(\Phi^\infty) \le \liminf_{n\to\infty} \widetilde{E}(\Phi^n)$. Moreover, $\Phi^\infty \in \mathcal{D}_1$ by (5.56) which implies the existence of minimizer of the problem (5.26).

If the matrix B is positive semi-definite and at least one of the parameters λ, γ_1 and γ_2 is nonzero, $-2|\lambda| \le \sigma \le 0$, the uniqueness of $(|\phi_1^\infty|, |\phi_2^\infty|)^T$ follows from the strict convexity of $\widetilde{E}$. For the case $\delta \neq 0$ and $\lambda = \gamma_1 = \gamma_2 = \sigma = 0$, the uniqueness is easy to derive. □

Remark 5.1 *Under the same conditions, we can prove the existence of the minimization problem (5.12). The proof is straightforward.*

Notice that the the results in Lemma 5.1, Remark 5.1 and Theorem 5.1, we immediately have the following existence and uniqueness results for the ground states of (5.12):

Theorem 5.2 *(Existence and uniqueness of (5.12)) Suppose $V(\mathbf{x}) \ge 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and at least one of the following condition holds,*

(i) $d = 1$;

(ii) $d = 2$ *and* $\beta_{11} \ge -C_b$, $\beta_{22} \ge -C_b$, *and* $\beta_{12} \ge -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$;

(iii) $d = 3$ *and B is either positive semi-definite or nonnegative,*

there exists a ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (5.12). In addition, if $\sigma \ge -2|\lambda|$, $\widetilde{\Phi}_g := (e^{i\theta_1}|\phi_1^g|, e^{i\theta_2}|\phi_2^g|)$ is also a ground state of (5.12) with θ_1 and θ_2 two constants satisfying $\theta_1 - \theta_2 = \pm\pi$ when $\lambda > 0$ and $\theta_1 - \theta_2 = 0$ when $\lambda < 0$, respectively. Furthermore, if the matrix B is positive semi-definite and at least one of the parameters δ, λ, γ_1 and γ_2 is nonzero, $-2|\lambda| \le \sigma \le 0$, then the ground state $(|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ is unique. In contrast, if one of the following conditions holds,

(i) $d = 2$ *and* $\beta_{11} < -C_b$ *or* $\beta_{22} < -C_b$ *or* $\beta_{12} < -C_b - \sqrt{C_b + \beta_{11}}\sqrt{C_b + \beta_{22}}$;

(ii) $d = 3$ *and* $\beta_{11} < 0$ *or* $\beta_{22} < 0$ *or* $\beta_{12} < 0$ *with* $\beta_{12}^2 > \beta_{11}\beta_{22}$.

there exists no ground state of (5.12).

Proof: The first part of the theorem follows from Theorem 5.1. We are going to prove the nonexistence results.

In 2D case, i.e. $d = 2$, let $\varphi(\mathbf{x}) \in H^1(\mathbb{R}^2)$ such that $\|\varphi\|_2 = 1$ and $C_b = \|\nabla\varphi\|_2^2/\|\varphi\|_4^4$ [155]. Consider $\Phi^\varepsilon = (\phi_1^\varepsilon, \phi_2^\varepsilon)^T$, where $\phi_1^\varepsilon(\mathbf{x}) = \sqrt{\theta}\varepsilon^{-1}\varphi(\mathbf{x}/\varepsilon)$, $\phi_2^\varepsilon(\mathbf{x}) = \sqrt{1-\theta}\varepsilon^{-1}\varphi(\mathbf{x}/\varepsilon)$, $\theta \in [0,1]$, $\varepsilon > 0$. When $\beta_{11} < -C_b$, choose $\theta = 1$, we have

$$E_s(\Phi^\varepsilon) = \frac{1}{2\varepsilon^2}\|\nabla\varphi\|_2^2 + \frac{\beta_{11}}{2\varepsilon^2}\|\varphi\|_4^4 + \mathcal{O}(1) = \frac{1+\frac{\beta_{11}}{C_b}}{2\varepsilon^2}\|\nabla\varphi\|_2^2 + \mathcal{O}(1), \quad \varepsilon \to 0^+,$$

thus $\lim_{\varepsilon\to 0^+} E_s(\Phi^\varepsilon) = -\infty$. When $\beta_{22} < -C_b$, choose $\theta = 0$, similarly we can draw the same conclusion. When $\beta_{11} \geq -C_b$, $\beta_{22} \geq -C_b$ and $\beta_{12} < -C_b - \sqrt{C_b+\beta_{11}}\sqrt{C_b+\beta_{22}}$, choose $\theta = \frac{\beta_{22}-\beta_{12}}{\beta_{11}+\beta_{22}-2\beta_{12}}$, then

$$\beta_\theta := \theta^2\beta_{11} + 2\beta_{12}\theta(1-\theta) + \beta_{22}(1-\theta)^2 = \frac{\beta_{11}\beta_{22}-\beta_{12}^2}{\beta_{11}+\beta_{22}-2\beta_{12}} < -C_b,$$

and

$$E_s(\Phi^\varepsilon) = \frac{1+\frac{\beta_\theta}{C_b}}{2\varepsilon^2}\|\nabla\varphi\|_2^2 + \mathcal{O}(1), \quad \varepsilon \to 0^+,$$

then $\lim_{\varepsilon\to 0} E_s(\Phi^\varepsilon) = -\infty$. Thus there exists no ground state in these cases.

In three dimensions (3D) case, i.e. $d = 3$, choose $\Phi^\varepsilon = (\phi_1^\varepsilon, \phi_2^\varepsilon)^T$, where $\phi_1^\varepsilon(\mathbf{x}) = \frac{\sqrt{\theta}}{(\varepsilon\pi)^{3/4}}\exp(-|\mathbf{x}|^2/2\varepsilon)$, $\phi_2^\varepsilon(\mathbf{x}) = \frac{\sqrt{1-\theta}}{(\varepsilon\pi)^{3/4}}\exp(-|\mathbf{x}|^2/2\varepsilon)$, $\theta \in [0,1]$, $\varepsilon > 0$. When $\beta_{11} < 0$, choosing $\theta = 1$, we obtain

$$E_s(\Phi^\varepsilon) = C_1\varepsilon^{-1} + \frac{\beta_{11}}{2}(2\pi\varepsilon)^{-3/2} + \mathcal{O}(1), \quad \varepsilon \to 0^+,$$

which shows $\lim_{\varepsilon\to 0^+} E(\Phi^\varepsilon) = -\infty$. When $\beta_{22} < 0$, choose $\theta = 0$, the same conclusion holds. When $\beta_{11} \geq 0$, $\beta_{22} \geq 0$, $\beta_{12} < 0$ and $\beta_{12}^2 > \beta_{11}\beta_{22}$, choose $\theta = \frac{\beta_{22}-\beta_{12}}{\beta_{11}+\beta_{22}-2\beta_{12}} \in (0,1)$, then

$$\beta_\theta := \theta^2\beta_{11} + 2\beta_{12}\theta(1-\theta) + \beta_{22}(1-\theta)^2 = \frac{\beta_{11}\beta_{22}-\beta_{12}^2}{\beta_{11}+\beta_{22}-2\beta_{12}} < 0,$$

and

$$E_s(\Phi^\varepsilon) = C_1\varepsilon^{-1} + \frac{\beta_\theta}{2}(2\pi\varepsilon)^{-3/2} + \mathcal{O}(1), \quad \varepsilon \to 0^+,$$

thus $\lim_{\varepsilon\to 0^+} E_s(\Phi^\varepsilon) = -\infty$. The above results imply that there exists no ground state in such cases. □

When B is nonnegative, we have the following uniqueness results for the ground states of (5.12):

Theorem 5.3 *Suppose* $V(\mathbf{x}) \ge 0$ *satisfying* $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$*, the matrix* B *is nonnegative satisfying* $\beta_{11} = \beta_{22} \ge 0$*, at least one of the parameters* δ*,* λ*,* γ_1 *and* γ_2 *is nonzero,* $-2|\lambda| \le \sigma \le 0$*, and* $\delta \ne 0$ *if* $\beta_{12} - \beta_{11} > 0$*, then the ground state* $\Phi_g = (|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ *of (5.12) is unique.*

Proof: If B is nonnegative and $\beta_{11} = \beta_{22} \ge \beta_{12} \ge 0$ which immediately implies that B is positive semi-definite, since at least one of the parameters δ, λ, γ_1 and γ_2 is nonzero, $\sigma \le 0$ and $|\lambda| + \frac{\sigma}{2} \ge 0$, the uniqueness of the ground state Φ_g follows immediately from Theorem 5.1.

If $\beta_{12} > \beta_{11} = \beta_{22} \ge 0$, for any $\Phi = (\phi_1, \phi_2)^T \in \mathcal{D}_1$, let

$$\varphi_1 = \frac{1}{\sqrt{2}}(\phi_1 + \phi_2), \qquad \varphi_2 = \frac{1}{\sqrt{2}}(\phi_1 - \phi_2). \tag{5.58}$$

Suppose that $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is a nonnegative minimizer of (5.26), then the corresponding $(\varphi_1^g, \varphi_2^g)^T$ is a minimizer of the following energy functional

$$\begin{aligned}
&\widehat{E}(\varphi_1, \varphi_2) \\
&= \int_{\mathbb{R}^d} \left[\frac{1}{2}\left(|\nabla\varphi_1|^2 + |\nabla\varphi_2|^2\right) + V(\mathbf{x})\left(|\varphi_1|^2 + |\varphi_2|^2\right) + (3\beta_{11} - \beta_{12})|\varphi_1|^2|\varphi_2|^2 + \delta \mathrm{Re}(\varphi_1\bar{\varphi}_2) \right. \\
&\left. + (\sigma - 2|\lambda|)\,|\varphi_1|^2 + \frac{\beta_{11} + \beta_{12}}{2}\left[|\varphi_1|^4 + |\varphi_2|^4\right] \right] d\mathbf{x} - \sigma\left(\int_{\mathbb{R}^d} \varphi_1^2(\mathbf{x})\, d\mathbf{x}\right)^2, \qquad (5.59)
\end{aligned}$$

under the constraint $\int_{\mathbb{R}^d}(|\varphi_1(\mathbf{x})|^2 + |\varphi_2(\mathbf{x})|^2)\, d\mathbf{x} = 1$.

Noticing that the matrix $\begin{pmatrix} \beta_{11} + \beta_{12} & 3\beta_{11} - \beta_{12} \\ 3\beta_{11} - \beta_{12} & \beta_{11} + \beta_{12} \end{pmatrix}$ is positive semi-definite in this case and δ is nonzero, using the results in the Theorem 5.1, we can obtain the uniqueness of the ground state $(\varphi_1^g, \varphi_2^g)^T$ to the problem (5.59) with $\varphi_1^g \ge 0$. Thus the uniqueness of the ground state $\Phi_g = (|\phi_1^g|, -\mathrm{sign}(\lambda)|\phi_2^g|)^T$ of (5.12) follows immediately. □

Theorem 5.4 *Suppose* $V(\mathbf{x}) \ge 0$ *satisfying* $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ *and* $\lambda = \sigma = 0$*.*

(i) If $\delta \ge 0$*,* $\beta_{12} \ge \beta_{22}$ *and* $\beta_{11} > \beta_{22} \ge 0$*, then the ground state* $\Phi_g = (\phi_1^g, \phi_2^g)^T$ *of (5.12) must satisfy* $\phi_1^g = 0$ *and* $|\phi_2^g|$ *is unique.*

(ii) If $\delta \le 0$*,* $\beta_{12} \ge \beta_{11}$ *and* $\beta_{22} > \beta_{11} \ge 0$*, then the ground state* $\Phi_g = (\phi_1^g, \phi_2^g)^T$ *of (5.12) must satisfy* $\phi_2^g = 0$ *and* $|\phi_1^g|$ *is unique.*

Proof: (i) Suppose $\Phi_g = (\phi_1^g, \phi_2^g)^T$ be a nonnegative minimizer of (5.12). Consider

$$\phi_1(\mathbf{x}) = 0, \quad \phi_2(\mathbf{x}) = \sqrt{|\phi_1^g(\mathbf{x})|^2 + |\phi_2^g(\mathbf{x})|^2}, \qquad \mathbf{x} \in \mathbb{R}^d. \tag{5.60}$$

Then, $\Phi = (\phi_1, \phi_2)^T \in \mathcal{D}_1$ and satisfies

$$\begin{aligned}
&\int_{\mathbb{R}^d} |\nabla\phi_2(\mathbf{x})|^2 d\mathbf{x} \leq \int_{\mathbb{R}^d} \left[|\nabla\phi_1^g(\mathbf{x})|^2 + |\nabla\phi_2^g(\mathbf{x})|^2\right] d\mathbf{x}, \\
&\int_{\mathbb{R}^d} V(\mathbf{x}) \left(|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2\right) d\mathbf{x} = \int_{\mathbb{R}^d} V(\mathbf{x}) \left(|\phi_1^g(\mathbf{x})|^2 + |\phi_2^g(\mathbf{x})|^2\right) d\mathbf{x}, \\
&\int_{\mathbb{R}^d} \frac{\beta_{22}}{2} |\phi_2(\mathbf{x})|^4 d\mathbf{x} \leq \int_{\mathbb{R}^d} \frac{1}{2} \left[\beta_{11}|\phi_1^g|^4 + \beta_{22}|\phi_2^g|^4 + 2\beta_{12}|\phi_1^g|^2|\phi_2^g|^2\right] d\mathbf{x}.
\end{aligned} \tag{5.61}$$

Thus,

$$E_s(\Phi) = E_s(\phi_1, \phi_2) \leq E_s(\phi_1^g, \phi_2^g) = E_s(\Phi_g) \leq E_s(\Phi). \tag{5.62}$$

So, the above inequalities must be equalities, which leads to our conclusion. The uniqueness of $|\phi_2^g|$ is also easy to see.

(ii) Follow the analogous arguments as in part (i) and the details are omitted. $\square$

Lastly, we stress that, if B is not positive semi-definite, the uniqueness of the ground state of (5.12) may not hold. Actually, we have the following result in contrast with Theorem 5.3.

Theorem 5.5 *Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim\limits_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, $\delta = \sigma = 0$ and $\beta_{12} > \beta_{11} = \beta_{22} \geq 0$, then there exists a constant $\Lambda_0 > 0$, such that for $\lambda \in (-\Lambda_0, \Lambda_0)$, the ground state $\Phi_g = (|\phi_1^g|, -sign(\lambda)|\phi_2^g|)^T$ of (5.12) is not unique.*

Proof: Let $\Phi_1 = (\phi^g, \phi^g)^T$ be the nonnegative minimizer of (5.25) in the subset of $\mathcal{D}_1$ $\left\{\Phi = (\phi_1, \phi_2)^T \in, \phi_1 = \phi_2\right\}$ and $\Phi_2 = (0, \phi)^T$ be the nonnegative minimizer of (5.25) in the set $\left\{\Phi = (\phi_1, \phi_2)^T \in \mathcal{D}_1, \phi_1 = 0\right\}$, then we know

$$\begin{aligned}
\widetilde{E}(\Phi_1) &= \min_{\Phi = (\phi_1, \phi_1)^T \in \mathcal{D}_1} \widetilde{E}(\Phi) \\
&= \min_{\|\phi\|_2 = 1} \int_{\mathbb{R}^d} \left\{\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta_{11} + \beta_{12}}{4}|\phi|^4\right\} d\mathbf{x} - |\lambda|,
\end{aligned} \tag{5.63}$$

and

$$\widetilde{E}(\Phi_2) = \min_{\|\phi\|_2 = 1} \int_{\mathbb{R}^d} \left\{\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta_{11}}{2}|\phi|^4\right\} d\mathbf{x}. \tag{5.64}$$

Since $\beta_{12} > \beta_{11}$, we have

$$\begin{aligned}\Lambda_0 &= \min_{\|\phi\|_2=1} \int_{\mathbb{R}^d} \left\{ \frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta_{11}+\beta_{12}}{4}|\phi|^4 \right\} d\mathbf{x} \\ &\quad - \min_{\|\phi\|_2=1} \int_{\mathbb{R}^d} \left\{ \frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta_{11}}{2}|\phi|^4 \right\} d\mathbf{x} \\ &\quad > 0.\end{aligned}$$

Thus, for $\lambda \in (-\Lambda_0, \Lambda_0)$, $\widetilde{E}(\Phi_1) > \widetilde{E}(\Phi_2)$, which implies that for ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ of (5.12), $|\phi_1^g| \neq |\phi_2^g|$. But under the assumption, we can see that if $\Phi_g = (\phi_1^g, \phi_2^g)^T$ is a ground state of (5.12), then $(\phi_2^g, \phi_1^g)^T$ is also a ground state. So, the minimizer $\Phi_g = (|\phi_1^g|, -\text{sign}(\lambda)|\phi_2^g|)^T$ of (5.12) can not be unique. □

Remark 5.2 *In the above theorem, for ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$, we have $(|\phi_1^g|, |\phi_2^g|)$ is unique under the permutation of subindex.*

Remark 5.3 *When $\delta = \lambda = \sigma = 0$ and $\beta_{11} = \beta_{12} = \beta_{22} \geq 0$, the nonnegative ground state Φ_g of (5.12) is not unique.*

Remark 5.4 *Similar to the results in [38, 40, 57], for any fixed $\beta_{11} \geq 0$ and $\beta_{22} \geq 0$, the phase of two components of the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ will be segregated when $\beta_{12} \to \infty$, i.e. Φ_g will converge to a state such that $\phi_1^g \cdot \phi_2^g = 0$.*

Remark 5.5 *If the potential $V(\mathbf{x})$ in the two equations in (5.1) is chosen different in different equations, i.e. $V_j(\mathbf{x})$ in the jth ($j = 1, 2$) equation, if they satisfy $V_j(\mathbf{x}) \geq 0$, $\lim_{|\mathbf{x}|\to\infty} V_j(\mathbf{x}) = \infty$ ($j = 1, 2$), then the conclusions in the above Lemmas and Theorem 5.1-5.2 are still valid under the similar conditions.*

5.2.2 For the case without optical resonator and Josephson junction, i.e. problem (5.14)

If $\alpha = 0$ or 1 in the nonconvex minimization problem (5.14), it reduces to a single component problem and the results were established in [98]. Thus here we assume $\alpha \in (0, 1)$. Denote

$$\beta'_{11} := \alpha\beta_{11}, \quad \beta'_{22} := (1-\alpha)\beta_{22}, \quad \beta'_{12} := \sqrt{\alpha(1-\alpha)}\beta_{12}, \quad \alpha' := \alpha(1-\alpha).$$

Then the following conclusions can be drawn.

Theorem 5.6 *(Existence and uniqueness of (5.14)) Suppose* $V(\mathbf{x}) \geq 0$ *satisfying* $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ *and at least one of the following condition holds,*

(i) $d = 1$;

(ii) $d = 2$ *and* $\beta'_{11} \geq -C_b$, $\beta'_{22} \geq -C_b$, *and* $\beta'_{12} \geq -\sqrt{(C_b + \beta'_{11})(C_b + \beta'_{22})}$;

(iii) $d = 3$ *and* B *is either positive semi-definite or nonnegative,*

then there exists a ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ *of (5.14). In addition,* $\widetilde{\Phi}_g := (e^{i\theta_1}|\phi_1^g|, e^{i\theta_2}|\phi_2^g|)$ *is also a ground state of (5.14) with two constants* θ_1 *and* θ_2*. Furthermore, if the matrix* B *is positive semi-definite, the ground state* $(|\phi_1^g|, |\phi_2^g|)^T$ *of (5.14) is unique. In contrast, if one of the following conditions holds,*

(i) $d = 2$ *and* $\beta'_{11} < -C_b$ *or* $\beta'_{22} < -C_b$ *or* $\beta'_{12} < -\frac{1}{2\sqrt{\alpha'}}(\alpha\beta'_{11} + (1-\alpha)\beta'_{22} + C_b))$;

(ii) $d = 3$ *and* $\beta_{11} < 0$ *or* $\beta_{22} < 0$ *or* $\beta_{12} < -\frac{1}{2\alpha'}(\alpha^2\beta_{11} + (1-\alpha)^2\beta_{22})$.

there exists no ground states of (5.14).

Proof: The proof is similar to those of Theorems 5.1 and 5.2 and it is omitted here for brevity.

□

5.3 Properties of the ground states

In this section, we will show some properties of the stationary states and find the limiting behavior of the ground states when either $|\lambda| \to \infty$ or $|\delta| \to \infty$.

Theorem 5.7 *Suppose that* $V(\mathbf{x}) \geq 0$ *and* $\beta_{11} = \beta_{12} = \beta_{22} = \sigma = 0$, *for the stationary states of (5.8) under the constraint (5.9), we have*

(i) The ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ *is the global minimizer of* $E(\Phi)$ *over the unit sphere* S.

(ii) Any excited state $\Phi_j = (\phi_1^j, \phi_2^j)^T$ $(j = 1, 2, \ldots)$ *is a saddle point of* $E(\Phi)$ *over the unit sphere* S.

Proof: Let $\Phi_e = (\phi_1^e, \phi_2^e)^T$ be the solution of (5.8) under the constraint (5.9) with $\beta_{11} = \beta_{12} = \beta_{22} = 0$ and μ_e be the corresponding eigenvalue. Obviously, $\|\Phi_e\|_2 = 1$ and $\mu_e = E(\Phi_e)$. For any function $\Phi = (\phi_1, \phi_2)^T$ with $E(\Phi) < \infty$ and $\|\Phi_e + \Phi\|_2 = 1$, we have

$$\begin{aligned}
\|\Phi\|_2^2 &= \|(\Phi_e + \Phi) - \Phi_e\|_2^2 = \|(\phi_1^e + \phi_1) - \phi_1^e\|_2^2 + \|(\phi_2^e + \phi_2) - \phi_2^e\|_2^2 \\
&= \|\Phi_e + \Phi\|_2^2 - \|\Phi_e\|_2^2 - \int_{\mathbb{R}^d} \left[\phi_1^e \bar{\phi}_1 + \bar{\phi}_1^e \phi_1 + \phi_2^e \bar{\phi}_2 + \bar{\phi}_2^e \phi_2\right] d\mathbf{x} \\
&= -\int_{\mathbb{R}^d} \left[\phi_1^e \bar{\phi}_1 + \bar{\phi}_1^e \phi_1 + \phi_2^e \bar{\phi}_2 + \bar{\phi}_2^e \phi_2\right] d\mathbf{x}. \qquad (5.65)
\end{aligned}$$

From (5.11) with $\Psi = \Phi_e + \Phi$, noticing (5.8) and (5.65) and integration by parts, we get

$$\begin{aligned}
E(\Phi_e + \Phi) &= E(\Phi_e) + E(\Phi) + 2\,\mathrm{Re} \int_{\mathbb{R}^d} \left[-\frac{1}{2}\nabla^2 \phi_1^e + (V(\mathbf{x}) + \delta)\phi_1^e + \lambda \phi_2^e\right] \bar{\phi}_1 \, d\mathbf{x} \\
&\quad + 2\,\mathrm{Re} \int_{\mathbb{R}^d} \left[-\frac{1}{2}\nabla^2 \phi_2^e + V(\mathbf{x})\phi_2^e + \lambda \phi_1^e\right] \bar{\phi}_2 \, d\mathbf{x} \\
&= E(\Phi_e) + E(\Phi) + \mu_e \int_{\mathbb{R}^d} \left[\phi_1^e \bar{\phi}_1 + \bar{\phi}_1^e \phi_1 + \phi_2^e \bar{\phi}_2 + \bar{\phi}_2^e \phi_2\right] d\mathbf{x} \\
&= E(\Phi_e) + E(\Phi) - \mu_e \|\Phi\|_2^2 \\
&= E(\Phi_e) + \left[E(\Phi/\|\Phi\|_2) - \mu_e\right] \|\Phi\|_2^2. \qquad (5.66)
\end{aligned}$$

(i) Taking $\Phi_e = \Phi_g$ and $\mu_e = \mu_g$ in (5.66) and noticing $E(\Phi/\|\Phi\|_2) \geq \mu_g$ for any $\Phi \neq 0$, we get immediately that Φ_g is a global minimizer of $E(\Phi)$ over S.

(ii) Taking $\Phi_e = \Phi_j$ and $\mu_e = \mu_j$ in (5.66), since $E(\Phi_g) < E(\Phi_j)$ and it is easy to find an eigenfunction Φ of (5.8) satisfying $\|\Phi\| = 1$ such that $E(\Phi) > E(\Phi_j)$, we get immediately that Φ_j is a saddle point of the energy functional $E(\Phi)$ over S. □

When $|\lambda| \to \infty$ or $|\delta| \to \infty$, we have the following limiting behavior of the ground states of (5.12).

Theorem 5.8 *Suppose $V(\mathbf{x}) \geq 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$ and B is either positive semi-definite or nonnegative. For fixed $V(\mathbf{x})$, B, σ and δ, let $\Phi^\lambda = (\phi_1^\lambda, \phi_2^\lambda)^T$ be a ground state of (5.12) with respect to λ. Then when $|\lambda| \to \infty$, we have*

$$\| \, |\phi_j^\lambda| - \phi^g \|_2 \to 0, \quad j = 1, 2, \qquad E(\Phi^\lambda) \approx 2E_1(\phi^g) - |\lambda|, \qquad (5.67)$$

where ϕ^g is the unique positive minimizer [98] of

$$E_1(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla \phi|^2 + V_1(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4\right] d\mathbf{x} \qquad (5.68)$$

under the constraint

$$\|\phi\|^2 = \|\phi\|_2^2 = \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 \, d\mathbf{x} = \frac{1}{2}, \tag{5.69}$$

with

$$V_1(\mathbf{x}) = V(\mathbf{x}) + \frac{\delta}{2}, \qquad \beta = \frac{\beta_{11} + \beta_{22} + 2\beta_{12}}{2}. \tag{5.70}$$

Proof: Without loss of generality, we assume $\lambda < 0$. In the case of $|\lambda|$ sufficient large, we can assume that the ground states $\Phi^\lambda = (\phi_1^\lambda, \phi_2^\lambda)^T$ satisfy $\phi_j^\lambda \geq 0$, $j = 1, 2$. Since $(\phi^g, \phi^g)^T \in \mathcal{D}_1$, we have

$$\widetilde{E}(\phi_1^\lambda, \phi_2^\lambda) \leq \widetilde{E}(\phi^g, \phi^g). \tag{5.71}$$

Noticing

$$\int_{\mathbb{R}^d} -2|\lambda| \cdot |\phi_1| \cdot |\phi_2| \, d\mathbf{x} = |\lambda| \int_{\mathbb{R}^d} (|\phi_1| - |\phi_2|)^2 - |\lambda|, \tag{5.72}$$

we have

$$\widetilde{E}(\phi^g, \phi^g) = 2E_1(\phi^g) - |\lambda| - \frac{\sigma}{4}. \tag{5.73}$$

Plugging (5.73) into (5.71) and noticing (5.72), there exists a constant $C > 0$ such that

$$\|\phi_1^\lambda\|_{H^1} + \|\phi_2^\lambda\|_{H^1} \leq C, \qquad \|\phi_1^\lambda - \phi_2^\lambda\|_2 \leq \frac{C}{|\lambda|}, \qquad |\lambda| > 0, \tag{5.74}$$

this immediately implies

$$\phi_1^\lambda - \phi_2^\lambda \longrightarrow 0 \text{ in } L^2, \qquad \text{as } |\lambda| \to \infty. \tag{5.75}$$

Using the similar arguments as in the proof of Theorem 5.1, we can see that there exists $\Phi^\infty = (\phi_1^\infty, \phi_2^\infty)^T \in \mathcal{D}_1$ such that

$$\begin{aligned} &\phi_1^\lambda \rightharpoonup \phi_1^\infty, \qquad \phi_2^\lambda \rightharpoonup \phi_2^\infty, \qquad \text{in } L^2 \cap L^4 \cap L_V^2, \\ &\nabla\phi_1^\lambda \rightharpoonup \nabla\phi_1^\infty, \qquad \nabla\phi_2^\lambda \rightharpoonup \nabla\phi_2^\infty, \qquad \text{in } L^2, \end{aligned} \tag{5.76}$$

and

$$\widetilde{E}(\phi_1^\infty, \phi_2^\infty) \leq \liminf_{|\lambda| \to \infty} \widetilde{E}(\phi_1^\lambda, \phi_2^\lambda). \tag{5.77}$$

These together with (5.75) imply that

$$\phi_1^\infty = \phi_2^\infty := \phi^\infty. \tag{5.78}$$

Plugging (5.78) into (5.25), we obtain

$$\begin{aligned}\widetilde{E}(\phi^\infty,\phi^\infty) &= 2E_1(\phi^\infty)-|\lambda|-\frac{\sigma}{4}\le \liminf_{|\lambda|\to\infty}\widetilde{E}(\phi_1^\lambda,\phi_2^\lambda)\le \limsup_{|\lambda|\to\infty}\widetilde{E}(\phi_1^\lambda,\phi_2^\lambda)\\ &\le 2E_1(\phi^g)-|\lambda|-\frac{\sigma}{4},\end{aligned} \tag{5.79}$$

and

$$E_1(\phi^\infty)\le E_1(\phi^g). \tag{5.80}$$

Since ϕ_1^λ and ϕ_2^λ are nonnegative and ϕ_1^λ converges weakly to ϕ^∞ in H^1, there exists a subsequence such that $\phi_1^{\lambda_n}$ converges to ϕ^∞ a.e. in any compact subset, which shows ϕ^∞ is nonnegative. Recalling that $\|\phi^\infty\|^2=\|\Phi^\lambda\|^2/2=1/2$ and ϕ^g is the unique positive minimizer of (5.68) under the constraint (5.69), we conclude that ϕ^∞ must be equal to ϕ^g. Therefore, all inequalities above must hold as equalities. Thus, with (5.75), we can obtain the norm convergence,

$$\begin{aligned}&\|\phi_1^\lambda\|_2\to\|\phi^g\|_2, \qquad \|\phi_2^\lambda\|_2\to\|\phi^g\|_2,\\ &\|\nabla\phi_1^\lambda\|_2\to\|\nabla\phi^g\|_2, \qquad \|\nabla\phi_2^\lambda\|_2\to\|\nabla\phi^g\|_2.\end{aligned} \tag{5.81}$$

Now, the weak convergence and the norm convergence would imply the conclusion since H^1 is a Hilbert space. □

Theorem 5.9 *Suppose $V(\mathbf{x})\ge 0$ satisfying $\lim_{|\mathbf{x}|\to\infty}V(\mathbf{x})=\infty$ and B is either positive semi-definite or nonnegative. For fixed $V(\mathbf{x})$, B, σ and λ, let $\Phi^\delta=(\phi_1^\delta,\phi_2^\delta)^T$ be a ground state of (5.12) with respect to δ. Then when $\delta\to+\infty$, we have*

$$\|\phi_1^\delta\|_2\to 0, \quad \|\,|\phi_2^\delta|-\phi^g\|_2\to 0, \qquad E(\Phi^\delta)\approx E_2(\phi^g), \tag{5.82}$$

and when $\delta\to-\infty$, we have

$$\|\,|\phi_1^\delta|-\phi^g\|_2\to 0, \quad \|\phi_2^\delta\|_2\to 0, \qquad E(\Phi^\delta)\approx E_2(\phi^g)+\delta, \tag{5.83}$$

where ϕ^g is the unique positive minimizer [98] of

$$E_2(\phi)=\int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\phi|^2+V(\mathbf{x})|\phi|^2+\frac{\beta}{2}|\phi|^4\right]d\mathbf{x} \tag{5.84}$$

under the constraint

$$\|\phi\|^2=\|\phi\|_2^2=\int_{\mathbb{R}^d}|\phi|^2\,d\mathbf{x}=1, \tag{5.85}$$

with $\beta=\beta_{22}$ when $\delta>0$, and $\beta=\beta_{11}$ when $\delta<0$.

Proof: Using the fact $(0,\phi^g)^T \in \mathcal{D}_1$ when $\delta > 0$ and $(\phi^g, 0)^T \in \mathcal{D}_1$ when $\delta < 0$, the results can be established by a similar argument as in Theorem 5.8. $\square$

5.4 Numerical methods

In this section, we will propose and analyze efficient and accurate numerical methods for computing the ground states of (5.12) without optical resonator, i.e. $\gamma = \nu = \sigma = 0$. This is motivated by the research of atomic laser, produced by a two-component BEC without optical resonator. In this section and the following sections, we will always assume that there is no optical resonator in (5.1).

5.4.1 Continuous normalized gradient flow and its discretization

In order to compute the ground state of two-component BEC with an internal atomic Josephson junction (5.12), we construct the following continuous normalized gradient flow (CNGF):

$$\begin{aligned}\frac{\partial \phi_1(\mathbf{x},t)}{\partial t} &= \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - \delta - (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\right]\phi_1 - \lambda\phi_2 + \mu_\Phi(t)\phi_1,\\ \frac{\partial \phi_2(\mathbf{x},t)}{\partial t} &= \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\right]\phi_2 - \lambda\phi_1 + \mu_\Phi(t)\phi_2,\end{aligned} \tag{5.86}$$

where $\Phi(\mathbf{x},t) = (\phi_1(\mathbf{x},t), \phi_2(\mathbf{x},t))^T$ and $\mu_\Phi(t)$ is chosen such that the above CNGF is mass or normalization conservative and it is given as

$$\begin{aligned}\mu_\Phi(t) &= \frac{1}{\|\Phi(\cdot,t)\|^2}\int_{\mathbb{R}^d}\left[\frac{1}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) + V(\mathbf{x})(|\phi_1|^2 + |\phi_2|^2) + \delta|\phi_1|^2\right.\\ &\qquad \left. + \beta_{11}|\phi_1|^4 + \beta_{22}|\phi_2|^4 + 2\beta_{12}|\phi_1|^2|\phi_2|^2 + 2\lambda\,\mathrm{Re}(\phi_1\bar{\phi}_2)\right]d\mathbf{x}\\ &= \frac{\mu(\Phi(\cdot,t))}{\|\Phi(\cdot,t)\|^2}, \qquad t \ge 0.\end{aligned} \tag{5.87}$$

For the above CNGF, we have

Theorem 5.10 *For any given initial data*

$$\Phi(\mathbf{x},0) = (\phi_1^0(\mathbf{x}), \phi_2^0(\mathbf{x}))^T := \Phi^{(0)}(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d, \tag{5.88}$$

satisfying $\|\Phi^{(0)}\|^2 = 1$*, the CNGF (5.86) is mass or normalization conservative and energy diminishing, i.e.*

$$\|\Phi(\cdot, t)\|^2 \equiv \|\Phi^{(0)}\|^2 = 1, \qquad E(\Phi(\cdot, t)) \le E(\Phi(\cdot, s)), \qquad 0 \le s \le t. \tag{5.89}$$

Proof: Follow the analogue proofs in [15] for single-component BEC and in [26] for spin-1 BEC. We omitted the details here. □

Using an argument similar to that in [132], when $V(\mathbf{x}) \ge 0$ satisfying $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, B is either positive semi-definite or nonnegative, and $\|\Phi^{(0)}\| = 1$, we may get as $t \to \infty$, $\Phi(\mathbf{x}, t)$ approaches to a steady state solution, which is a critical point of the energy functional $E(\Phi)$ over the unit sphere S or an eigenfunction of the nonlinear eigenvalue problem (5.8) under the constraint (5.9). In addition, when the initial data in (5.88) is chosen properly, e.g. its energy is less than that of the first excited state, the ground state Φ_g can be obtained from the steady state solution of (5.86), i.e.

$$\Phi_g(\mathbf{x}) = \lim_{t\to\infty} \Phi(\mathbf{x}, t), \qquad \mathbf{x} \in \mathbb{R}^d. \tag{5.90}$$

For practical computation, here we also present a second-order in both space and time full discretization for the above CNGF (5.86). For simplicity of notation, we introduce the method for the case of one spatial dimension (1D) in a bounded domain $U = (a, b)$ with homogeneous Dirichlet boundary condition

$$\Phi(a, t) = \Phi(b, t) = 0, \qquad t \ge 0. \tag{5.91}$$

Generalizations to higher dimensions are straightforward for tensor product grids.

Choose time step $k = \Delta t > 0$ and let time steps be $t_n = n\,k = n\,\Delta t$ for $n = 0, 1, 2, \ldots$; and choose spatial mesh size $h = \Delta x > 0$ with $h = (b-a)/M$ for M a positive integer and let the grid points be $x_j = a + j\,h$, $j = 0, 1, 2, \ldots, M$. Let $\Phi_j^n = (\phi_{1,j}^n, \phi_{2,j}^n)^T$ be the numerical approximation of $\Phi(x_j, t_n)$ and Φ^n be the solution vector with component Φ_j^n. In addition, denote $\Phi_j^{n+1/2} = (\phi_{1,j}^{n+1/2}, \phi_{2,j}^{n+1/2})^T$ with

$$\phi_{l,j}^{n+1/2} = \frac{1}{2}\left(\phi_{l,j}^{n+1} + \phi_{l,j}^n\right), \qquad j = 0, 1, 2, \ldots, M, \qquad l = 1, 2. \tag{5.92}$$

Then a second-order full discretization for the CNGF (5.86) is given, for $j = 1, 2, \ldots, M-1$

and $n \geq 0$, as

$$\begin{aligned}
\frac{\phi_{1,j}^{n+1}-\phi_{1,j}^{n}}{k} &= \frac{\phi_{1,j+1}^{n+1/2}-2\phi_{1,j}^{n+1/2}+\phi_{1,j-1}^{n+1/2}}{2h^2} - \left[V(x_j)+\delta-\mu_{\Phi,h}^{n+1/2}\right]\phi_{1,j}^{n+1/2} - \lambda\phi_{2,j}^{n+1/2} \\
&-\frac{1}{2}\left[\beta_{11}\left(|\phi_{1,j}^{n+1}|^2+|\phi_{1,j}^{n}|^2\right)+\beta_{12}\left(|\phi_{2,j}^{n+1}|^2+|\phi_{2,j}^{n}|^2\right)\right]\phi_{1,j}^{n+1/2}, \qquad (5.93)\\
\frac{\phi_{2,j}^{n+1}-\phi_{2,j}^{n}}{k} &= \frac{\phi_{2,j+1}^{n+1/2}-2\phi_{2,j}^{n+1/2}+\phi_{2,j-1}^{n+1/2}}{2h^2} - \left[V(x_j)-\mu_{\Phi,h}^{n+1/2}\right]\phi_{2,j}^{n+1/2} - \lambda\phi_{1,j}^{n+1/2} \\
&-\frac{1}{2}\left[\beta_{12}\left(|\phi_{1,j}^{n+1}|^2+|\phi_{1,j}^{n}|^2\right)+\beta_{22}\left(|\phi_{2,j}^{n+1}|^2+|\phi_{2,j}^{n}|^2\right)\right]\phi_{2,j}^{n+1/2}, \qquad (5.94)
\end{aligned}$$

where

$$\mu_{\Phi,h}^{n+1/2} = \frac{D_{\Phi,h}^{n+1/2}}{h\sum_{j=0}^{M-1}\left(|\phi_{1,j}^{n+1/2}|^2+|\phi_{2,j}^{n+1/2}|^2\right)}, \qquad n \geq 0, \qquad (5.95)$$

with

$$\begin{aligned}
D_{\Phi,h}^{n+1/2} &= h\sum_{j=0}^{M-1}\left\{\sum_{l=1}^{2}\left(\frac{1}{2h^2}|\phi_{l,j+1}^{n+1/2}-\phi_{l,j}^{n+1/2}|^2+V(x_j)|\phi_{l,j}^{n+1/2}|^2\right)+\delta|\phi_{1,j}^{n+1/2}|^2\right. \\
&+\frac{1}{2}\beta_{11}(|\phi_{1,j}^{n+1}|^2|+|\phi_{1,j}^{n}|^2)|\phi_{1,j}^{n+1/2}|^2+\frac{1}{2}\beta_{22}(|\phi_{2,j}^{n+1}|^2+|\phi_{2,j}^{n}|^2)|\phi_{2,j}^{n+1/2}|^2 \\
&+\frac{1}{2}\beta_{12}\left[(|\phi_{2,j}^{n+1}|^2+|\phi_{2,j}^{n}|^2)|\phi_{1,j}^{n+1/2}|^2+(|\phi_{1,j}^{n+1}|^2|+|\phi_{1,j}^{n}|^2)|\phi_{2,j}^{n+1/2}|^2\right] \\
&\left.+2\lambda\ \mathrm{Re}\left(\phi_{1,j}^{n+1/2}\bar{\phi}_{2,j}^{n+1/2}\right)\right\}. \qquad (5.96)
\end{aligned}$$

The boundary condition (5.91) is discretized as

$$\phi_{1,0}^{n+1}=\phi_{1,M}^{n+1}=\phi_{2,0}^{n+1}=\phi_{2,M}^{n+1}=0, \quad n=0,1,2,\ldots. \qquad (5.97)$$

The initial data (5.88) is discretized as

$$\phi_{1,j}^{0}=\phi_1^0(x_j), \qquad \phi_{2,j}^{0}=\phi_2^0(x_j), \qquad j=0,1,\ldots,M. \qquad (5.98)$$

Similarly, for the above full discretization for the CNGF, we have

Theorem 5.11 *For any given time step $k>0$ and mesh size $h>0$ as well as initial data $\Phi^{(0)}$ in (5.88) satisfying $\|\Phi^0\|=1$, the full discretization (5.93)-(5.98) for CNGF (5.86) is mass or normalization conservative and energy diminishing, i.e.*

$$N_{\Phi,h}^{n} := h\sum_{j=0}^{M-1}\sum_{l=1}^{2}|\phi_{l,j}^{n}|^2 \equiv N_{\Phi,h}^{0} := h\sum_{j=0}^{M-1}\sum_{l=1}^{2}|\phi_l^0(x_j)|^2, \qquad n\geq 0, \qquad (5.99)$$

$$E_{\Phi,h}^{n} \leq E_{\Phi,h}^{n-1} \leq \cdots \leq E_{\Phi,h}^{0}, \qquad n \geq 0, \qquad (5.100)$$

where the discretized energy $E^n_{\Phi,h}$ *is defined as*

$$E^n_{\Phi,h} = h\sum_{j=0}^{M-1}\left\{\sum_{l=1}^{2}\left(\frac{1}{2h^2}|\phi^n_{l,j+1}-\phi^n_{l,j}|^2+V(x_j)|\phi^n_{l,j}|^2\right)+\delta|\phi^n_{1,j}|^2 \right.$$
$$\left.+\frac{1}{2}\beta_{11}|\phi^n_{1,j}|^4+\frac{1}{2}\beta_{22}|\phi^n_{2,j}|^4+\beta_{12}|\phi^n_{1,j}|^2|\phi^n_{2,j}|^2+2\lambda\, Re\left(\phi^n_{1,j}\bar{\phi}^n_{2,j}\right)\right\}. \quad (5.101)$$

Proof: Follow the analogous arguments in [26] for spin-1 BEC and we omitted the details here. □

In the above full discretization, at every time step, we need to solve a fully nonlinear system which is very tedious in practical computation. Below we present a more efficient discretization for the CNGF (5.86) for computing the ground states.

5.4.2 Gradient flow with discrete normalization and its discretization

Another more efficient way to discretize the CNGF (5.86) is through the construction of the following gradient flow with discrete normalization (GFDN):

$$\begin{aligned}\frac{\partial\phi_1}{\partial t} &= \left[\frac{1}{2}\nabla^2-V(\mathbf{x})-\delta-(\beta_{11}|\phi_1|^2+\beta_{12}|\phi_2|^2)\right]\phi_1-\lambda\phi_2,\\ \frac{\partial\phi_2}{\partial t} &= \left[\frac{1}{2}\nabla^2-V(\mathbf{x})-(\beta_{12}|\phi_1|^2+\beta_{22}|\phi_2|^2)\right]\phi_2-\lambda\phi_1,\quad t_n\le t<t_{n+1},\end{aligned} \quad (5.102)$$

followed by a projection step as

$$\phi_l(\mathbf{x},t_{n+1}) := \phi_l(\mathbf{x},t^+_{n+1}) = \sigma_l^{n+1}\,\phi_l(\mathbf{x},t^-_{n+1}),\qquad l=1,2,\quad n\ge 0, \quad (5.103)$$

where $\phi_l(\mathbf{x},t^\pm_{n+1}) = \lim_{t\to t^\pm_{n+1}}\phi_l(\mathbf{x},t)$ $(l=1,2)$ and σ_l^{n+1} $(l=1,2)$ are chosen such that

$$\|\Phi(\mathbf{x},t_{n+1})\|^2 = \|\phi_1(\mathbf{x},t_{n+1})\|^2+\|\phi_2(\mathbf{x},t_{n+1})\|^2 = 1,\qquad n\ge 0. \quad (5.104)$$

The above GFDN (5.102)-(5.103) can be viewed as applying the first-order splitting method to the CNGF (5.86) and the projection step (5.103) is equivalent to solve the following ordinary differential equations (ODEs)

$$\frac{\partial\phi_1(\mathbf{x},t)}{\partial t} = \mu_\Phi(t)\phi_1,\qquad \frac{\partial\phi_2(\mathbf{x},t)}{\partial t} = \mu_\Phi(t)\phi_2,\qquad t_n\le t\le t_{n+1}, \quad (5.105)$$

which immediately suggests that the projection constants in (5.103) are chosen as

$$\sigma_1^{n+1} = \sigma_2^{n+1}, \qquad n \geq 0. \tag{5.106}$$

Plugging (5.106) and (5.103) into (5.104), we obtain

$$\sigma_1^{n+1} = \sigma_2^{n+1} = \frac{1}{\|\Phi(\cdot, t_{n+1}^-)\|} = \frac{1}{\sqrt{\|\phi_1(\cdot, t_{n+1}^-)\|^2 + \|\phi_2(\cdot, t_{n+1}^-)\|^2}}, \qquad n \geq 0. \tag{5.107}$$

In fact, the gradient flow (5.102) can be viewed as applying the steepest decent method to the energy functional $E(\Phi)$ in (5.12) without constraints, and (5.103) project the solution back to the unit sphere S. In addition, (5.102) can also be obtained from the CGPEs (5.1) by the change of variable $t \to -i\ t$, that is why this kind of algorithm is usually called as the imaginary time method in physics literatures [9,15,50,126]. From numerical point of view, the GFDN is much easier to discretize since the gradient flow (5.102) can be solved via traditional techniques and the normalization (5.104) is simply achieved by a projection (5.103) at the end of each time step.

For the above GFDN, we have

Theorem 5.12 *Suppose $V(\mathbf{x}) \geq 0$ and $\beta_{11} = \beta_{12} = \beta_{22} = 0$, then for any time step $k > 0$ and initial data $\Phi^{(0)}$ in (5.88) satisfying $\|\Phi^{(0)}\| = 1$, the GFDN (5.102)-(5.103) is energy diminishing, i.e.*

$$E(\Phi(\cdot, t_{n+1})) \leq E(\Phi(\cdot, t_n) \leq \cdots \leq E(\Phi(\cdot, 0)) = E(\Phi^0), \qquad n = 0, 1, 2, \dots\ . \tag{5.108}$$

Proof: Follow the analogous arguments in [15] for single-component BEC and we omit the details here. □

Again, for practical computation, here we also present a modified backward Euler finite difference (MBEFD) discretization for the above GFDN (5.102)-(5.103) in a bounded domain $U=(a,b)$ with homogeneous Dirichlet boundary condition (5.91):

$$\begin{aligned}
\frac{\phi_{1,j}^{*}-\phi_{1,j}^{n}}{k} &= \frac{1}{2h^2}\left[\phi_{1,j+1}^{*}-2\phi_{1,j}^{*}+\phi_{1,j-1}^{*}\right]-\left[\left(V(x_j)+\delta+\alpha\right]\phi_{1,j}^{*}-\lambda\phi_{2,j}^{*}\right. \\
&\quad -\left(\beta_{11}|\phi_{1,j}^{n}|^2+\beta_{12}|\phi_{2,j}^{n}|^2\right)\phi_{1,j}^{*}+\alpha\phi_{1,j}^{n}, \quad 1\le j\le M-1, \\
\frac{\phi_{2,j}^{*}-\phi_{2,j}^{n}}{k} &= \frac{1}{2h^2}\left[\phi_{2,j+1}^{*}-2\phi_{2,j}^{n}+\phi_{2,j-1}^{*}\right]-\left[V(x_j)+\alpha\right]\phi_{1,j}^{*}-\lambda\phi_{1,j}^{*} \qquad (5.109)\\
&\quad -\left(\beta_{12}|\phi_{1,j}^{n}|^2+\beta_{22}|\phi_{2,j}^{n}|^2\right)\phi_{2,j}^{*}+\alpha\phi_{2,j}^{n}, \quad 1\le j\le M-1, \\
\phi_{l,j}^{n+1} &= \frac{\phi_{l,j}^{*}}{\|\Phi^*\|_h}, \qquad j=0,1,\ldots,M, \quad n\ge 0, \quad l=1,2;
\end{aligned}$$

where $\alpha\ge 0$ is a stabilization parameter chosen such that the time step k is independent of the internal atomic Josephson junction λ and

$$\|\Phi^*\|_h := \sqrt{h\sum_{j=1}^{M-1}\left[|\phi_{1,j}^{*}|^2+|\phi_{2,j}^{*}|^2\right]}. \qquad (5.110)$$

The initial and boundary conditions are discretized similarly as those for CNGF.

For the above full discretization for the GFDN, we have

Theorem 5.13 *Suppose $V(\mathbf{x})\ge 0$ and $\beta_{11}=\beta_{12}=\beta_{22}=0$, if $\alpha\ge|\lambda|+\max(0,-\delta)$, then the MBEFD discretization (5.109) is energy diminishing for any time step $k>0$ and initial data $\Phi^{(0)}$ satisfying $\|\Phi^{(0)}\|_h=1$, i.e.*

$$E_{\Phi,h}^{n+1}\le E_{\Phi,h}^{n}\le\cdots\le E_{\Phi,h}^{0}=E_{\Phi^{(0)},h}, \qquad n\ge 0, \qquad (5.111)$$

where the discretized energy $E_{\Phi,h}^{n}$ is defined in (5.101) with $\beta_{11}=\beta_{12}=\beta_{22}=0$.

Proof: Denote

$$\begin{aligned}
&\Phi^n=(\phi_{1,1}^n,\phi_{1,2}^n,\ldots,\phi_{1,M-1}^n,\phi_{2,1}^n,\phi_{2,2}^n,\ldots,\phi_{2,M-1}^n)^T,\\
&F=\mathrm{diag}(V(x_1),V(x_2),\ldots,V(x_{M-1}),V(x_1),V(x_2),\ldots,V(x_{M-1})),\\
&D=\begin{pmatrix} G & 0\\ 0 & G\end{pmatrix}, \quad D_1=\begin{pmatrix}\delta I_{M-1} & \lambda I_{M-1}\\ \lambda I_{M-1} & 0\end{pmatrix}, \quad D_2=\begin{pmatrix}(\alpha+\delta)I_{M-1} & \lambda I_{M-1}\\ \lambda I_{M-1} & \alpha I_{M-1}\end{pmatrix},
\end{aligned}$$

where I_{M-1} is the $(M-1)\times(M-1)$ identity matrix and G is an $(M-1)\times(M-1)$ tridiagonal matrix with $1/h^2$ at the diagonal entries and $-1/2h^2$ at the off-diagonal entries. Let

$$T=D+F+D_2=D+F+D_1+\alpha I_{2M-2}. \qquad (5.112)$$

When $\beta_{11} = \beta_{12} = \beta_{22} = 0$, the MBEFD discretization (5.109) reads

$$\begin{aligned}
&\frac{\Phi^* - \Phi^n}{k} = -(D + F + D_2)\Phi^* + \alpha\Phi^n = -T\Phi^* + \alpha\Phi^n, \\
&\Phi^{n+1} = \frac{\Phi^*}{\|\Phi^*\|_h}, \quad n \geq 0,
\end{aligned} \tag{5.113}$$

and the discretized energy $E^n_{\Phi,h}$ in (5.101) with $\beta_{11} = \beta_{12} = \beta_{22} = 0$ can be written as

$$E^n_{\Phi,h} = h(\Phi^n)^T(D + F + D_1)\bar{\Phi}^n = h\,(\Phi^n, T\Phi^n) - \alpha\|\Phi^n\|^2_h, \tag{5.114}$$

where $(\cdot, \cdot)$ is the standard inner product. From (5.113), we have

$$(I + k\,T)\Phi^* = (1 + \alpha\,k)\Phi^n, \qquad n \geq 0. \tag{5.115}$$

If $\alpha \geq |\lambda| + \max(0, -\delta)$, then T is positive semi-definite, notice (5.114) and (5.115), using Lemma 2.8 in [15], we get

$$\begin{aligned}
E^{n+1}_{\Phi,h} - \alpha\|\Phi^{n+1}\|^2_h &= h(\Phi^{n+1}, T\Phi^{n+1}) = \frac{(\Phi^*, T\Phi^*)}{(\Phi^*, \Phi^*)} \leq \frac{((1+k\alpha)\Phi^n, (1+k\alpha)T\Phi^n)}{((1+k\alpha)\Phi^n, (1+k\alpha)\Phi^n)} \\
&= h(\Phi^n, T\Phi^n) = E^n_{\Phi,h} - \alpha\|\Phi^n\|^2_h, \qquad n \geq 0.
\end{aligned} \tag{5.116}$$

Thus the conclusion follows immediately from the above inequality and the fact that $\|\Phi^n\|_h = \|\Phi^{n+1}\|_h = 1$. □

In fact, when $\alpha = 0$, the MBEFD discretization (5.109) collapses to the standard backward Euler finite difference scheme [15]. In addition, from the proof in the above Theorem, in practical computation, we can choose $\alpha = |\lambda| + \max(0, -\delta)$.

5.5 Numerical results

In this section, we will report the ground states of (5.12) in 1D computed by our numerical method MBEFD (5.109). In our computation, the ground state is reached when $\|\Phi^{n+1} - \Phi^n\| \leq \varepsilon := 10^{-7}$. In addition, for ground state of two-component BEC with an internal atomic Josephson junction (5.12), we have $\lambda \leftrightarrow -\lambda \iff \phi^g_2 \leftrightarrow -\phi^g_2$, and thus we only present results for $\lambda \leq 0$.

Example 1. Ground states of two-component BEC with an internal atomic Josephson junction when B is positive definite, i.e. we take $d = 1$, $V(x) = \frac{1}{2}x^2$ and $\beta_{11} : \beta_{12} : \beta_{22} =$

$(1 : 0.94 : 0.97)\beta$ in (5.12) [9, 87, 88]. In this case, since $\lambda \le 0$ and B is positive definite when $\beta > 0$, thus we know that the positive ground state $\Phi_g = (\phi_1, \phi_2)^T$ is unique. In our computations, we take the computational domain $U = [-16, 16]$ with mesh size $h = \frac{1}{32}$ and time step $k = 0.1$. The initial data in (5.88) is chosen as

$$\phi_1^0(x) = \phi_2^0(x) = \frac{1}{\pi^{1/4}\sqrt{2}} e^{-x^2/2}, \qquad x \in \mathbb{R}. \tag{5.117}$$

In fact, we have checked with other types of initial data in (5.88) and the computed ground state is the same.

Fig. 5.1 plots the ground states Φ_g when $\delta = 0$ and $\lambda = -1$ for different β, and Fig. 5.2 depicts similar results when $\delta = 0$ and $\beta = 100$ for different $\lambda \le 0$. Fig. 5.3 shows mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states when $\delta = 0$ for different λ and β. Fig. 5.4 shows similar results when $\beta = 100$ and $\delta = 0, 1$ for different λ, and Fig. 5.5 for results when $\beta = 100$ and $\lambda = 0, -5$ for different δ.

From Figs. 5.1-5.5 and additional numerical results not shown here for brevity, we can draw the following conclusions for the ground states in this case: (i) the positive ground state is unique when at least one of the parameters β, λ and δ is nonzero which confirm the results in Theorem 5.1 (cf. Figs. 5.1 & 5.2); (ii) when $\beta = 0$ and $\delta = 0$, $\phi_1 = \phi_2$ when $\lambda < 0$, and $\phi_1 = -\phi_2$ when $\lambda > 0$ (cf. Fig. 5.1); (iii) for fixed β and δ, when $\lambda \to -\infty$, $\phi_1 - \phi_2 \to 0$ and when $\lambda \to +\infty$, $\phi_1 + \phi_2 \to 0$ (cf. Fig. 5.2) which confirm the analytical results in Theorem 5.8; (iv) when $\delta = 0$, $N(\phi_1)$ decreases and $N(\phi_2)$ increases when $\lambda \ne 0$ (cf. Fig. 5.3) which is due to $\beta_{11} > \beta_{22}$; (v) for fixed δ and λ, when $\beta \gg 1$, $E = O(\beta^{1/3})$ and $\mu = O(\beta^{1/3})$ which can be confirmed by a re-scaling $\mathbf{x} \to \varepsilon^{1/2}\mathbf{x}$ and $\Phi \to \varepsilon^{-d/4}\Phi$ with $\varepsilon = \beta^{-d/(d+2)}$ in the energy functional $E(\Phi)$ in (5.11) and the chemical potential $\mu(\Phi)$ in (5.10) [10, 167]; (vi) for fixed $\beta > 0$ and δ, when $|\lambda| \to \infty$, then $N(\phi_1) - N(\phi_2) \to 0$, $E \approx -|\lambda| + C_1$ and $\mu \approx -|\lambda| + C_2$ with C_1 and C_2 two constants independent of λ (cf. Fig. 5.4) which confirm the analytical results in Theorem 5.8; (vii) for fixed $\beta > 0$ and λ, when $\delta \to +\infty$, $N(\phi_1) \to 0$, $N(\phi_2) \to 1$, $E \approx C_3$ and $\mu \approx C_4$ with C_3 and C_4 two constants independent of δ; and when $\delta \to -\infty$, $N(\phi_1) \to 1$, $N(\phi_2) \to 0$, $E \approx \delta + C_5$ and $\mu \approx \delta + C_6$ with C_5 and C_6 two constants independent of δ (cf. Fig. 5.5) which confirm the results in Theorem 5.9. In addition, when $\delta = 0$ and $\lambda = 0$, $N(\phi_1) = 1/3$ and $N(\phi_2) = 2/3$ which are independent of β (cf. Fig. 5.3). In fact, in this case, the energy functional can be written as

$$E(\Phi) = \int_U \left[\frac{1}{2}\left(|\nabla\phi_1|^2 + |\nabla\phi_2|^2\right) + V(\mathbf{x})\left(|\phi_1|^2 + |\phi_2|^2\right) + \frac{\beta}{2}\left(|\phi_1|^4 + 0.97|\phi_2|^4 + 2\times 0.94|\phi_1|^2|\phi_2|^2\right)\right] d\mathbf{x}. \quad (5.118)$$

Denote $\rho(\mathbf{x}) = \sqrt{|\phi_1(\mathbf{x})|^2 + |\phi_2(\mathbf{x})|^2}$, using the Cauchy inequality, we have

$$\begin{aligned} E(\Phi) &\geq \int_U \left[\frac{1}{2}|\nabla\rho|^2 + V(\mathbf{x})|\rho|^2 + \frac{0.94\beta}{2}|\rho|^4 + \frac{\beta}{2}\left(0.06|\phi_1|^4 + 0.03|\phi_2|^4\right)\right] d\mathbf{x} \\ &\geq \int_U \left[\frac{1}{2}|\nabla\rho|^2 + V(\mathbf{x})|\rho|^2 + \frac{0.94\beta}{2}|\rho|^4 + \frac{0.02\beta}{2}|\rho|^4\right] d\mathbf{x}, \end{aligned}$$

and the above equality holds only if $2|\phi_1|^2 = |\phi_2|^2$. Notice that the functional $E_2(\rho) = \int_U \left(\frac{1}{2}|\nabla\rho|^2 + V(\mathbf{x})|\rho|^2 + \frac{0.96\beta}{2}|\rho|^4\right) d\mathbf{x}$ admits a unique positive minimizer ρ_g under constraint $\|\rho\|_2 = 1$ [98], then $\Phi_g = (\sqrt{1/3}\rho_g, \sqrt{2/3}\rho_g)^T$ is a ground state of the original problem, which justifies our numerical observation in Fig. 2.4.

Example 2. Ground states of two-component BEC with an internal atomic Josephson junction when B is nonnegative, i.e. we take $d = 1$, $V(x) = \frac{1}{2}x^2 + 24\cos^2(x)$ and $\beta_{11} : \beta_{12} : \beta_{22} = (1.03 : 1 : 0.97)\beta$ in (5.12) [9, 74, 75]. In our computations, we take the computational domain $U = [-16, 16]$ with mesh size $h = \frac{1}{32}$ and time step $k = 0.1$.

Fig. 5.6 plots the ground states Φ_g when $\delta = 0$ and $\lambda = -1$ for different β, and Fig. 5.7 depicts similar results when $\delta = 0$ and $\beta = 100$ for different λ. Fig. 5.8 shows mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states when $\delta = 0$ for different λ and β.

From Figs. 5.6-5.8 and additional numerical results not shown here for brevity, same conclusions as those in (ii)-(vii) in **Example 1** can be drawn. Moreover, the numerical results show that the positive ground state is unique in this case. Due to the appearance of the optical lattice potential $24\cos^2(x)$ in the trapping potential $V(x)$, there are several peaks in the ground state and the distance between two nearby peaks is roughly as π which is the period of the optical lattice potential (cf. Figs. 5.6-5.7). In addition, when $\delta = 0$, $\lambda = 0$, $N(\phi_1) = 0$ and $N(\phi_2) = 1$ are independent of β (cf. Fig. 5.8), which can be explained by Theorem 5.4.

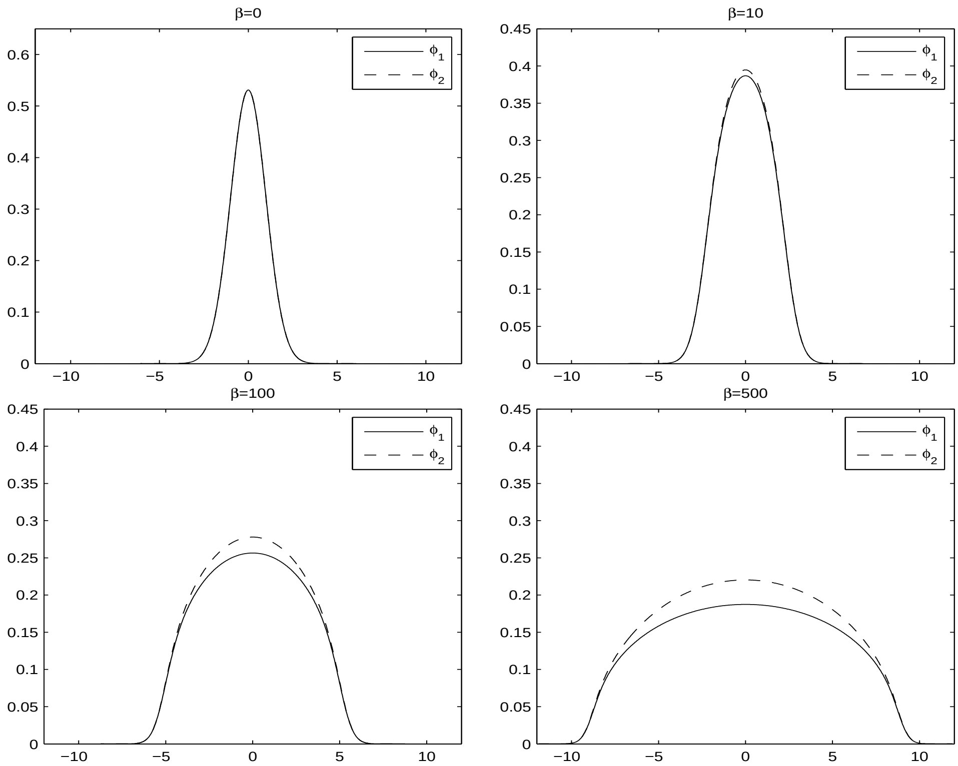

Figure 5.1: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in **Example 1** when $\delta = 0$ and $\lambda = -1$ for different β.

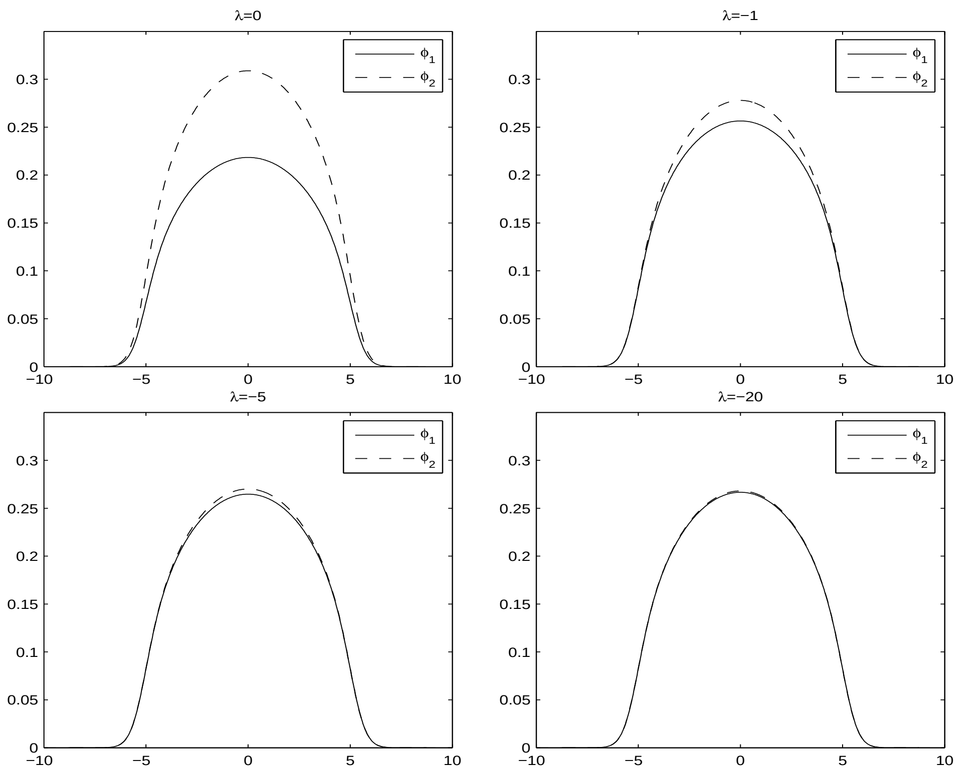

Figure 5.2: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in **Example 1** when $\delta = 0$ and $\beta = 100$ for different λ.

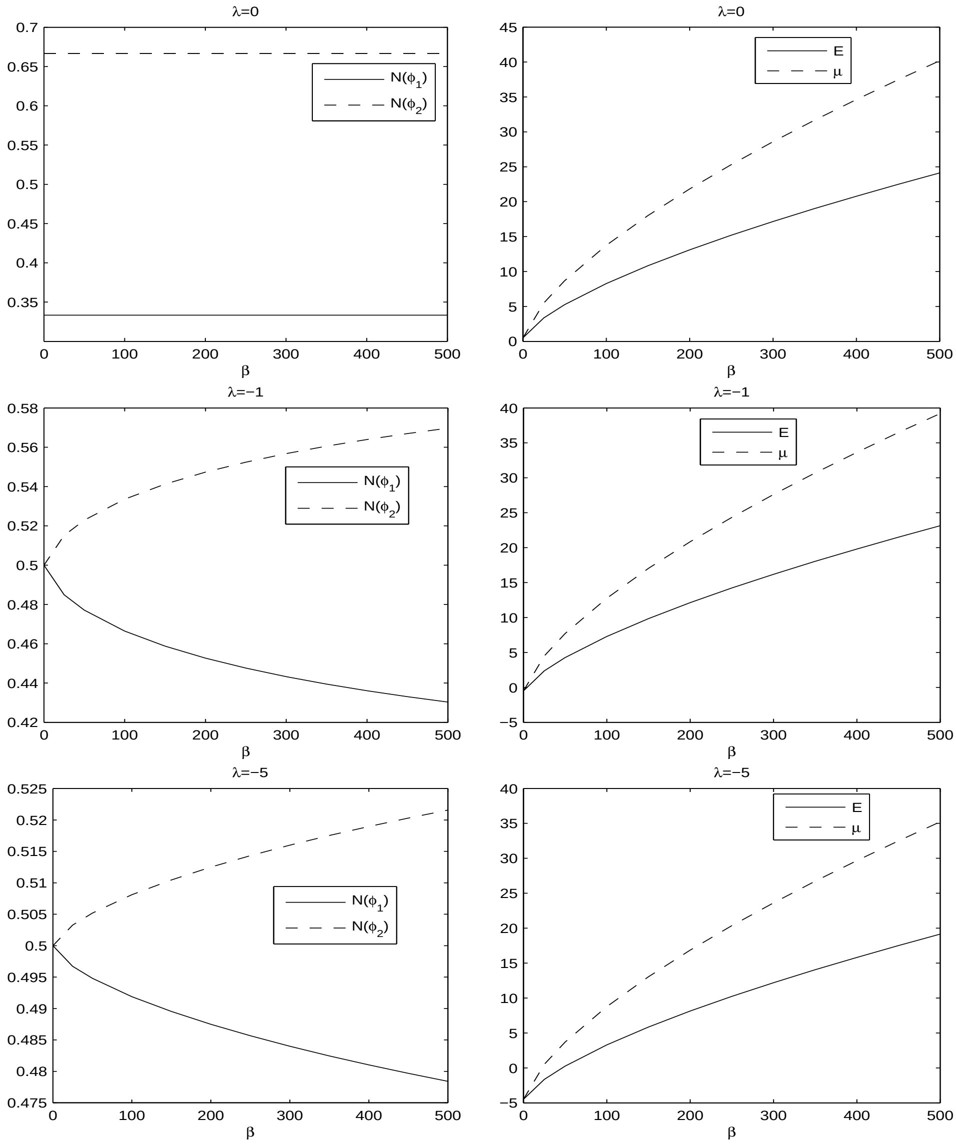

Figure 5.3: Mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states in **Example 1** when $\delta = 0$ for different λ and β.

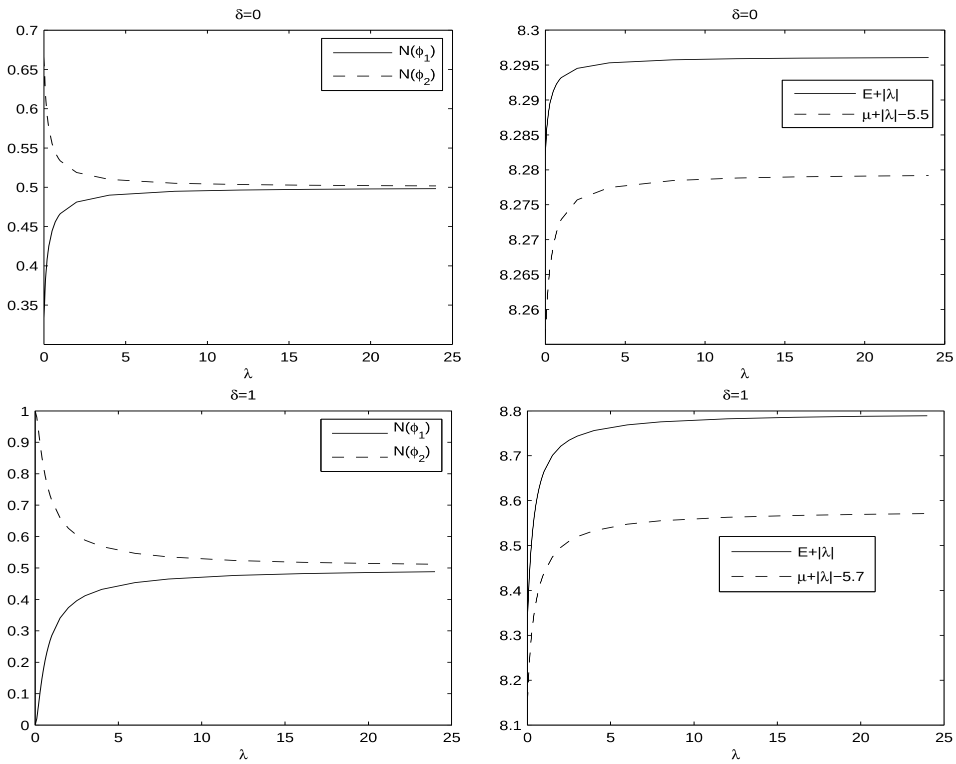

Figure 5.4: Mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states in **Example 1** when $\beta = 100$ and $\delta = 0, 1$ for different λ.

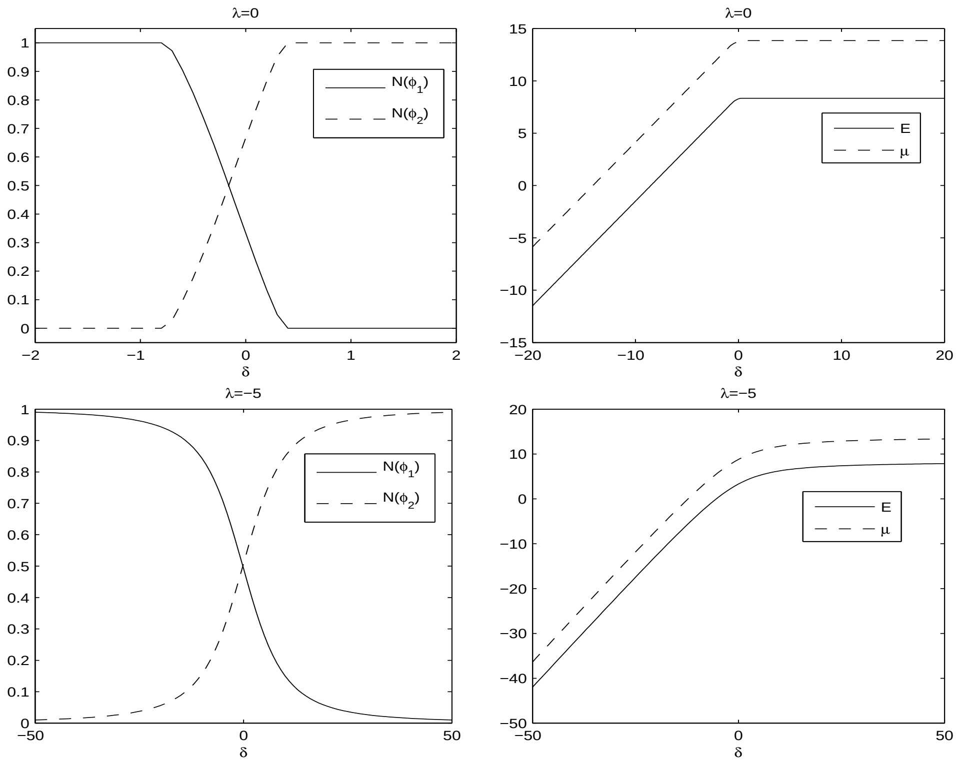

Figure 5.5: Mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states in **Example 1** when $\beta = 100$ and $\lambda = 0, -5$ for different δ.

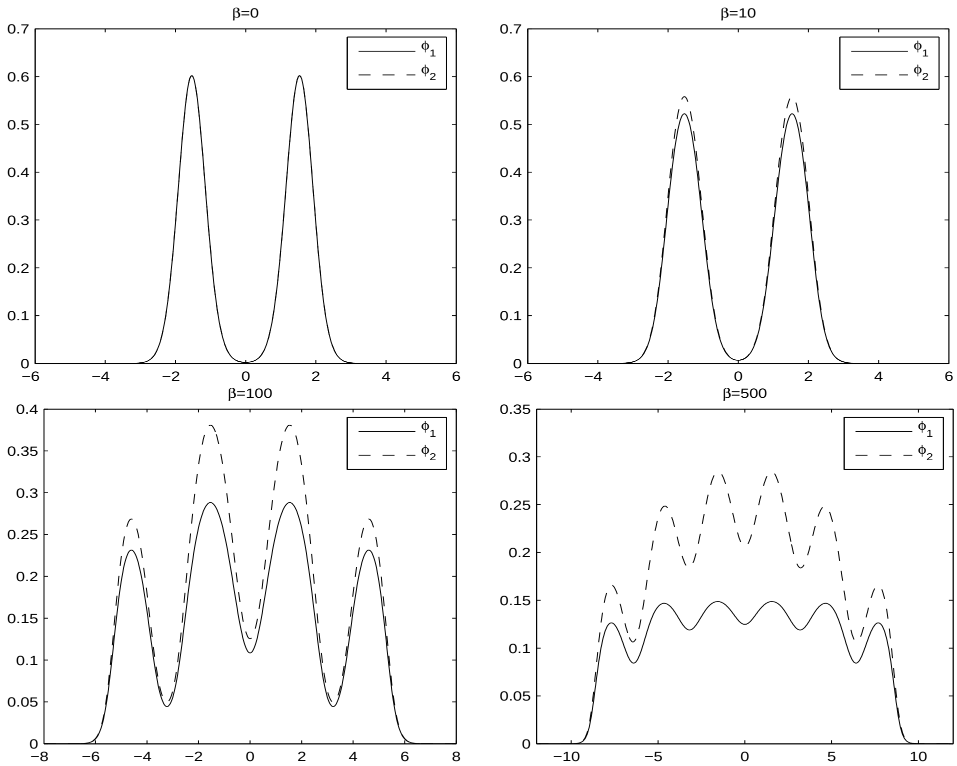

Figure 5.6: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in **Example 2** when $\delta = 0$ and $\lambda = -1$ for different β.

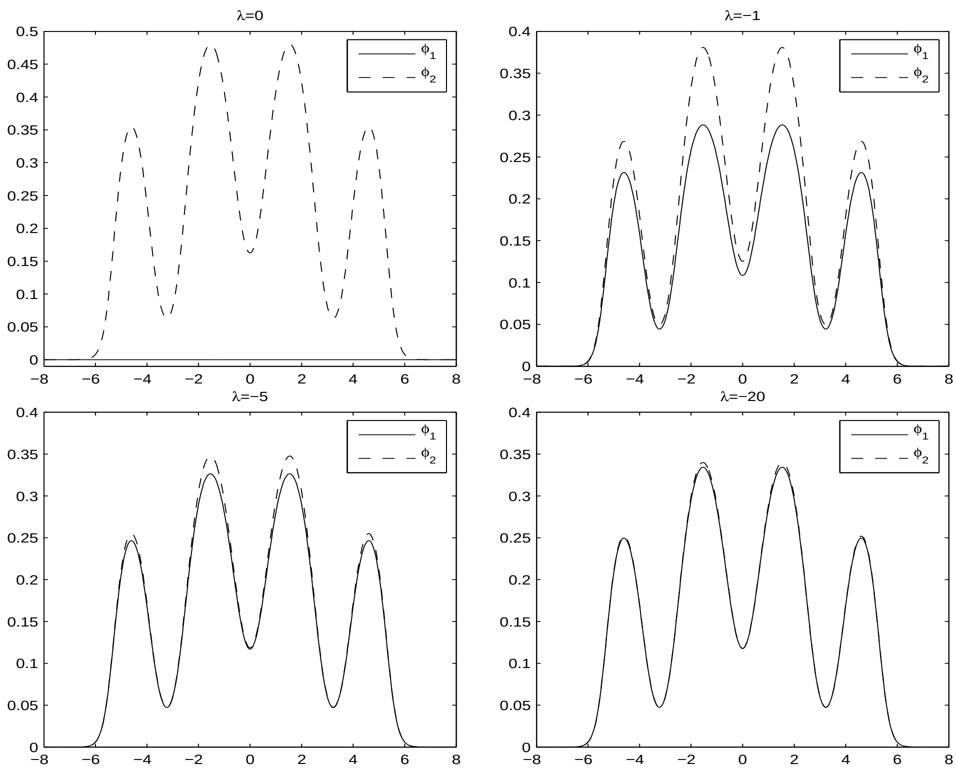

Figure 5.7: Ground states $\Phi_g = (\phi_1, \phi_2)^T$ in **Example 2** when $\delta = 0$ and $\beta = 100$ for different λ.

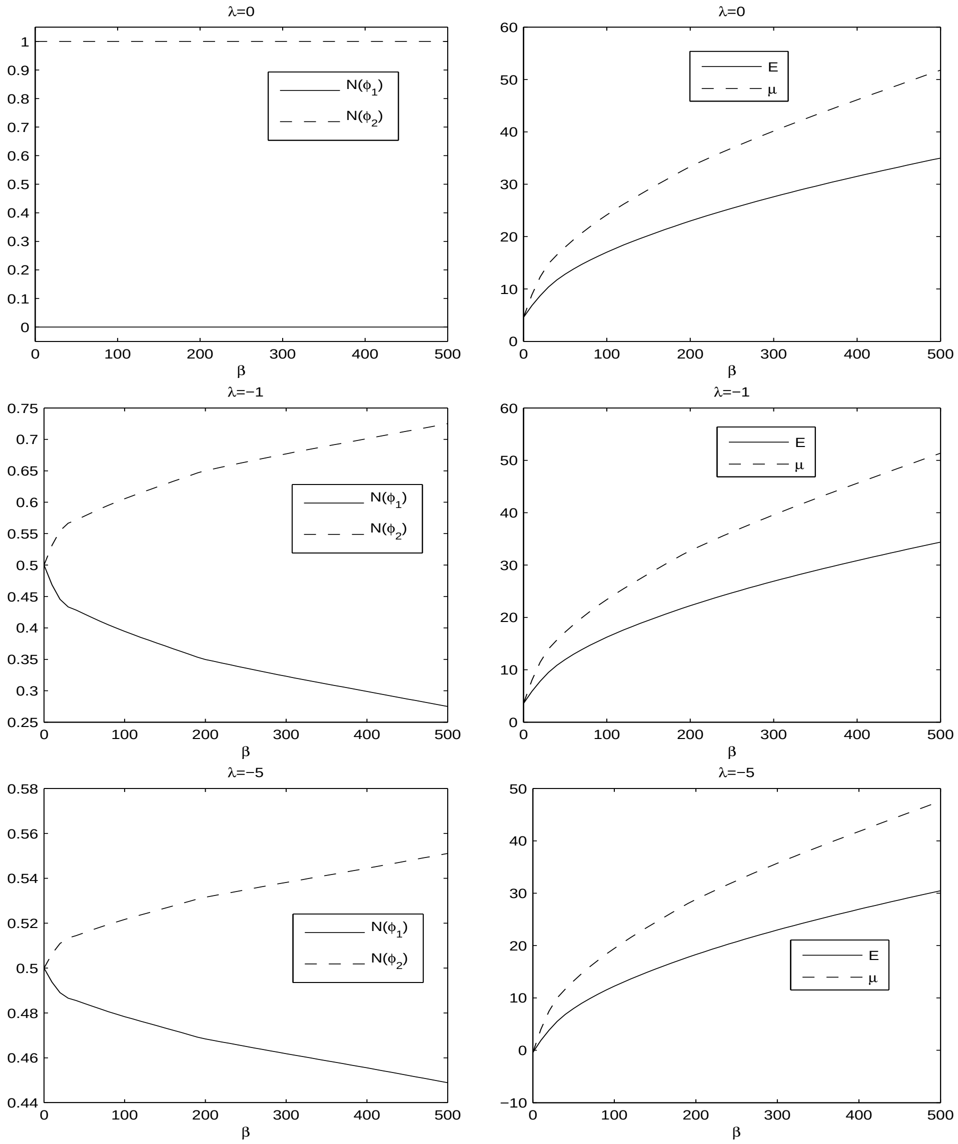

Figure 5.8: Mass of each component $N(\phi_j) = \|\phi_j\|^2$ $(j = 1, 2)$, energy $E := E(\Phi_g)$ and chemical potential $\mu := \mu(\Phi_g)$ of the ground states in **Example 2** when $\delta = 0$ for different λ and β.

Chapter 6

Optimal error estimates of finite difference methods for the Gross-Pitaevskii equation with angular momentum rotation

In this chapter, we prove the convergence rates of finite difference methods applied to the GPE with rotational frame in two and three dimensions (2D and 3D). Optimal convergence rates will be established for both the conservative Crank-Nicolson finite difference method and the nonconservative semi-implicit finite difference method.

6.1 The equation

Recalling equation (1.12), the Gross-Pitaevskii equation (GPE) with an angular momentum rotation term in d-dimensions ($d = 2, 3$) for modeling a rotating Bose-Einstein condensate (BEC) [4, 20, 117] reads as

$$i\partial_t\psi(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) - \Omega L_z + \beta|\psi(\mathbf{x},t)|^2\right]\psi(\mathbf{x},t), \quad \mathbf{x} \in U \subset \mathbb{R}^d,\ t > 0, \tag{6.1}$$

with the homogeneous Dirichlet boundary condition

$$\psi(\mathbf{x},t) = 0, \qquad \mathbf{x} \in \Gamma = \partial U, \quad t \geq 0, \tag{6.2}$$

and initial condition

$$\psi(\mathbf{x},0) = \psi_0(\mathbf{x}), \qquad \mathbf{x} \in U. \tag{6.3}$$

Here $\mathbf{x} = (x, y)$ in two dimensions (2D), i.e. $d = 2$, and resp. $\mathbf{x} = (x, y, z)$ in three dimensions (3D), i.e. $d = 3$, are the cartesian coordinates, U is a bounded computational domain, $\psi := \psi(\mathbf{x}, t)$ is the complex-valued wave function, Ω is a dimensionless constant corresponding to the angular speed of the laser beam in experiments, β is a dimensionless constant characterizing the interaction between particles in the rotating BEC. $V(\mathbf{x})$ is a real-valued function corresponding to the external trap potential and it is chosen as a harmonic potential, i.e. a quadratic polynomial, in most experiments. L_z is the z-component of the angular momentum defined as (1.13) or equivalently as

$$L_z = -i\partial_\theta, \tag{6.4}$$

where (r, θ) and (r, θ, z) are the polar coordinates in 2D and cylindrical coordinates in 3D, respectively. In fact, GPE (6.1) conserves the total *mass*

$$N(\psi(\cdot, t)) := \int_U |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} \equiv N(\psi(\cdot, 0)) = N(\psi_0), \qquad t \geq 0, \tag{6.5}$$

and the *energy*

$$E(\psi(\cdot, t)) := \int_U \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{1}{2}\beta|\psi|^4 - \Omega\bar{\psi}L_z\psi\right] d\mathbf{x} \equiv E(\psi_0), \qquad t \geq 0. \tag{6.6}$$

Because of the observation of quantized vortices in rotating BEC [2, 41, 106] which is related to superfluidity, theoretical studies of BEC and quantized vortices based on the above GPE have stimulated great research interests in quantum physics and computational mathematics communities. For mathematical analysis of the above GPE, well-posedness of the equation can be found in [43, 76, 77, 97] and references therein. For the numerical methods, as introduced in chapter 1, different efficient and accurate numerical methods including the time-splitting pseudospectral method [23, 78, 121, 142], finite difference method [3, 5], and Runge-Kutta or Crank-Nicolson pseudospectral method [41, 55] have been developed for the GPE without the angular momentum rotation term, i.e. $\Omega = 0$. For $\Omega \neq 0$, efficient numerical methods also have been developed [16, 25, 27].

Error estimates for different numerical methods of NLSE, e.g. the GPE (6.1) without the angular momentum rotation ($\Omega = 0$) and/or $d = 1$, have been established in the literatures. For the analysis of splitting error of the time-splitting or split-step method for NLSE, we refer to [32, 54, 103, 110, 143] and references therein. For the error estimates of the implicit Runge-Kutta finite element method for NLSE, we refer to [6, 114]. Error bounds of conservative Crank-Nicolson finite difference (CNFD) method for NLSE in 1D was established in [46,67]. In fact, their proofs for CNFD rely strongly on the conservative property of the method and the discrete version of the Sobolev inequality in 1D

$$\|f\|_{L^\infty}^2 \leq \|\nabla f\|_{L^2} \cdot \|f\|_{L^2}, \qquad \forall f \in H^1(U) \text{ with } U \subset \mathbb{R},$$

which immediately imply *a priori* uniform bound for $\|f\|_{L^\infty}$. However, the extension of the discrete version of the above Sobolev inequality is no longer valid in 2D and 3D. Thus the techniques used in [46, 67] for obtaining error bounds of CNFD for NLSE only work for conservative schemes in 1D and they cannot be extended to either high dimensions or non-conservative finite difference schemes. To our knowledge, no error estimates are available in the literatures of finite difference methods for NLSE either in high dimensions or for non-conservative scheme. However, the GPE with the angular momentum rotation is either in 2D or 3D [16, 20, 25, 117]. Here, we are going to use different techniques to establish optimal error bounds of CNFD and semi-implicit finite difference (SIFD) method for the GPE (6.1) with the angular momentum rotation in 2D and 3D. Based on our results, both CNFD and SIFD have the same second-order convergence rate in space and time. In our analysis, besides the standard techniques of the energy method, for SIFD, we adopt the mathematical induction; for CNFD, we first derive the l^2-norm error estimate and then obtain *a priori* bound of the numerical solution in the l^∞-norm by using the inverse inequality.

In this chapter and the next chapter, we denote C a generic constant which is independent of mesh size h and time step τ, and use the notation $p \lesssim q$ to represent that there exists a generic constant C which is independent of time step τ and mesh size h such that $|p| \leq C\, q$.

6.2 Finite difference methods and main results

In this section, we introduce SIFD and CNFD methods for the GPE (6.1) in 2D on a rectangle $U = [a, b] \times [c, d]$, and resp. in 3D on a cube $U = [a, b] \times [c, d] \times [e, f]$, and state our main error estimate results.

6.2.1 Numerical methods

For the simplicity of notation, we only present the methods in 2D, i.e. $d = 2$ and $U = [a, b] \times [c, d]$ in (6.1). Extensions to 3D are straightforward, and the error estimates in l^2-norm and discrete H^1-norm are the same in 2D and 3D. Choose time step $\tau := \Delta t$ and denote time steps as $t_n := n\,\tau$ for $n = 0, 1, 2, \ldots$; choose mesh sizes $\Delta x := \frac{b-a}{M}$ and $\Delta y := \frac{d-c}{K}$ with M and K two positive integers and denote $h := h_{\max} = \max\{\Delta x,\ \Delta y\}$ and grid points as

$$x_j := a + j\,\Delta x, \quad j = 0, 1, \ldots, M; \qquad y_k := c + k\,\Delta y, \quad k = 0, 1, \ldots, K.$$

Define the index sets

$$\mathcal{T}_{MK} = \{(j,k) \mid j = 1, 2, \ldots, M-1,\ k = 1, 2, \ldots, K-1\},$$
$$\mathcal{T}^0_{MK} = \{(j,k) \mid j = 0, 1, 2 \ldots, M,\ k = 0, 1, 2 \ldots, K\}.$$

Let ψ^n_{jk} be the numerical approximation of $\psi(x_j, y_k, t_n)$ for $(j,k) \in \mathcal{T}^0_{MK}$ and $n \geq 0$ and denote $\psi^n \in \mathbb{C}^{(M+1)\times(K+1)}$ be the numerical solution at time $t = t_n$. Introduce the following finite difference operators:

$$\delta^+_x \psi^n_{jk} = \frac{1}{\Delta x}(\psi^n_{j+1\,k} - \psi^n_{jk}), \quad \delta^+_y \psi^n_{jk} = \frac{1}{\Delta y}(\psi^n_{j\,k+1} - \psi^n_{jk}), \quad \delta^+_t \psi^n_{jk} = \frac{1}{\tau}(\psi^{n+1}_{jk} - \psi^n_{jk}),$$
$$\delta^-_x \psi^n_{jk} = \frac{1}{\Delta x}(\psi^n_{jk} - \psi^n_{j-1\,k}), \quad \delta^-_y \psi^n_{jk} = \frac{1}{\Delta y}(\psi^n_{jk} - \psi^n_{j\,k-1}), \quad \delta^-_t \psi^n_{jk} = \frac{1}{\tau}(\psi^n_{jk} - \psi^{n-1}_{jk}),$$
$$\delta_x \psi^n_{jk} = \frac{\psi^n_{j+1\,k} - \psi^n_{j-1\,k}}{2\,\Delta x}, \quad \delta_y \psi^n_{jk} = \frac{\psi^n_{j\,k+1} - \psi^n_{j\,k-1}}{2\,\Delta y}, \quad \delta_t \psi^n_{jk} = \frac{\psi^{n+1}_{jk} - \psi^{n-1}_{jk}}{2\tau},$$
$$\delta^2_x \psi^n_{jk} = \frac{\psi^n_{j+1\,k} - 2\psi^n_{jk} + \psi^n_{j-1\,k}}{(\Delta x)^2}, \quad \delta^2_y \psi^n_{jk} = \frac{\psi^n_{j\,k+1} - 2\psi^n_{jk} + \psi^n_{j\,k-1}}{(\Delta y)^2}, \quad (j,k) \in \mathcal{T}_{MK},$$
$$\delta^+_\nabla \psi^n_{jk} = (\delta^+_x \psi^n_{jk}, \delta^+_y \psi^n_{jk}), \quad \delta^2_\nabla \psi^n_{jk} = \delta^2_x \psi^n_{jk} + \delta^2_y \psi^n_{jk}, \quad L^h_z \psi^n_{jk} = -i(x_j \delta_y \psi^n_{jk} - y_k \delta_x \psi^n_{jk}).$$

Then the *conservative Crank-Nicolson finite difference* (CNFD) discretization of the GPE (6.1) reads

$$i\delta^+_t \psi^n_{jk} = \big[-\frac{1}{2}\delta^2_\nabla + V_{jk} - \Omega L^h_z + \frac{\beta}{2}(|\psi^{n+1}_{jk}|^2 + |\psi^n_{jk}|^2) \big] \psi^{n+1/2}_{jk}, \; (j,k) \in \mathcal{T}_{MK},\ n \geq 0, \quad (6.7)$$

where

$$V_{jk} = V(x_j, y_k), \qquad \psi^{n+1/2}_{jk} = \frac{1}{2}\left(\psi^{n+1}_{jk} + \psi^n_{jk}\right), \qquad (j,k) \in \mathcal{T}^0_{MK}, \quad n = 0, 1, 2, \ldots.$$

The boundary condition (6.2) is discretized as

$$\psi_{0k}^n = \psi_{Mk}^n = 0, \quad \psi_{j0}^n = \psi_{jK}^n = 0, \qquad (j,k) \in \mathcal{T}_{MK}^0, \quad n = 0, 1, \dots , \tag{6.8}$$

and the initial condition (6.3) is discretizaed as

$$\psi_{jk}^0 = \psi_0(x_j, y_k), \qquad (j,k) \in \mathcal{T}_{MK}^0. \tag{6.9}$$

As proved in section 6.4, the above CNFD method conserves the mass and energy in the discretized level. However, it is a fully implicit method, i.e. at each time step, a fully nonlinear system must be solved, which may be very expensive, especially in 2D and 3D. In fact, if the fully nonlinear system is not solved numerically to extremely high accuracy, e.g. at machine accuracy, then the mass and energy of the numerical solution obtained in practical computation are no longer conserved. This motivates us also consider the following discretization for the GPE.

The *semi-implicit finite difference* (SIFD) discretization for the GPE (6.1) is to use Crank-Nicolson/leap-frog schemes for discretizing linear/nonlinear terms, respectively, as

$$i\delta_t \psi_{jk}^n = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right] \frac{\psi_{jk}^{n+1} + \psi_{jk}^{n-1}}{2} + \beta|\psi_{jk}^n|^2\psi_{jk}^n, \; (j,k) \in \mathcal{T}_{MK}, \; n \ge 1. \tag{6.10}$$

Again, the boundary condition (6.2) and initial condition (6.3) are discretized in (6.8) and (6.9), respectively. In addition, the first step can be computed by any explicit second or higher order time integrator, e.g. the second-order modified Euler method, as

$$\psi_{jk}^1 = \psi_{jk}^0 - i\tau \left[\left(-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right)\psi_{jk}^{(1)} + \beta|\psi_{jk}^{(1)}|^2\psi_{jk}^{(1)}\right], \qquad (j,k) \in \mathcal{T}_{MK}, \tag{6.11}$$

$$\psi_{jk}^{(1)} = \psi_{jk}^0 - i\frac{\tau}{2}\left[\left(-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right)\psi_{jk}^0 + \beta|\psi_{jk}^0|^2\psi_{jk}^0\right].$$

For this SIFD method, at each time step, only a linear system is to be solved, which is much more cheaper than that of the CNFD method in practical computation.

6.2.2 Main error estimate results

Before we state our main error estimate results, we denote the space

$$X_{MK} = \left\{u = (u_{jk})_{(j,k)\in\mathcal{T}_{MK}^0} \mid u_{0k} = u_{Mk} = u_{j0} = u_{jK} = 0, \; (j,k) \in \mathcal{T}_{MK}^0\right\} \subset \mathbb{C}^{(M+1)\times(K+1)},$$

and define norms and inner product over X_{MK} as

$$\|u\|_2^2 = \Delta x\, \Delta y \sum_{j=0}^{M-1}\sum_{k=0}^{K-1} |u_{jk}|^2, \quad \|\delta_\nabla^+ u\|_2^2 = \Delta x\, \Delta y \sum_{j=0}^{M-1}\sum_{k=0}^{K-1} \left(\left|\delta_x^+ u_{jk}\right|^2 + \left|\delta_y^+ u_{jk}\right|^2\right), \tag{6.12}$$

$$\|u\|_\infty = \sup_{(j,k)\in \mathcal{T}_{MK}^0} |u_{jk}|, \quad \|u\|_p^p = \Delta x\, \Delta y \sum_{j=0}^{M-1}\sum_{k=0}^{K-1} |u_{jk}|^p, \quad 0 < p < \infty, \tag{6.13}$$

$$\mathcal{E}(u) = \frac{1}{2}\|\delta_\nabla^+ u\|_2^2 + \Delta x\, \Delta y \sum_{j=1}^{M-1}\sum_{k=1}^{K-1} \left[V_{jk}|u_{jk}|^2 - \Omega\, \bar{u}_{jk}\, L_z^h u_{jk}\right], \quad \forall u \in X_{MK}, \tag{6.14}$$

$$E_h(u) = \frac{1}{2}\|\delta_\nabla^+ u\|_2^2 + \frac{\beta}{2}\|u\|_4^4 + \Delta x\, \Delta y \sum_{j=1}^{M-1}\sum_{k=1}^{K-1} \left[V_{jk}|u_{jk}|^2 - \Omega\, \bar{u}_{jk}\, L_z^h u_{jk}\right], \tag{6.15}$$

$$(u, v) = \Delta x\, \Delta y \sum_{j=0}^{M-1}\sum_{k=0}^{K-1} u_{jk}\bar{v}_{jk}, \quad \langle u, v\rangle = \Delta x\, \Delta y \sum_{j=1}^{M-1}\sum_{k=1}^{K-1} u_{jk}\bar{v}_{jk}, \quad \forall u, v \in X_{MK}. \tag{6.16}$$

We also make the following assumptions:

(A) Assumption on the trapping potential $V(\mathbf{x})$ and rotation speed Ω, i.e. there exists a constant $\gamma > 0$ such that

$$V(\mathbf{x}) \in C^1(U), \qquad V(\mathbf{x}) \geq \frac{1}{2}\gamma^2(x^2 + y^2), \quad \forall \mathbf{x} \in U, \qquad |\Omega| < \gamma;$$

Assumption on the exact solution ψ, i.e. let $0 < T < T_{\max}$ with $T_{\max}$ the maximal existing time of the solution [43, 76]:

$$\text{(B)} \qquad \psi \in C^4([0,T]; L^\infty(U)) \cap C^3([0,T]; W^{2,\infty}(U)) \cap C^2([0,T]; W^{3,\infty}(U)) \cap C^1([0,T]; W^{4,\infty}(U)) \cap C^0([0,T]; W^{5,\infty}(U) \cap H_0^1(U)).$$

Define the 'error' function $e^n \in X_{MK}$ as

$$e_{jk}^n = \psi(x_j, y_k, t_n) - \psi_{jk}^n, \qquad (j,k) \in \mathcal{T}_{MK}^0, \quad n \geq 0. \tag{6.17}$$

Then for the SIFD method, we have

Theorem 6.1 *Assume $h \lesssim h_{\min} := \min\{\Delta x, \Delta y\}$ and $\tau \lesssim h$, under Assumption (A) and (B), there exist $h_0 > 0$ and $0 < \tau_0 < \frac{1}{4}$ sufficiently small, when $0 < h \leq h_0$ and $0 < \tau \leq \tau_0$, we have the following optimal error estimate for the SIFD method (6.10) with (6.8), (6.9) and (6.11)*

$$\|e^n\|_2 \lesssim h^2 + \tau^2, \quad \|\delta_\nabla^+ e^n\|_2 \lesssim h^{3/2} + \tau^{3/2}, \qquad 0 \leq n \leq \frac{T}{\tau}. \tag{6.18}$$

In addition, if either $\Omega = 0$ *and* $\partial_{\mathbf{n}} V(\mathbf{x})|_{\partial U} = 0$ *or* $\psi \in C^0([0,T]; H_0^2(U))$*, where* $\partial_{\mathbf{n}} = \nabla \cdot \mathbf{n}$ *denotes the normal derivative with* $\mathbf{n}$ *being the unit outer normal vector on the boundary, we have the optimal error estimates*

$$\|e^n\|_2 + \|\delta_\nabla^+ e^n\|_2 \lesssim h^2 + \tau^2, \quad 0 \le n \le \frac{T}{\tau}. \tag{6.19}$$

Similarly, for the CNFD method, we have

Theorem 6.2 *Suppose* $h \lesssim h_{\min} := \min\{\Delta x, \Delta y\}$, $\tau \lesssim h$ *and either* $\beta \ge 0$ *or* $\beta < 0$ *with* $\|\psi^0\|_2^2 < \frac{1}{|\beta|}\left(1 - \frac{\Omega^2}{\gamma^2}\right)$*, under Assumption (A), there exists* $h_0 > 0$ *sufficiently small, when* $0 < h \le h_0$*, the discretization (6.7) with (6.8) and (6.9) admits a unique solution* ψ^n $(0 \le n \le \frac{T}{\tau})$*. Furthermore, under Assumption (B), there exist* $h_0 > 0$ *and* $\tau_0 > 0$ *sufficiently small, when* $0 < h \le h_0$ *and* $0 < \tau \le \tau_0$*, we have the following error estimate*

$$\|e^n\|_2 \lesssim h^2 + \tau^2, \qquad \|\delta_\nabla^+ e^n\|_2 \lesssim h^{3/2} + \tau^{3/2}, \qquad 0 \le n \le \frac{T}{\tau}. \tag{6.20}$$

In addition, if either $\Omega = 0$ *and* $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ *or* $\psi \in C^0([0,T]; H_0^2(U))$*, we have the optimal error estimates*

$$\|e^n\|_2 + \|\delta_\nabla^+ e^n\|_2 \lesssim h^2 + \tau^2, \quad 0 \le n \le \frac{T}{\tau}. \tag{6.21}$$

6.3 Error estimates for the SIFD method

In this section, we establish optimal error estimates for the SIFD method (6.10) with (6.8), (6.9) and (6.11) in l^2-norm, discrete H^1-norm and l^∞-norm. Let $\psi^n \in X_{MK}$ be the numerical solution of the SIFD method and $e^n \in X_{MK}$ be the error function.

From (6.14) and (6.16), we have

Lemma 6.1 *The following equalities hold*

$$\langle \delta_x u, v \rangle = -\langle u, \delta_x v \rangle, \qquad \langle \delta_x^2 u, v \rangle = -\left(\delta_x^+ u, \delta_x^+ v\right), \tag{6.22}$$

$$\langle \delta_y u, v \rangle = -\langle u, \delta_y v \rangle, \qquad \langle \delta_y^2 u, v \rangle = -\left(\delta_y^+ u, \delta_y^+ v\right), \qquad \forall u, v \in X_{MK}, \tag{6.23}$$

$$\|u\|_2^2 \lesssim \|\delta_\nabla^+ u\|_2^2, \qquad \|u\|_4^4 \le \|u\|_2^2 \cdot \|\delta_\nabla^+ u\|_2^2, \qquad \forall u \in X_{MK}. \tag{6.24}$$

In addition, under the assumption (A), we have

$$\frac{1}{2}\left(1 - \frac{\Omega^2}{\gamma^2}\right) \|\delta_\nabla^+ u\|_2^2 \le \mathcal{E}(u) \lesssim \|\delta_\nabla^+ u\|_2^2 + \|u\|_2^2 \lesssim \|\delta_\nabla^+ u\|_2^2, \qquad \forall u \in X_{MK}. \tag{6.25}$$

Proof: The equality (6.22) follows from (6.16) by using summation by parts as

$$\begin{aligned}
\langle \delta_x u, v\rangle &= \Delta x\,\Delta y \sum_{j=1}^{M-1}\sum_{k=1}^{K-1} \frac{u_{j+1\,k}-u_{j-1\,k}}{2\Delta x}\,\bar{v}_{jk}\\
&= \Delta x\,\Delta y \sum_{j=1}^{M-1}\sum_{k=1}^{K-1} u_{jk}\,\frac{\bar{v}_{j-1\,k}-\bar{v}_{j+1\,k}}{2\Delta x} = -\langle u, \delta_x v\rangle\,,\\
\left\langle \delta_x^2 u, v\right\rangle &= \Delta x\,\Delta y \sum_{j=1}^{M-1}\sum_{k=1}^{K-1} \frac{u_{j+1\,k}-2u_{jk}+u_{j-1\,k}}{(\Delta x)^2}\,\bar{v}_{jk}\\
&= \Delta x\,\Delta y \sum_{j=0}^{M-1}\sum_{k=0}^{K-1} \frac{u_{j+1\,k}-u_{jk}}{\Delta x}\,\frac{\bar{v}_{j,k}-\bar{v}_{j+1\,k}}{\Delta x}\\
&= -\left(\delta_x^+ u, \delta_x^+ v\right), \qquad \forall u, v\in X_{MK}.
\end{aligned}$$

Similarly, we can get (6.23). For $u\in X_{MK}$, we have

$$\begin{aligned}
\left|(u_{jk})^2\right| &= \left|\sum_{l=0}^{j-1}\left[(u_{l+1\,k})^2-(u_{lk})^2\right]\right| = \Delta x\left|\sum_{l=0}^{j-1}[u_{l+1\,k}+u_{lk}]\delta_x^+ u_{lk}\right|\\
&\le \Delta x\sum_{l=0}^{j-1}|u_{l+1\,k}+u_{lk}|\cdot\left|\delta_x^+ u_{lk}\right|\\
&\le \sqrt{2}\Delta x\sqrt{\sum_{l=0}^{M-1}|\delta_x^+ u_{lk}|^2}\sqrt{\sum_{l=0}^{M-1}|u_{lk}|^2}, \qquad (j,k)\in\mathcal{T}_{MK}.
\end{aligned} \tag{6.26}$$

Similarly, we have

$$\left|(u_{jk})^2\right| \le \sqrt{2}\Delta y\sqrt{\sum_{m=0}^{K-1}|\delta_y^+ u_{jm}|^2}\sqrt{\sum_{m=0}^{K-1}|u_{jm}|^2}, \qquad (j,k)\in\mathcal{T}_{MK}. \tag{6.27}$$

Combining (6.26) and (6.27), using the Cauchy inequality, we get

$$\begin{aligned}
\|u\|_4^4 &= \Delta x\Delta y\sum_{j=0}^{M-1}\sum_{k=0}^{K-1}|u_{jk}|^4 = \Delta x\Delta y\sum_{j=0}^{M-1}\sum_{k=0}^{K-1}|u_{jk}|^2\cdot|u_{jk}|^2\\
&\le 2(\Delta x\Delta y)^2\sum_{j=0}^{M-1}\sum_{k=0}^{K-1}\left(\sqrt{\sum_{l=0}^{M-1}|\delta_x^+ u_{lk}|^2}\sqrt{\sum_{l=0}^{M-1}|u_{lk}|^2}\sqrt{\sum_{m=0}^{K-1}|\delta_y^+ u_{jm}|^2}\sqrt{\sum_{m=0}^{K-1}|u_{jm}|^2}\right)\\
&= 2(\Delta x\Delta y)^2\sum_{k=0}^{K-1}\left(\sqrt{\sum_{l=0}^{M-1}|\delta_x^+ u_{lk}|^2}\sqrt{\sum_{l=0}^{M-1}|u_{lk}|^2}\right)\sum_{j=0}^{M-1}\left(\sqrt{\sum_{m=0}^{K-1}|\delta_y^+ u_{jm}|^2}\sqrt{\sum_{m=0}^{K-1}|u_{jm}|^2}\right)\\
&\le 2(\Delta x\Delta y)^2\sqrt{\sum_{k=0}^{K-1}\sum_{l=0}^{M-1}|\delta_x^+ u_{lk}|^2}\sqrt{\sum_{k=0}^{K-1}\sum_{l=0}^{M-1}|u_{lk}|^2}\sqrt{\sum_{j=0}^{M-1}\sum_{m=0}^{K-1}|\delta_y^+ u_{jm}|^2}\sqrt{\sum_{j=0}^{M-1}\sum_{m=0}^{K-1}|u_{jm}|^2}\\
&\le \|\delta_\nabla^+ u\|_2^2\cdot\|u\|_2^2, \qquad u\in X_{MK}.
\end{aligned}$$

The first inequality in (6.24) can be proved in a similar way. From (6.14), summation by parts, we get

$$\begin{aligned}\sum_{j=1}^{M-1}\sum_{k=1}^{K-1}\bar{u}_{jk}\,L_z^h u_{jk} &= -i\sum_{j=1}^{M-1}\sum_{k=1}^{K-1}\bar{u}_{jk}\,\left(x_j\delta_y u_{jk}-y_k\delta_x u_{jk}\right)\\ &= -i\sum_{j=1}^{M-1}\sum_{k=1}^{K-1}u_{jk}\,\left(x_j\delta_y \bar{u}_{jk}-y_k\delta_x \bar{u}_{jk}\right)\\ &= \sum_{j=1}^{M-1}\sum_{k=1}^{K-1}u_{jk}\,\bar{L}_z^h\bar{u}_{jk}\quad\in\mathbb{R},\qquad \forall u\in X_{MK},\end{aligned}\tag{6.28}$$

which immediately implies that $\mathcal{E}(u)\in\mathbb{R}$ for all $u\in X_{MK}$. In addition, using the Cauchy inequality and triangular inequality, noticing Assumption (A), we get for $u\in X_{MK}$

$$\begin{aligned}-\Omega\sum_{j=1}^{M-1}\sum_{k=1}^{K-1}\bar{u}_{jk}\,L_z^h u_{jk} =&\frac{\Omega}{2}\sum_{j=1}^{M-1}\sum_{k=1}^{K-1}i\bar{u}_{jk}\,\left[x_j\left(\delta_y^+u_{jk}+\delta_y^+u_{j,k-1}\right)-y_k\left(\delta_x^+u_{jk}+\delta_x^+u_{j-1,k}\right)\right]\\ \geq& -\sum_{j=0}^{M-1}\sum_{k=0}^{K-1}\left[V_{jk}|u_{jk}|^2+\frac{\Omega^2}{2\gamma^2}\left(|\delta_x^+u_{jk}|^2+|\delta_y^+u_{jk}|^2\right)\right].\end{aligned}\tag{6.29}$$

Plugging (6.29) into (6.14) and noticing (6.12), we get (6.25) immediately. □

From now on, without loss of generality, we assume that $\Delta x=\Delta y=h$. From (6.25) in Lemma 6.1, we have

Lemma 6.2 *(Solvability of the difference equations) Under the Assumption (A), for any given initial data $\psi^0\in X_{MK}$, there exists a unique solution $\psi^n\in X_{MK}$ of (6.11) for $n=1$ and (6.10) for $n>1$.*

Proof: The assertion for $n=1$ is obviously true. In SIFD (6.11), for given $\psi^{n-1},\psi^n\in X_{MK}$ $(n\geq 1)$, we first prove the uniqueness. Suppose there exist two solutions $\psi^{(1)},\psi^{(2)}\in X_{MK}$ satisfying the SIFD scheme (6.10), i.e. for $(j,k)\in\mathcal{T}_{MK}$,

$$i\frac{\psi_{jk}^{(1)}-\psi_{jk}^{n-1}}{2\tau}=\left[-\frac{1}{2}\delta_\nabla^2+V_{jk}-\Omega L_z^h\right]\frac{\psi_{jk}^{(1)}+\psi_{jk}^{n-1}}{2}+\beta|\psi_{jk}^n|^2\psi_{jk}^n,\tag{6.30}$$

$$i\frac{\psi_{jk}^{(2)}-\psi_{jk}^{n-1}}{2\tau}=\left[-\frac{1}{2}\delta_\nabla^2+V_{jk}-\Omega L_z^h\right]\frac{\psi_{jk}^{(2)}+\psi_{jk}^{n-1}}{2}+\beta|\psi_{jk}^n|^2\psi_{jk}^n.\tag{6.31}$$

Denote $u=\psi^{(1)}-\psi^{(2)}\in X_{MK}$ and subtract (6.31) from (6.30), we have

$$i\frac{u_{jk}}{\tau}=\left[-\frac{1}{2}\delta_\nabla^2+V_{jk}-\Omega L_z^h\right]u_{jk},\qquad (j,k)\in\mathcal{T}_{MK}.\tag{6.32}$$

Multiplying both sides of (6.32) by $\bar{u}_{jk}$ and summing together for $(j,k) \in \mathcal{T}_{MK}$, using the summation by parts formula and taking imaginary parts, using (6.25) from Lemma 6.1, we obtain $\|u\|_2^2 = 0$, which implies $u = 0$. Hence $\psi^{(1)} = \psi^{(2)}$, i.e. the solution of (6.10) is unique.

Next, we prove the existence. For $(j,k) \in \mathcal{T}_{MK}$, rewrite equation (6.10) as

$$i\psi_{jk}^{n+1} + \tau\left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right]\psi_{jk}^{n+1} + P_{jk} = 0, \tag{6.33}$$

where $P \in X_{MK}$ is defined as

$$P_{jk} = -i\psi_{jk}^{n-1} + 2\tau\beta|\psi_{jk}^n|^2\psi_{jk}^n + \tau\left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right]\psi_{jk}^{n-1}. \tag{6.34}$$

Consider the map $G : \psi^* \in X_{MK} \to G(\psi^*) \in X_{MK}$ defined as

$$G(\psi^*)_{jk} = i\psi_{jk}^* + \tau\left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right]\psi_{jk}^* + P_{jk}, \quad (j,k) \in \mathcal{T}_{MK}. \tag{6.35}$$

We know that G is continuous from X_{MK} to X_{MK}. Noticing (6.25) in Lemma 6.1, we have

$$\mathrm{Im}(G(\psi^*), \psi^*) = \|\psi^*\|_2^2 + \mathrm{Im}(P, \psi^*) \geq \|\psi^*\|_2^2 - \|P\|_2\|\psi^*\|_2, \tag{6.36}$$

which immediately implies

$$\lim_{\|\psi^*\|_2 \to \infty} \frac{|(P(\psi^*), \psi^*)|}{\|\psi^*\|_2} = \infty. \tag{6.37}$$

Hence $G : X_{MK} \to X_{MK}$ is surjective [94] and there exists a solution $\psi^{n+1} \in X_{MK}$ satisfying $G(\psi^{n+1}) = 0$. Then ψ^{n+1} satisfies the equation (6.10). The proof is complete. □

Define the local truncation error $\eta^n \in X_{MK}$ of the SIFD method (6.10) with (6.8), (6.9) and (6.11) for $n \geq 1$ as

$$\begin{aligned} \eta_{jk}^n \;:=\; & i\delta_t\psi(x_j, y_k, t_n) - \left[-\frac{1}{2}\delta_\nabla^2 - \Omega L_z^h + V_{jk}\right]\frac{\psi(x_j, y_k, t_{n-1}) + \psi(x_j, y_k, t_{n+1})}{2} \\ & -\beta|\psi(x_j, y_k, t_n)|^2\psi(x_j, y_k, t_n), \qquad (j,k) \in \mathcal{T}_{MK}, \end{aligned} \tag{6.38}$$

and by noticing (6.9) for $n = 0$ as

$$\eta_{jk}^0 := i\delta_t^+\psi(x_j, y_k, 0) - \left(-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right)\psi_{jk}^{(1)} - \beta|\psi_{jk}^{(1)}|^2\psi_{jk}^{(1)}, \; (j,k) \in \mathcal{T}_{MK}, \tag{6.39}$$

$$\psi_{jk}^{(1)} = \psi_0(x_j, y_k) - i\frac{\tau}{2}\left[\left(-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right)\psi_0(x_j, y_k) + \beta|\psi_0(x_j, y_k)|^2\psi_0(x_j, y_k)\right].$$

Then we have

Lemma 6.3 *(Local truncation error) Assuming $V(\mathbf{x}) \in C(\overline{U})$, under the Assumption (B), we have*

$$\|\eta^n\|_\infty \lesssim \tau^2 + h^2, \qquad 0 \le n \le \frac{T}{\tau} - 1, \quad \text{and} \qquad \|\delta_\nabla^+ \eta^0\|_\infty \lesssim \tau + h. \tag{6.40}$$

In addition, assuming $V(\mathbf{x}) \in C^1(\overline{U})$ and $\tau \lesssim h$, we have for $1 \le n \le \frac{T}{\tau} - 1$

$$|\delta_\nabla^+ \eta_{jk}^n| \lesssim \begin{cases} \tau^2 + h^2, & 1 \le j \le M-2,\ 1 \le k \le K-2, \\ \tau + h, & j = 0, M-1, \ \text{or}\ k = 0, K-1. \end{cases} \tag{6.41}$$

Furthermore, assuming either $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ or $u \in C([0,T]; H_0^2(U))$, we have

$$\|\delta_\nabla^+ \eta^n\|_\infty \lesssim \tau^2 + h^2, \qquad 1 \le n \le \frac{T}{\tau} - 1. \tag{6.42}$$

Proof: First, we prove (6.40) and (6.42) when $n = 0$. Rewriting $\psi_{jk}^{(1)}$ and then using Taylor's expansion at $(x_j, y_k, 0)$, noticing (6.1) and (6.3), we get

$$\begin{aligned}
\psi_{jk}^{(1)} &= \psi\left(x_j, y_k, \frac{\tau}{2}\right) + i\frac{\tau}{2}\Bigg[\left(\frac{1}{2}\delta_\nabla^2 - V_{jk} + \Omega L_z^h\right)\psi_0(x_j, y_k) - \beta|\psi_0(x_j, y_k)|^2\psi_0(x_j, y_k) \\
&\quad + i\frac{\psi\left(x_j, y_k, \frac{\tau}{2}\right) - \psi_0(x_j, y_k)}{\tau/2}\Bigg] \\
&= \psi\left(x_j, y_k, \frac{\tau}{2}\right) + i\frac{\tau}{2}\Bigg[\frac{h}{6}\Big[\partial_{xxx}\psi_0\left(x_j + h\theta_{jk}^{(2)}, y_k\right) + \partial_{yyy}\psi_0\left(x_j, y_k + h\theta_{jk}^{(3)}\right) \\
&\quad - 3i\Omega\left(x_j \partial_{yy}\psi_0\left(x_j, y_k + h\theta_{jk}^{(4)}\right) - y_k \partial_{xx}\psi_0\left(x_j + h\theta_{jk}^{(2)}, y_k\right)\right)\Big] \\
&\quad + i\frac{\tau}{4}\partial_{tt}\psi\left(x_j, y_k, \tau\theta_{jk}^{(1)}\right)\Bigg] = \psi\left(x_j, y_k, \frac{\tau}{2}\right) + O\left(\tau^2 + \tau h\right), \quad (j,k) \in \mathcal{T}_{MK},
\end{aligned} \tag{6.43}$$

where $\theta_{jk}^{(1)} \in [0, 1/2]$ and $\theta_{jk}^{(2)}$, $\theta_{jk}^{(3)}$, $\theta_{jk}^{(4)}$, $\theta_{jk}^{(5)} \in [-1, 1]$ are constants. Similarly, using Taylor's expansion at $(x_j, y_k, \tau/2)$ in (6.39), noticing (6.1) and (6.43), using triangle inequality and the Assumption (B), we get

$$\begin{aligned}
|\eta_{jk}^0| &\lesssim \tau^2\|\partial_{ttt}\psi\|_{L^\infty} + h^2\left[\|\partial_{xxxx}\psi\|_{L^\infty} + \|\partial_{yyyy}\psi\|_{L^\infty} + \|\partial_{xxx}\psi\|_{L^\infty} + \|\partial_{yyy}\psi\|_{L^\infty}\right] \\
&\quad + \tau^2\left[\|\partial_{ttxx}\psi\|_{L^\infty} + \|\partial_{ttyy}\psi\|_{L^\infty} + \|\partial_{ttx}\psi\|_{L^\infty} + \|\partial_{tty}\psi\|_{L^\infty} + \|\partial_{tt}\psi\|_{L^\infty}\ \|\psi\|_{L^\infty}^2\right] \\
&\quad + \tau h\left[\|\psi_0\|_{W^{5,\infty}(U)} + \|\psi\|_{L^\infty}^2\ \|\psi_0\|_{W^{3,\infty}(U)}\right] + O\left(h^4 + \tau^4\right) \\
&\lesssim \tau^2 + h^2, \qquad (j,k) \in \mathcal{T}_{MK},
\end{aligned}$$

where the L^∞-norm means $\|f\|_{L^\infty} := \sup_{0 \le t \le T} \sup_{\mathbf{x} \in U} |f(\mathbf{x}, t)|$. This immediately implies (6.40) when $n = 0$ as

$$\|\eta^0\|_\infty = \max_{(j,k) \in \mathcal{T}_{MK}^0} |\eta_{jk}^0| \lesssim \tau^2 + h^2.$$

Similarly, noticing $\tau \lesssim h$,

$$|\delta_\nabla^+ \eta_{jk}^0| \lesssim \frac{1}{h}|\eta_{jk}^0| \lesssim \tau + h, \qquad (j,k) \in \mathcal{T}_{MK},$$

which immediately implies (6.42) when $n = 0$. Now we prove (6.40), (6.41) and (6.42) when $n \geq 1$. Using Taylor's expansion at (x_j, y_k, t_n) in (6.38), noticing (6.1), using triangle inequality and the Assumption (B), we have

$$\begin{aligned}
|\eta_{jk}^n| &\lesssim h^2 \left[\|\partial_{xxxx}\psi\|_{L^\infty} + \|\partial_{yyyy}\psi\|_{L^\infty} + \|\partial_{yyy}\psi\|_{L^\infty} + \|\partial_{xxx}\psi\|_{L^\infty}\right] \\
&\quad + \tau^2 \left[\|\partial_{ttt}\psi\|_{L^\infty} + \|\partial_{ttxx}\psi\|_{L^\infty} + \|\partial_{ttyy}\psi\|_{L^\infty} + \|\partial_{ytt}\psi\|_{L^\infty} + \|\partial_{xtt}\psi\|_{L^\infty}\right] \\
&\lesssim \tau^2 + h^2, \qquad (j,k) \in \mathcal{T}_{MK}, \qquad 1 \leq n \leq \frac{T}{\tau} - 1,
\end{aligned}$$

which implies (6.40) for $n \geq 1$ and (6.41) for $j = 0, M-1$ or $k = 0, K-1$. Similarly, we have

$$\begin{aligned}
|\delta_\nabla^+ \eta_{jk}^n| &\lesssim h^2 \left[\|\partial_{xxxx}\nabla\psi\|_{L^\infty} + \|\partial_{yyyy}\nabla\psi\|_{L^\infty} + \|\partial_{yyy}\nabla\psi\|_{L^\infty} + \|\partial_{xxx}\nabla\psi\|_{L^\infty}\right] \\
&\quad + \tau^2 \left[\|\partial_{ttt}\nabla\psi\|_{L^\infty} + \|\partial_{ttxx}\nabla\psi\|_{L^\infty} + \|\partial_{ttyy}\nabla\psi\|_{L^\infty} \right. \\
&\quad \left. + \|\partial_{ytt}\nabla\psi\|_{L^\infty} + \|\partial_{xtt}\nabla\psi\|_{L^\infty}\right] \\
&\lesssim \tau^2 + h^2, \qquad 1 \leq j \leq M-2,\ 1 \leq k \leq K-2, \qquad 1 \leq n \leq \frac{T}{\tau} - 1, \quad (6.44)
\end{aligned}$$

which immediately implies (6.41) for $n \geq 1$. In addition, if $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$, using the equation (6.1), we obtain the following derivatives of ψ on the boundary are 0, i.e.

$$\partial_{xx}\psi\big|_{\partial U} = \partial_{yy}\psi\big|_{\partial U} = \partial_{xxxx}\psi\big|_{\partial U} = \partial_{yyyy}\psi\big|_{\partial U} = 0. \qquad (6.45)$$

Hence (6.44) holds for the boundary case, i.e. $j = 0, M-1$ or $k = 0, K-1$, and we could obtain (6.42) for $n \geq 1$. If $\psi \in C^0([0,T]; H_0^2(U))$, using the equation (6.1), we obtain that

$$\partial_x^m \partial_y^n \psi\big|_{\partial U} = 0, \qquad m \geq 0,\ n \geq 0,\ m + n \leq 4, \qquad (6.46)$$

and similarly (6.44) holds for $j = 0, M-1$ or $k = 0, K-1$, then we could obtain (6.42) for $n \geq 1$. Thus, the proof is complete. □

Theorem 6.3 *(l^2-norm estimate) Assume $\tau \lesssim h$, under the Assumptions (A) and (B), there exist $h_0 > 0$ and $0 < \tau_0 < \frac{1}{4}$ sufficiently small, when $0 < h \leq h_0$ and $0 < \tau \leq \tau_0$, we have*

$$\|e^n\|_2 \lesssim \tau^2 + h^2, \qquad \|\psi^n\|_\infty \leq 1 + M_1, \qquad 0 \leq n \leq \frac{T}{\tau}, \qquad (6.47)$$

where $M_1 = \max_{0\le t\le T} \|\psi(\cdot,t)\|_{L^\infty(U)}$.

Proof: We will prove this theorem by the method of mathematical induction. From (6.3) and (6.9), it is straightforward to see that (6.47) is valid when $n = 0$. From (6.11) and (6.39), noticing (6.40), we get

$$|e_{jk}^1| = \left|\psi(x_j, y_k, t_1) - \psi_{jk}^1\right| = \left|-i\tau\eta_{jk}^0\right| \lesssim \tau\left(\tau^2 + h^2\right) \lesssim \tau^2 + h^2, \qquad (j,k) \in \mathcal{T}_{MK}, \quad (6.48)$$

which immediately implies the first inequality in (6.47) when $n = 1$. This, together with the triangle inequality, when τ and h are sufficiently small, we obtain

$$|\psi_{jk}^1| \le |\psi(x_j, y_k, t_1)| + |e_{jk}^1| \le M_1 + C\left(\tau^2 + h^2\right) \le 1 + M_1, \qquad (j,k) \in \mathcal{T}_{MK},$$

which immediately implies the second inequality in (6.47) when $n = 1$. Now we assume that (6.47) is valid for all $0 \le n \le m - 1 \le \frac{T}{\tau} - 1$, then we need to show that it is still valid when $n = m$. In order to do so, subtracting (6.38) from (6.10), noticing (6.2) and (6.8), we obtain the following equation for the 'error' function $e^n \in X_{MK}$:

$$i\delta_t e_{jk}^n = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right]\frac{e_{jk}^{n+1} + e_{jk}^{n-1}}{2} + \xi_{jk}^n + \eta_{jk}^n, \qquad (j,k) \in \mathcal{T}_{MK}, \quad n \ge 1, \quad (6.49)$$

where $\xi^n \in X_{MK}$ $(n \ge 1)$ is defined as

$$\begin{aligned} \xi_{jk}^n &= \beta|\psi(x_j, y_k, t_n)|^2\psi(x_j, y_k, t_n) - \beta|\psi_{jk}^n|^2\psi_{jk}^n \\ &= \beta|\psi(x_j, y_k, t_n)|^2 e_{jk}^n + \beta(\overline{e_{jk}^n}\psi_{jk}^n + \overline{\psi(x_j, y_k, t_n)}e_{jk}^n)\psi_{jk}^n, \qquad (j,k) \in \mathcal{T}_{MK}. \quad (6.50) \end{aligned}$$

Noticing (6.47), we have the following estimate

$$\|\xi^n\|_2^2 \le 9\beta^2(1 + M_1)^4\|e^n\|_2^2, \qquad \|\delta_\nabla^+\xi^n\|_2^2 \lesssim \|\delta_\nabla^+ e^n\|_2^2 + \|e^n\|_2^2, \qquad 1 \le n \le m - 1. \quad (6.51)$$

Multiplying both sides of (6.49) by $\overline{e_{jk}^{n+1} + e_{jk}^{n-1}}$ and summing all together for $(j,k) \in \mathcal{T}_{MK}$, taking imaginary parts, using the triangular and Cauchy inequalities, noticing (6.40) and (6.51) , we have for $1 \le n \le m - 1$

$$\begin{aligned} \|e^{n+1}\|_2^2 - \|e^{n-1}\|_2^2 &= 2\tau\,\mathrm{Im}\left(\xi^n + \eta^n, e^{n+1} + e^{n-1}\right) \\ &\le 2\tau\left[\|e^{n+1}\|_2^2 + \|e^{n-1}\|_2^2 + \|\eta^n\|_2^2 + \|\xi^n\|_2^2\right] \\ &\le C\tau(h^2 + \tau^2)^2 + 2\tau\left(\|e^{n+1}\|_2^2 + \|e^{n-1}\|_2^2\right) + 18\tau\beta^2(1 + M_1)^4\|e^n\|_2^2. \end{aligned}$$

When $\tau \leq \frac{1}{4}$, we have

$$\|e^{n+1}\|_2^2 - \|e^{n-1}\|_2^2 \leq C\tau \left[(h^2+\tau^2)^2 + \|e^{n-1}\|_2^2 + \beta^2(1+M_1)^4\|e^n\|_2^2\right].$$

Summing the above inequality for $n = 1, 2, \ldots, m-1$, we get

$$\|e^m\|_2^2 + \|e^{m-1}\|_2^2 \leq CT(h^2+\tau^2)^2 + C\tau\left[1+\beta^2(M_1+1)^4\right]\sum_{l=1}^{m-1}\|e^l\|_2^2, \ 1 \leq m \leq \frac{T}{\tau}. \quad (6.52)$$

Using the discrete Gronwall inequality [46, 67, 95] and noticing $\|e^0\|_2 = 0$ and $\|e^1\|_2 \lesssim h^2 + \tau^2$, we immediately obtain the first inequality in (6.47) for $n = m$. Using the inverse inequality, triangle inequality and l^2-norm estimate, noticing $\tau \lesssim h$, we obtain

$$\begin{aligned} |\psi_{jk}^m| &\leq |\psi(x_j, y_k, t_m)| + |e_{jk}^m| \leq M_1 + \|e^m\|_\infty \leq M_1 + \frac{C}{h}\|e^m\|_2 \\ &\leq M_1 + \frac{C}{h}\left(h^2+\tau^2\right) \leq M_1 + Ch, \qquad (j,k) \in \mathcal{T}_{MK}^0. \end{aligned}$$

Thus there exists a constant $h_0 > 0$ sufficiently small, when $0 < h \leq h_0$ and $0 < \tau \lesssim h$, we have

$$\|\psi^m\|_\infty \leq 1 + M_1, \qquad 1 \leq m \leq \frac{T}{\tau},$$

which is the second inequality in (6.47) when $n = m$. Therefore the proof of the theorem is completed by the method of mathematical induction. □

Combining Theorem 6.3 and Lemmas 6.1, 6.2 and 6.3, we are now ready to prove the main Theorem 6.1.

Proof of Theorem 6.1: We first prove the optimal discrete semi-H^1 norm convergence rate in the case of either $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ or $\psi \in C^0([0,T]; H_0^2(U))$. From (6.9), we know $e^0 = 0$ and thus (6.18) is valid for $n = 0$. From (6.11) and (6.39), noticing (6.40), we get

$$\begin{aligned} |\delta_\nabla^+ e_{jk}^1| &= \left|\delta_\nabla^+\left(\psi(x_j, y_k, t_1) - \psi_{jk}^1\right)\right| = \left|-i\tau\delta_\nabla^+\eta_{jk}^0\right| \\ &\lesssim \tau(\tau+h) \lesssim \tau^2 + h^2, \qquad (j,k) \in \mathcal{T}_{MK}, \end{aligned} \quad (6.53)$$

which immediately implies (6.18) when $n = 1$. Multiplying both sides of (6.49) by $\overline{e_{jk}^{n+1} - e_{jk}^{n-1}}$, summing over index $(j,k) \in \mathcal{T}_{MK}$ and summation by parts, taking real part and noticing (6.13), we have

$$\mathcal{E}(e^{n+1}) - \mathcal{E}(e^{n-1}) = -2\,\mathrm{Re}\left\langle \xi^n + \eta^n, e^{n+1} - e^{n-1}\right\rangle, \qquad n \geq 1. \quad (6.54)$$

Rewriting (6.49) as

$$e_{jk}^{n+1} - e_{jk}^{n-1} = -2i\tau \left[\xi_{jk}^n + \eta_{jk}^n + \chi_{jk}^n\right], \qquad (j,k) \in \mathcal{T}_{MK}, \tag{6.55}$$

where $\chi^n \in X_{MK}$ is defined as

$$\chi_{jk}^n = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_h^z\right] \frac{e_{jk}^{n+1} + e_{jk}^{n-1}}{2}, \qquad (j,k) \in \mathcal{T}_{MK}, \tag{6.56}$$

then plugging (6.55) into (6.54), we obtain

$$\begin{aligned} \mathcal{E}(e^{n+1}) - \mathcal{E}(e^{n-1}) &= -4\tau \operatorname{Im} \langle \xi^n + \eta^n, \xi^n + \eta^n + \chi^n \rangle \\ &= -4\tau \operatorname{Im} \langle \xi^n + \eta^n, \chi^n \rangle, \qquad n \geq 1. \end{aligned} \tag{6.57}$$

From (6.56) and (6.50), noticing (6.22), (6.23) and (6.25), we have

$$\begin{aligned} |\langle \xi^n, \chi^n \rangle| &= \frac{1}{2} \left| \left\langle \xi^n, \left(-\frac{1}{2}\delta_\nabla^2 + V - \Omega L_z^h\right) \left(e^{n+1} + e^{n-1}\right) \right\rangle \right| \\ &\lesssim \left|\left\langle \delta_\nabla^+ \xi^n, \delta_\nabla^+ \left(e^{n+1} + e^{n-1}\right)\right\rangle\right| + \left|\left\langle \xi^n, V\left(e^{n+1} + e^{n-1}\right)\right\rangle\right| \\ &\quad + \left| \left\langle \xi^n, \Omega L_z^h \left(e^{n+1} + e^{n-1}\right) \right\rangle \right| \\ &\lesssim \|\delta_\nabla^+ e^{n+1}\|_2^2 + \|\delta_\nabla^+ e^n\|_2^2 + \|\delta_\nabla^+ e^{n-1}\|_2^2 + \|e^{n+1}\|_2^2 + \|e^n\|_2^2 + \|e^{n-1}\|_2^2 \\ &\quad + \|\delta_\nabla^+ \xi^n\|_2^2 + \|\xi^n\|_2^2 \\ &\lesssim \|\delta_\nabla^+ e^{n+1}\|_2^2 + \|\delta_\nabla^+ e^n\|_2^2 + \|\delta_\nabla^+ e^{n-1}\|_2^2, \qquad 1 \leq n \leq \frac{T}{\tau} - 1. \end{aligned} \tag{6.58}$$

Similarly, noticing (6.51), (6.40) and (6.42), we have

$$\begin{aligned} |\langle \eta^n, \chi^n \rangle| &= \frac{1}{2} \left| \left\langle \eta^n, \left(-\frac{1}{2}\delta_\nabla^2 + V - \Omega L_z^h\right) \left(e^{n+1} + e^{n-1}\right) \right\rangle \right| \\ &\lesssim \left|\left\langle \delta_\nabla^+ \eta^n, \delta_\nabla^+ \left(e^{n+1} + e^{n-1}\right)\right\rangle\right| + \left|\left\langle \eta^n, V\left(e^{n+1} + e^{n-1}\right)\right\rangle\right| \\ &\quad + \left| \left\langle \eta^n, \Omega L_z^h \left(e^{n+1} + e^{n-1}\right) \right\rangle \right| \\ &\lesssim \|\delta_\nabla^+ e^{n+1}\|_2^2 + \|\delta_\nabla^+ e^n\|_2^2 + \|\delta_\nabla^+ e^{n-1}\|_2^2 + \|e^{n+1}\|_2^2 + \|e^n\|_2^2 + \|e^{n-1}\|_2^2 \\ &\quad + \|\delta_\nabla^+ \eta^{n+1}\|_2^2 + \|\eta^n\|_2^2 \\ &\lesssim \|\delta_\nabla^+ e^{n+1}\|_2^2 + \|\delta_\nabla^+ e^n\|_2^2 + \|\delta_\nabla^+ e^{n-1}\|_2^2 + (\tau^2 + h^2)^2, \quad 1 \leq n \leq \frac{T}{\tau} - 1. \end{aligned} \tag{6.59}$$

Plugging (6.58) and (6.59) into (6.57), using (6.25) and the triangle inequality, we get

$$\begin{aligned} \mathcal{E}(e^{n+1}) - \mathcal{E}(e^{n-1}) &\lesssim \tau(\tau^2 + h^2)^2 + \tau\left[\|\delta_\nabla^+ e^{n+1}\|_2^2 + \|\delta_\nabla^+ e^n\|_2^2 + \|\delta_\nabla^+ e^{n-1}\|_2^2\right] \\ &\lesssim \tau(\tau^2 + h^2)^2 + \tau\left[\mathcal{E}(e^{n+1}) + \mathcal{E}(e^n) + \mathcal{E}(e^{n-1})\right], \ 1 \leq n \leq \frac{T}{\tau} - 1. \end{aligned}$$

There exists $\tau_0 > 0$ sufficiently small, when $0 < \tau \le \tau_0$, we have

$$\mathcal{E}(e^{n+1}) - \mathcal{E}(e^{n-1}) \lesssim \tau(\tau^2 + h^2)^2 + \tau\left[\mathcal{E}(e^n) + \mathcal{E}(e^{n-1})\right], \qquad 1 \le n \le \frac{T}{\tau} - 1. \quad (6.60)$$

Summing the above inequality for $1 \le n \le m-1 \le \frac{T}{\tau} - 1$, we get

$$\mathcal{E}(e^m) + \mathcal{E}(e^{m-1}) \lesssim T(\tau^2 + h^2)^2 + \mathcal{E}(e^1) + \mathcal{E}(e^0) + \tau\sum_{l=1}^{m-1}\mathcal{E}(e^l), \qquad 1 \le m \le \frac{T}{\tau}.$$

Using the discrete Gronwall inequality [95], noticing (6.47) and (6.53), we have

$$\begin{aligned}\|\delta_\nabla^+ e^m\|_2^2 &\lesssim \mathcal{E}(e^m) \le \mathcal{E}(e^m) + \mathcal{E}(e^{m-1}) \lesssim (\tau^2 + h^2)^2 + \mathcal{E}(e^1) + \mathcal{E}(e^0) \\ &\lesssim (\tau^2 + h^2)^2 + \|e^1\|_2^2 + \|\delta_\nabla^+ e^1\|_2^2 \lesssim (\tau^2 + h^2)^2, \qquad 1 \le m \le \frac{T}{\tau}.\end{aligned}$$

This together with (6.47) imply (6.18). For the case of the Assumption (A) and (B) without further assumptions, we will lose half order convergence rate because of the boundary (6.41). Notice that the reminder term is $O(h^2 + \tau^2)^{3/2}$ instead of $O(h^2 + \tau^2)$ in (6.59), and the the remaining proof is the same. Hence, we will have the 3/2 order convergence rate for discrete semi-H^1 norm. The proof is complete. $\Box$

Similar as the proof of Theorem 6.1, we can get error estimate for the mass and energy in the discretized level as

Lemma 6.4 *(Estimates on mass and energy) Under the same conditions of Theorem 6.1, with only Assumption (A) and (B), we have for* $0 \le n \le \frac{T}{\tau}$

$$\begin{aligned}\left|\, \|\psi^n\|_2^2 - N(\psi_0)\right| &= \left|\, \|\psi^n\|_2^2 - N(\psi(\cdot, t_n))\right| \\ &\le \left|\, \|\psi^n\|_2^2 - \|\Pi_h\psi(t_n)\|_2^2\right| + \left|\|\Pi_h\psi(t_n)\|_2^2 - N(\psi(\cdot, t_n))\right| \lesssim h^{3/2} + \tau^{3/2}, \\ |E_h(\psi^n) - E(\psi_0)| &= |E_h(\psi^n) - E(\psi(\cdot, t_n))| \\ &\le |E_h(\psi^n) - E_h(\Pi\psi(t_n))| + |E_h(\Pi\psi(t_n)) - E(\psi(\cdot, t_n))| \lesssim h^{3/2} + \tau^{3/2},\end{aligned}$$

where $\Pi_h : X := \{f \in C(\bar{U}) \mid f|_{\partial U} = 0\} \to X_{MK}$ *is the standard project operator defined as*

$$(\Pi_h f)_{jk} = f(x_j, y_k), \quad f \in X, \qquad (\Pi_h\psi(t_n))_{jk} = \psi(x_j, y_k, t_n), \qquad (j,k) \in \mathcal{T}_{MK}^0. \quad (6.61)$$

In addition, assume either $\Omega = 0$ *and* $\partial_{\mathbf{n}}V(\mathbf{x}) = 0$ *or* $\psi \in C([0,T]; H_0^2(U))$*, then we have*

$$\left|\, \|\psi^n\|_2^2 - N(\psi_0)\right| + |E_h(\psi^n) - E(\psi_0)| \lesssim h^2 + \tau^2, \quad 0 \le n \le \frac{T}{\tau}. \qquad (6.62)$$

In addition, from Theorem 6.1 and using the inverse inequality [145], we get immediately the error estimate in l^∞-norm for the SIFD method as

Lemma 6.5 *(l^∞-norm estimate) Under the same conditions of Theorem 6.1 and assume $h < 1$, we have the following error estimate for the SIFD with Assumption (A) and (B)*

$$\|e^n\|_\infty \lesssim \begin{cases} (h^{3/2} + \tau^{3/2})|\ln(h)|, & d = 2, \\ h + \tau, & d = 3. \end{cases}$$

In addition, if either $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ or $\psi \in C^0([0,T]; H_0^2(U))$, we have

$$\|e^n\|_\infty \lesssim \begin{cases} (h^2 + \tau^2)|\ln(h)|, & d = 2, \\ h^{3/2} + \tau^{3/2}, & d = 3. \end{cases}$$

Remark 6.1 *If the cubic nonlinear term $\beta|\psi|^2\psi$ in (6.1) is replaced by a general nonlinearity $f(|\psi|^2)\psi$, the numerical discretization SIFD and its error estimates in l^2-norm, l^∞-norm and discrete H^1-norm are still valid provided that the nonlinear real-valued function $f(\rho) \in C^2([0,\infty))$.*

6.4 Error estimates for the CNFD method

In this section, we prove optimal error estimate for the CNFD method (6.7) with (6.8) and (6.9) in l^2-norm, discrete H^1-norm and l^∞-norm. Let $\psi^n \in X_{MK}$ be the numerical solution of the CNFD method and $e^n \in X_{MK}$ be the error function.

Lemma 6.6 *(Conservation of mass and energy) For the CNFD scheme (6.7) with (6.8) and (6.9), for any mesh size $h > 0$, time step $\tau > 0$ and initial data ψ_0, it conserves the mass and energy in the discretized level, i.e.*

$$\|\psi^n\|_2^2 \equiv \|\psi^0\|_2^2, \qquad E_h(\psi^n) \equiv E_h(\psi^0), \qquad n = 0, 1, 2, \dots . \tag{6.63}$$

Proof: Follow the analogous arguments of the CNFD method for the NLSE [46, 67] and we omit the details here for brevity. □

Lemma 6.7 *(Solvability of the difference equations) For any given ψ^n, there exists a solution ψ^{n+1} of the CNFD discretization (6.7) with (6.8) and (6.9). In addition, assume*

$\tau \lesssim h$ and either $\beta \geq 0$ or $\beta < 0$ with $\|\psi^0\|_2^2 < \frac{1}{|\beta|}\left(1 - \frac{\Omega^2}{\gamma^2}\right)$, under the Assumption (A), there exists $h_0 > 0$ sufficiently small, when $0 < h \leq h_0$, the solution is unique.

Proof: First, we prove the existence of a solution of the CNFD discretization (6.7). In order to do so, for any given $\psi^n \in X_{MK}$, we rewrite the equation (6.7) as

$$\psi^{n+1/2} = \psi^n + i\frac{\tau}{2}F^n(\psi^{n+1/2}), \qquad n = 0, 1, \dots , \tag{6.64}$$

where $F^n : X_{MK} \to X_{MK}$ defined as

$$(F^n(u))_{jk} = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right] u_{jk} + \frac{\beta}{2}(|2u_{jk} - \psi_{j,k}^n|^2 + |\psi_{j,k}^n|^2)u_{jk}, \qquad (j,k) \in \mathcal{T}_{MK}.$$

Define the map $G^n : X_{MK} \to X_{MK}$ as

$$G^n(u) = u - \psi^n - i\frac{\tau}{2}F^n(u), \qquad u \in X_{MK},$$

and it is easy to see that G^n is continuous from X_{MK} to X_{MK}. Moreover,

$$\mathrm{Re}\,(G^n(u), u) = \|u\|_2^2 - \mathrm{Re}(\psi^n, u) \geq \|u\|_2(\|u\|_2 - \|\psi^n\|_2), \qquad u \in X_{MK},$$

which immediately implies

$$\lim_{\|u\|_2 \to \infty} \frac{|\,(G^n(u), u)\,|}{\|u\|_2} = \infty.$$

Thus G^n is surjective. By using the Brouwer fixed point theorem (cf. [94]), it is easy to show that there exists a solution u^* with $G^n(u^*) = 0$, which implies that there exists a solution $\psi^{n+1/2}$ to the problem (6.64) and thus the CNFD discretization (6.7) is solvable for any given ψ^n. In addition, for the solution ψ^{n+1} to (6.7), using (6.63), we have

$$\|\delta_\nabla^+\psi^{n+1}\|_2^2 \leq C\, E_h(\psi^{n+1}) = C\, E_h(\psi^0), \qquad n = 0, 1, \dots ; \tag{6.65}$$

where when $\beta \geq 0$, we have $C = 2$; and when $\beta < 0$ with $\|\psi^0\|_2^2 < \frac{1}{|\beta|}(1 - \frac{\Omega^2}{\gamma^2})$, it comes from

$$\begin{aligned} E_h(\psi^0) &= E_h(\psi^{n+1}) \geq \frac{1}{2}\left(1 - \frac{\Omega^2}{\gamma^2}\right)\|\delta_\nabla^+\psi^{n+1}\|_2^2 - \frac{|\beta|}{2}\|\delta_\nabla^+\psi^{n+1}\|_2^2 \cdot \|\psi^{n+1}\|_2^2 \\ &= \frac{1}{2}\left(1 - \frac{\Omega^2}{\gamma^2}\right)\|\delta_\nabla^+\psi^{n+1}\|_2^2 - \frac{|\beta|}{2}\|\delta_\nabla^+\psi^{n+1}\|_2^2 \cdot \|\psi^0\|_2^2 \\ &= \frac{|\beta|}{2}\left[\frac{1}{|\beta|}\left(1 - \frac{\Omega^2}{\gamma^2}\right) - \|\psi^0\|_2^2\right]\|\delta_\nabla^+\psi^{n+1}\|_2^2. \end{aligned}$$

Thus assume $h < 1$, when $\beta \ge 0$ or $\beta < 0$ with $\|\psi^0\|_2^2 < \frac{1}{|\beta|}\left(1 - \frac{\Omega^2}{\gamma^2}\right)$, using (6.65) and the inverse inequality [145], we obtain

$$\|\psi^{n+1}\|_\infty \le C|\ln h|\,\|\delta_\nabla^+\psi^{n+1}\|_2 \le C|\ln h|\,E_h(\psi^0), \qquad n = 0, 1, \ldots . \tag{6.66}$$

Next, we show the uniqueness of the solution of the CNFD scheme (6.7). For given $\psi^n \in X_{MK}$, suppose that there are two solutions $u^{n+1} \in X_{MK}$ and $v^{n+1} \in X_{MK}$ to (6.7). From (6.66), we get

$$\|u^{n+1}\|_\infty \le C\,E_h(\psi^0)\,|\ln h|, \qquad \|v^{n+1}\|_\infty \le C\,E_h(\psi^0)\,|\ln h|. \tag{6.67}$$

Denoting $w := u^{n+1} - v^{n+1} \in X_{MK}$, from (6.7), we have

$$i\frac{w_{jk}}{\tau} \;=\; \left(-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right) w_{jk} + \hat{R}_{jk}, \qquad (j,k) \in \mathcal{T}_{MK}, \tag{6.68}$$

where

$$\hat{R}_{jk} = \frac{\beta}{2}(|u_{ij}^{n+1}|^2 + |\psi_{jk}^n|^2)w_{jk} + \frac{\beta}{2}(v_{jk}^{n+1} + \psi_{jk}^n)(|u_{jk}^{n+1}|^2 - |v_{jk}^{n+1}|^2), \qquad (j,k) \in \mathcal{T}_{MK}.$$

Multiplying both sides of (6.68) with $\bar{w}_{jk}$, summing for $(j,k) \in \mathcal{T}_{MK}$, and then taking imaginary parts, using (6.66) and (6.67), we have

$$\|w\|_2^2 \le \tau C\left[\|u^{n+1}\|_\infty^2 + \|v^{n+1}\|_\infty^2 + \|\psi^n\|_\infty^2\right]\|w\|_2^2 \le C\tau\left[E_h(\psi^0)\,\ln h\right]^2 \|w\|_2^2.$$

Thus under the assumption $\tau \lesssim h$, there exists $h_0 > 0$, when $0 < h \le h_0$, we have $C\tau(\ln h\,E_h(\psi^0))^2 < 1$ which immediately implies

$$\|w\|_2 = \|u^{n+1} - v^{n+1}\|_2 = 0 \qquad \Longrightarrow \qquad u^{n+1} = v^{n+1},$$

i.e. the solution of CNFD (6.7) is unique. □

Denote the local truncation error $\widetilde{\eta}^n \in X_{MK}$ $(n \ge 0)$ of the CNFD scheme (6.7) with (6.8) and (6.9) as

$$\begin{aligned}\widetilde{\eta}_{jk}^n :\;=\;& i\delta_t^+\psi(x_j,y_k,t_n) - \Big[-\frac{1}{2}\delta_\nabla^2 - \Omega L_z^h + V_{jk} + \frac{\beta}{2}\big(|\psi(x_j,y_k,t_{n+1})|^2 \\ &+|\psi(x_j,y_k,t_n)|^2\big)\Big]\times\frac{\psi(x_j,y_k,t_n)+\psi(x_j,y_k,t_{n+1})}{2}, \quad (j,k)\in\mathcal{T}_{MK}.\end{aligned} \tag{6.69}$$

Then we have

Lemma 6.8 *(Local truncation error) Assume $V(\mathbf{x}) \in L^\infty(U)$ and under the Assumption (B), we have*

$$\|\widetilde{\eta}^n\|_\infty \lesssim \tau^2 + h^2, \qquad 0 \le n \le \frac{T}{\tau} - 1. \tag{6.70}$$

In addition, assuming $V(\mathbf{x}) \in C^1(U)$ and $\tau \lesssim h$, we have for $1 \le n \le \frac{T}{\tau} - 1$

$$|\delta_\nabla^+ \widetilde{\eta}_{jk}^n| \lesssim \begin{cases} \tau^2 + h^2, & 1 \le j \le M-2,\ 1 \le k \le K-2, \\ \tau + h, & j = 0, M-1, \text{ or } k = 0, K-1. \end{cases} \tag{6.71}$$

In addition, if either $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ or $\psi \in C^0([0,T]; H_0^2(U))$, we have

$$\|\delta_\nabla^+ \widetilde{\eta}^n\|_\infty \lesssim \tau^2 + h^2, \qquad 1 \le n \le \frac{T}{\tau} - 1. \tag{6.72}$$

Proof: Follow the analogous line for Lemma 6.3 and we omit it here for brevity. □

Theorem 6.4 *(l^2-norm estimate) Assume $\tau \lesssim h$ and either $\beta \ge 0$ or $\beta < 0$ with $\|\psi^0\|_2^2 < \frac{1}{|\beta|}\left(1 - \frac{\Omega^2}{\gamma^2}\right)$, under the Assumption (A) and (B), there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small, when $0 < h \le h_0$ and $0 < \tau \le \tau_0$, we have*

$$\|e^n\|_2 \lesssim \tau^2 + h^2, \qquad \|\psi^n\|_\infty \le \sqrt{2}(1 + M_1), \qquad 0 \le n \le \frac{T}{\tau}. \tag{6.73}$$

Proof: Choose a smooth function $\alpha(\rho)$ ($\rho \ge 0$)$\in C^\infty([0,\infty))$ defined as

$$\alpha(\rho) = \begin{cases} 1, & 0 \le \rho \le 1, \\ \in [0,1], & 1 \le \rho \le 2, \\ 0, & \rho \ge 2. \end{cases} \tag{6.74}$$

Denote $M_0 = 2(1 + M_1)^2 > 0$ and define

$$F_{M_0}(\rho) = \alpha\left(\frac{\rho}{M_0}\right)\rho, \qquad 0 \le \rho < \infty,$$

then $F_{M_0}(\rho) \in C^\infty([0,\infty))$ and it is global Lipschitz, i.e.

$$|F_{M_0}(\rho_1) - F_{M_0}(\rho_2)| \le C_{M_0}\, |\sqrt{\rho_1} - \sqrt{\rho_2}|\,, \qquad 0 \le \rho_1, \rho_2 < \infty. \tag{6.75}$$

Choose $\phi^0 = \psi^0 \in X_{MK}$ and define $\phi^n \in X_{MK}$ ($n = 0, 1, \ldots$) as for $(j,k) \in \mathcal{T}_{MK}$

$$i\delta_t^+ \phi_{jk}^n = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h + \frac{\beta}{2}\left(F_{M_0}(|\phi_{jk}^{n+1}|^2) + F_{M_0}\left(|\phi_{jk}^n|^2\right)\right)\right]\phi_{jk}^{n+1/2}, \tag{6.76}$$

where

$$\phi_{jk}^{n+1/2} = \frac{1}{2}(\phi_{jk}^{n+1} + \phi_{jk}^{n}), \qquad (j,k) \in \mathcal{T}_{MK}^0, \quad n \geq 0.$$

In fact, ϕ^n can be viewed as another approximation of $\psi(\mathbf{x}, t_n)$. Define the 'error' function $\hat{e}^n \in X_{MK}$

$$\hat{e}_{jk}^n := \psi(x_j, y_k, t_n) - \phi_{jk}^n, \qquad (j,k) \in \mathcal{T}_{MK}^0, \quad n \geq 0,$$

and the local truncation error $\hat{\eta}^n \in X_{MK}$ of the scheme (6.76) as

$$\begin{aligned} \hat{\eta}_{jk}^n \;:=\; & i\delta_t^+ \psi(x_j, y_k, t_n) - \left[-\frac{1}{2}\delta_\nabla^2 - \Omega L_z^h + V_{jk} + \frac{\beta}{2}\bigg(F_{M_0}(|\psi(x_j, y_k, t_{n+1})|^2) \right. \qquad (6.77) \\ & \left. + F_{M_0}(|\psi(x_j, y_k, t_n)|^2) \bigg) \right] \times \frac{\psi(x_j, y_k, t_n) + \psi(x_j, y_k, t_{n+1})}{2}, \quad (j,k) \in \mathcal{T}_{MK}, \ n \geq 0. \end{aligned}$$

Similar as Lemma 6.8, we can prove

$$\|\hat{\eta}^n\|_\infty \lesssim \tau^2 + h^2, \qquad 0 \leq n \leq \frac{T}{\tau}.$$

Subtracting (6.77) from (6.76), we obtain

$$\begin{aligned} i\delta_t^+ \hat{e}_{j,k}^n \;=\; & \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h \right] \hat{e}_{jk}^{n+1/2} + \frac{\beta}{2}\left(F_{M_0}(|\phi_{jk}^{n+1}|^2) + F_{M_0}(|\phi_{jk}^n|^2) \right) \hat{e}_{jk}^{n+1/2} \\ & + \frac{\beta}{4}\left(\psi(x_j, y_k, t_{n+1}) + \psi(x_j, y_k, t_n) \right) \hat{\xi}_{jk}^n + \hat{\eta}_{jk}^n, \quad (j,k) \in \mathcal{T}_{MK}, \ n \geq 0, (6.78) \end{aligned}$$

where $\hat{\xi}^n \in X_{MK}$ defined as

$$\hat{\xi}_{jk}^n = F_{M_0}(|\phi_{jk}^{n+1}|^2) + F_{M_0}(|\phi_{jk}^n|^2) - F_{M_0}(|\psi(x_j, y_k, t_{n+1})|^2) - F_{M_0}(|\psi(x_j, y_k, t_n)|^2), \ (j,k) \in \mathcal{T}_{MK}^0.$$

This together with (6.75) implies

$$\left| \frac{\beta}{4}\left(\psi(x_j, y_k, t_{n+1}) + \psi(x_j, y_k, t_n) \right) \hat{\xi}_{jk}^n \right| \lesssim C\left(|\hat{e}_{jk}^{n+1}| + |\hat{e}_{jk}^n| \right), \qquad (j,k) \in \mathcal{T}_{MK}^0.$$

Multiplying both sides of (6.78) with $\overline{\hat{e}_{jk}^{n+1} + \hat{e}_{jk}^n}$, summing for $(j,k) \in \mathcal{T}_{MK}$, taking imaginary part and applying the Cauchy inequality, we obtain

$$\begin{aligned} \|\hat{e}^{n+1}\|_2^2 - \|\hat{e}^n\|_2^2 \;\lesssim\; & \tau\left(|\hat{\eta}^n|_\infty^2 + C(\|\hat{e}^{n+1}\|_2^2 + \|\hat{e}^n\|_2^2) \right) \\ \lesssim\; & \tau\left[(h^2 + \tau^2)^2 + (\|\hat{e}^{n+1}\|_2^2 + \|\hat{e}^n\|_2^2) \right], \qquad 0 \leq n \leq \frac{T}{\tau} - 1. \end{aligned}$$

Then there exists $\tau_0 > 0$ sufficiently small, when $0 < \tau \leq \tau_0$, applying the discrete Gronwall inequality [46, 67, 95], we get

$$\|\hat{e}^n\|_2 \lesssim \tau^2 + h^2, \qquad 0 \leq n \leq \frac{T}{\tau}.$$

Applying the inverse inequality in 2D, we have

$$\|\hat{e}^n\|_\infty \lesssim \frac{1}{h}\|\hat{e}^n\|_2 \lesssim h + \frac{\tau^2}{h} \lesssim h, \quad 0 \le n \le \frac{T}{\tau}, \tag{6.79}$$

which implies

$$\|\phi^n\|_\infty \le \|\Pi_h \psi(t_n)\|_\infty + \|\hat{e}^n\|_\infty \le \frac{\sqrt{M_0}}{2} + Ch, \quad 0 \le n \le \frac{T}{\tau}.$$

Thus under the assumption $\tau \lesssim h$, there exists $h_0 > 0$, when $0 < h \le h_0$, we have

$$\|\phi^n\|_\infty \le \frac{\sqrt{M_0}}{2} + \frac{\sqrt{M_0}}{2} = \sqrt{M_0} \qquad \Longrightarrow \qquad \|\phi^n\|_\infty^2 \le M_0, \qquad 0 \le n \le \frac{T}{\tau}. \tag{6.80}$$

Therefore, the discretization (6.76) collapses exactly to the CNFD discretization (6.7) with (6.8) and (6.9), i.e.

$$\psi^n = \phi^n, \qquad e^n = \hat{e}^n, \qquad 0 \le n \le \frac{T}{\tau}.$$

This together with (6.79) and (6.80) complete the proof. □

Again, combining Theorem 6.4 and Lemmas 6.7 and 6.8, we are now ready to prove the main Theorem 6.2.

Proof of Theorem 6.2: As in the proof of Theorem 6.1, we only prove the optimal convergence under the Assumption (A) and (B) with either $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ or $\psi \in C^0([0,T]; H_0^2(U))$. Subtracting (6.69) from (6.7), we get

$$i\delta_t^+ e_{jk}^n \;=\; \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right] e_{jk}^{n+1/2} + \widetilde{\xi}_{jk}^n + \widetilde{\eta}_{jk}^n, \quad (j,k) \in \mathcal{T}_{MK},\ n \ge 0, \tag{6.81}$$

where $\tilde{\xi}^n \in X_{MK}$ defined as

$$\begin{aligned}\widetilde{\xi}_{jk}^n \;=\;& \frac{\beta}{2}\left[e_{jk}^n\overline{\psi(x_j,y_k,t_n)} + \psi_{jk}^n\overline{e_{jk}^n} + e_{jk}^{n+1}\overline{\psi(x_j,y_k,t_{n+1})} + \psi_{jk}^{n+1}\overline{e_{jk}^{n+1}}\right]\psi_{jk}^{n+1/2}\\ &+\frac{\beta}{2}(|\psi(x_j,y_k,t_n)|^2 + |\psi(x_j,y_k,t_{n+1})|^2)e_{jk}^{n+1/2}, \qquad (j,k) \in \mathcal{T}_{MK}.\end{aligned}$$

Again, rewrite (6.81) as

$$e^{n+1} - e^n = -i\tau\left(\widetilde{\chi}^n + \widetilde{\xi}^n + \widetilde{\eta}^n\right), \qquad n \ge 0, \tag{6.82}$$

where $\widetilde{\chi}^n \in X_{MK}$ defined as

$$\widetilde{\chi}_{jk}^n = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h\right] e_{jk}^{n+1/2}, \qquad (j,k) \in \mathcal{T}_{MK}, \quad n \ge 0.$$

Multiplying both sides of (6.81) with $\overline{e_{jk}^{n+1} - e_{jk}^{n}}$, summing for $(j,k) \in \mathcal{T}_{MK}$, noticing (6.22), (6.23) and (6.82), taking real parts, we obtain

$$\begin{aligned}\mathcal{E}(e^{n+1}) - \mathcal{E}(e^n) &= -2\,\mathrm{Re}\left\langle \widetilde{\xi}^n + \widetilde{\eta}^n, e^{n+1} - e^n \right\rangle \\ &= -2\,\mathrm{Re}\left\langle \widetilde{\xi}^n + \widetilde{\eta}^n, -i\tau(\widetilde{\chi}^n + \widetilde{\xi}^n + \widetilde{\eta}^n) \right\rangle \\ &= 2\tau\ \mathrm{Im}\left\langle \widetilde{\xi}^n + \widetilde{\eta}^n, \widetilde{\chi}^n \right\rangle, \qquad 0 \le n \le \frac{T}{\tau} - 1.\end{aligned}$$

Similar as those in the proof of Theorem 6.1, we can prove

$$\left|\mathrm{Im}\left\langle \widetilde{\xi}^n + \widetilde{\eta}^n, \widetilde{\chi}^n \right\rangle\right| \lesssim (h^2+\tau^2)^2 + \mathcal{E}(e^{n+1}) + \mathcal{E}(e^n), \qquad 0 \le n \le \frac{T}{\tau} - 1.$$

Combining the above two inequalities, we get

$$\mathcal{E}(e^{n+1}) - \mathcal{E}(e^n) \lesssim \tau\left[(\tau^2+h^2)^2 + \mathcal{E}(e^{n+1}) + \mathcal{E}(e^n)\right], \qquad 0 \le n \le \frac{T}{\tau} - 1. \tag{6.83}$$

Then there exists $\tau_0 > 0$ sufficiently small, when $0 < \tau \le \tau_0$, using the discrete Gronwall inequality [46, 67, 95] and noticing $e^0 = 0$ and $\mathcal{E}(e^0) = 0$, we get

$$\mathcal{E}(e^n) \lesssim (\tau^2 + h^2)^2, \qquad 0 \le n \le \frac{T}{\tau},$$

which immediately implies (6.20). If we only have Assumption (A) and (B) without further assumption, the convergence rate will be $O(h^{3/2} + \tau^{3/2})$. The proof is the same as in Theorem 6.1, and we omit it here. □

Similarly, from Theorem 6.2 and using the inverse inequality [145], we get immediately the error estimate in l^∞-norm for the CNFD method as

Lemma 6.9 *(l^∞-norm estimate) Under the same conditions of Theorem 6.2 and assume $h < 1$, with Assumption (A) and (B), we have the following error estimate for the CNFD*

$$\|e^n\|_\infty \lesssim \begin{cases} (h^{3/2} + \tau^{3/2})|\ln(h)|, & d = 2, \\ h + \tau, & d = 3. \end{cases}$$

In addition, if either $\Omega = 0$ and $\partial_{\mathbf{n}} V(\mathbf{x}) = 0$ or $\psi \in C^0([0,T]; H_0^2(U))$, we have

$$\|e^n\|_\infty \lesssim \begin{cases} (h^2 + \tau^2)|\ln(h)|, & d = 2, \\ h^{3/2} + \tau^{3/2}, & d = 3. \end{cases}$$

Remark 6.2 *If the cubic nonlinear term $\beta|\psi|^2\psi$ in (6.1) is replaced by a general nonlinearity $f(|\psi|^2)\psi$, the numerical discretization CNFD and its error estimates in l^2-norm, l^∞-norm and discrete H^1-norm are still valid provided that the nonlinear real-valued function $f(\rho) \in C^3([0,\infty))$.*

6.5 Extension to other cases

In this section, we will discuss a discretization of the GPE with an angular momentum rotation (6.1) when U is a disk in 2D, and resp. a cylinder in 3D and its error estimates. As noticed in [16], the angular momentum rotation is constant coefficient in 2D with polar coordinates and 3D with cylindrical coordinates. Thus the original problem of GPE with an angular momentum rotation term defined in $\mathbb{R}^d$ ($d = 2, 3$) for rotating BEC is usually truncated onto a disk in 2D and a cylinder in 3D as bounded computational domain. Again, for simplicity of notation, we only consider SIFD in 2D, i.e. $d = 2$ and $U = \{\mathbf{x} \mid |\mathbf{x}| < R\}$ with $R > 0$ fixed. Extension to 3D are straightforward. In 2D with polar coordinate, the problem collapses

$$i\partial_t\psi = \left[-\frac{1}{2}\left(\frac{1}{r}\partial_r\left(r\partial_r\right) + \frac{1}{r^2}\partial_{\theta\theta}\right) + V_0(r) + W(r,\theta) + i\Omega\partial_\theta + \beta|\psi|^2\right]\psi, \quad (r,\theta) \in U, \tag{6.84}$$

with boundary condition

$$\psi(R,\theta) = 0, \qquad \psi(r,\theta) = \psi(r,\theta + 2\pi), \qquad 0 \le \theta \le 2\pi, \quad 0 \le r \le R, \tag{6.85}$$

and initial condition

$$\psi(r,\theta,0) = \psi_0(r,\theta), \qquad 0 \le r \le R, \quad 0 \le \theta \le 2\pi; \tag{6.86}$$

where $\psi = \psi(r,\theta,t)$ and here we split the external trapping potential $V(\mathbf{x})$ into a radial symmetry part $V_0(r)$ and a left-over part $W(\mathbf{x})$, i.e.

$$V(\mathbf{x}) = V_0(r) + W(r,\theta), \qquad \mathbf{x} \in U.$$

Let $M,\ K > 0$ be two positive integers, and $\Delta r := \frac{2R}{2M+1}$, $\Delta\theta := \frac{2\pi}{K}$, define the grid points

$$r_j = j\Delta r, \quad r_{j+\frac{1}{2}} = \left(j + \frac{1}{2}\right)\Delta r, \qquad j = 0, 1, \ldots, M; \qquad \theta_k = k\Delta\theta, \quad k = 0, 1, \ldots, K.$$

Let $\psi^n_{j+\frac{1}{2}\,k}$ be the approximation of $\psi(r_{j+\frac{1}{2}}, \theta_k, t_n)$ and ψ^n be the numerical solution at time $t = t_n$. We adopt the similar notations as those in section 6.2.

Then a *semi-implicit finite difference* (SIFD) discretization reads for $n \geq 1$

$$
\begin{aligned}
i\delta_t\psi^n_{j+\frac{1}{2}\,k} =& \frac{-r^{-1}_{j+\frac{1}{2}}}{4(\Delta r)^2}\left[r_{j+1}(\psi^{n+1}_{j+\frac{3}{2}\,k}+\psi^{n-1}_{j+\frac{3}{2}\,k})-(r_{j+1}+r_j)(\psi^{n+1}_{j+\frac{1}{2}\,k}+\psi^{n-1}_{j+\frac{1}{2}\,k})+r_j(\psi^{n+1}_{j-\frac{1}{2}\,k}+\psi^{n-1}_{j-\frac{1}{2}\,k})\right]\\
&-\frac{1}{4r^2_{j+\frac{1}{2}}(\Delta\theta)^2}\left[\psi^{n+1}_{j+\frac{1}{2}\,k+1}-2\psi^{n+1}_{j+\frac{1}{2}\,k}+\psi^{n+1}_{j+\frac{1}{2}\,k-1}+\psi^{n-1}_{j+\frac{1}{2}\,k+1}-2\psi^{n-1}_{j+\frac{1}{2}\,k}+\psi^{n-1}_{j+\frac{1}{2}\,k-1}\right]\\
&+\frac{V_0(r_{j+\frac{1}{2}})}{2}\left(\psi^{n+1}_{j+\frac{1}{2}\,k}+\psi^{n-1}_{j+\frac{1}{2}\,k}\right)+\frac{i\Omega}{2\Delta\theta}\left[\psi^{n+1}_{j+\frac{1}{2}\,k+1}-\psi^{n+1}_{j+\frac{1}{2}\,k-1}+\psi^{n-1}_{j+\frac{1}{2}\,k+1}-\psi^{n-1}_{j+\frac{1}{2}\,k-1}\right]\\
&+\beta|\psi^n_{j+\frac{1}{2}\,k}|^2\psi^n_{j+\frac{1}{2}\,k}+W(r_{j+\frac{1}{2}},\theta_k)\psi^n_{j+\frac{1}{2}\,k},\quad 0\leq j\leq M-1,\ 0<k\leq K. \qquad (6.87)
\end{aligned}
$$

The boundary condition (6.85) is discretized as

$$\psi_{M+\frac{1}{2}\,k}=0,\ 0\leq k\leq K;\qquad \psi_{j+\frac{1}{2}\,0}=\psi_{j+\frac{1}{2}\,K},\ \psi_{j+\frac{1}{2}\,K+1}=\psi_{j+\frac{1}{2}\,1},\quad 0\leq j\leq M;\ (6.88)$$

and the initial condition (6.86) is discretized as

$$\psi^0_{j+\frac{1}{2}\,k}=\psi_0(r_{j+\frac{1}{2}},\theta_k),\qquad 0\leq j\leq M,\quad 0\leq k\leq K. \qquad (6.89)$$

The first step ψ^1 can be obtained by using the same spatial discretization combining with any explicit second-order time integrator.

For this SIFD method, although it is implicit, however, at each time step, the linear system can be solved directly via fast direct Poisson solver via fast discrete Fourier transform in θ-direction with computational cost at $O\left(MK\,\ln K\right)$, i.e. it is very efficient in practical computation [16]. In fact, this method is also widely used in simulating quantized vortex dynamics of rotating Bose-Einstein condensate [16]. In addition, let $e^n_{j+1/2\,k} = \psi^n_{j+1/2\,k}-\psi(r_{j+\frac{1}{2}},\theta_k,t_n)$, similar as those in section 6.3, we can prove the following error estimate.

Theorem 6.5 *Assume $h_{\min} := \min\{\Delta r,\Delta\theta\} \lesssim h := h_{\max} = \max\{\Delta r,\Delta\theta\}$ and $\tau \lesssim h$, under Assumption (A) and (B), there exist $h_0>0$ and $0<\tau_0<\frac{1}{4}$ sufficiently small, when $0<h\leq h_0$ and $0<\tau\leq\tau_0$, we have the following optimal error estimate for the SIFD method (6.87) with (6.88), (6.89)*

$$\|e^n\|_2 \lesssim h^2+\tau^2,\quad \|\delta^+_\nabla e^n\|_2\lesssim h^{3/2}+\tau^{3/2},\qquad 0\leq n\leq\frac{T}{\tau}, \qquad (6.90)$$

where

$$\|e^n\|_2^2=\Delta r\Delta\theta\sum_{j=0}^{M-1}\sum_{k=0}^{K-1}r_{j+\frac{1}{2}}\left|e^n_{j+\frac{1}{2}\,k}\right|^2,\qquad n=0,1,\ldots,$$

$$\|\delta^+_\nabla e^n\|_2^2=\Delta r\Delta\theta\sum_{j=0}^{M-1}\sum_{k=0}^{K-1}\left[r_{j+1}\left|\frac{e^n_{j+\frac{3}{2}\,k}-e^n_{j+\frac{1}{2}\,k}}{\Delta r}\right|^2+\frac{1}{r_{j+\frac{1}{2}}}\left|\frac{e^n_{j+\frac{1}{2}\,k+1}-e^n_{j+\frac{1}{2}\,k}}{\Delta\theta}\right|^2\right].$$

In addition, assuming $\psi \in C^0([0,T]; H_0^2(U))$, *we have*

$$\|e^n\|_2 + \|\delta_\nabla^+ e^n\|_2 \lesssim h^2 + \tau^2, \qquad 0 \le n \le \frac{T}{\tau}. \tag{6.91}$$

The CNFD method and its error estimate can be extended to this case directly and we omit the details for brevity. Again, it is implicit and at every time step, a nonlinear system must be solved.

6.6 Numerical results

In this section, we report numerical results of the SIFD (6.10) and CNFD (6.7) discretizations of the GPE (6.1) to confirm the error estimates.

We take $d = 2$, $U = [-8, 8] \times [-8, 8]$, $V(\mathbf{x}) = \frac{1}{2}(x^2 + y^2)$, $\beta = 10$ in (6.1) and $\psi_0(\mathbf{x}) = \frac{2}{\sqrt{\pi}}(x + iy)e^{-(x^2+y^2)}$ in (6.3). For comparison, the numerical 'exact' solution ψ_e is obtained by the CNFD with a very fine mesh and a small time step, e.g. $h = 1/64$ and $\tau = 0.0001$. For SIFD scheme, at each time step, we use Gauss-Seidel iteration method to solve the linear system. For CNFD scheme, to solve the fully nonlinear system, at each iteration, the system is linearized, i.e. the CNFD (6.7) is linearized as

$$i\frac{\psi_{jk}^{(m)} - \psi_{jk}^n}{\tau} = \left[-\frac{1}{2}\delta_\nabla^2 + V_{jk} - \Omega L_z^h + \frac{\beta}{2}(|\psi_{jk}^n|^2 + |\psi_{jk}^{(m-1)}|^2)\right]\frac{1}{2}(\psi_{jk}^{(m)} + \psi_{jk}^n),\ m \ge 1,$$

and we solve this inner problem to get $\psi_{jk}^{(m)}$ by Gauss-Seidel iteration method. Then the solution ψ_{jk}^{n+1} is numerically reached once $\psi_{jk}^{(m)}$ converges.

Let $\psi_{h,\tau}$ be the numerical solution corresponding to mesh size h and time step τ and define the error function as $e := \psi_e - \psi_{h,\tau}$. The convergence rates are calculated as $\log_2(\|e(h,\tau)\|/\|e(h/2,\tau/2)\|)$ with the corresponding norms. Tab. 6.1 shows the errors $\|e\|_2$, $\|\delta_\nabla^+ e\|_2$ and $\|e\|_\infty$ for the CNFD method (6.7) with different Ω, h and τ; and Tab. 6.2 displays similar results for SIFD method (6.10). Figs. 6.1 & 6.2 depict time evolution of the errors between the discretized mass and energy with their continuous counter-parts, respectively, i.e. $\big|\,\|\psi^n\|_2^2 - N(\psi_0)\big|$ and $|E_h(\psi^n) - E(\psi_0)|$ of the SIFD method (6.10) for different Ω, h and τ. Fig. 3 displays similar results of the CNFD method (6.7) when the nonlinear system is iteratively solved up to a given accuracy $\varepsilon > 0$.

From Tabs. 6.1&6.2, they demonstrate the second-order convergence rate of both SIFD and CNFD methods in l^2-norm, l^∞-norm and discrete H^1-norm. From Figs. 6.1, 6.2 and

		$h = 1/4$ $\tau = 2^{-5}$	$h = 1/8$ $\tau = 2^{-6}$	$h = 1/16$ $\tau = 2^{-7}$	$h = 1/32$ $\tau = 2^{-8}$
$\Omega = 0$	$\|e\|_2$	5.424E-2	1.574E-2	3.907E-3	8.268E-4
	Rate	1.78	2.01	2.24	
	$\|\delta_\nabla^+ e\|_2$	2.257E-1	8.008E-2	2.066E-2	4.448E-3
	Rate	1.50	1.95	2.22	
	$\|e\|_\infty$	1.521E-2	3.273E-3	7.676E-3	1.585E-4
	Rate	2.22	2.09	2.28	
$\Omega = 0.5$	$\|e\|_2$	4.758E-2	1.408E-2	3.502E-3	7.425E-4
	Rate	1.76	2.01	2.24	
	$\|\delta_\nabla^+ e\|_2$	2.097E-1	7.535E-2	1.943E-2	4.186E-3
	Rate	1.48	1.96	2.21	
	$\|e\|_\infty$	1.259E-2	3.081E-3	7.233E-4	1.489E-4
	Rate	2.03	2.09	2.28	
$\Omega = 0.9$	$\|e\|_2$	4.406E-2	1.315E-2	3.272E-3	6.934E-4
	Rate	1.74	2.01	2.24	
	$\|\delta_\nabla^+ e\|_2$	2.007E-1	7.240E-2	1.863E-2	4.011E-3
	Rate	1.47	1.96	2.22	
	$\|e\|_\infty$	1.196E-2	3.105E-3	7.284E-4	1.494E-4
	Rate	1.95	2.09	2.29	

Table 6.1: Error analysis of the CNFD method (6.7) for the GPE (6.1) at time $t = 0.5$ for different Ω, mesh size h and time step τ.

6.3, we can draw the following conclusions: (i) the SIFD discretization approximates the mass very well (up to 4 significant digits, cf. Fig. 6.1) and the energy at second order accurate in practical computation when $\tau = O(h)$ are not too big (cf. Fig. 6.1). When the final computational time t increases, the errors in mass or energy are either oscillating or slightly increasing (cf. Figs. 6.1&6.2). An interesting observation is that, for fixed $h > 0$ small, when $\tau > 0$ very small, the errors in mass and energy increase with time, especially in long time (cf. Fig. 6.2). (ii) For the CNFD discretization, when the fully nonlinear system is iteratively solved at every time step to extremely high accuracy, e.g. machine accuracy, the solution obtained in practical computation conserves the mass and energy very well (cf. Fig. 6.3). However, if the nonlinear system is solved accurately but not extremely accurately, the solution obtained in practical computation doesn't conserve the mass and energy very well, especially in long time (cf. Fig. 6.3). (iii) From the accuracy point of view, SIFD method is the same accurate as CNFD method and it approximates the mass very well and the energy in the same order as the numerical solution in the

		$h = 1/4$ $\tau = 2^{-7}$	$h = 1/8$ $\tau = 2^{-8}$	$h = 1/16$ $\tau = 2^{-9}$	$h = 1/32$ $\tau = 2^{-10}$
$\Omega = 0$	$\|e\|_2$	4.943E-2	1.360E-2	3.285E-3	6.661E-4
	Rate	1.92	1.99	2.30	
	$\|\delta_\nabla^+ e\|_2$	2.084E-1	6.726E-2	1.663E-2	3.399E-3
	Rate	1.63	2.02	2.29	
	$\|e\|_\infty$	1.298E-2	2.867E-3	6.709E-4	1.346E-4
	Rate	2.18	2.10	2.32	
$\Omega = 0.5$	$\|e\|_2$	4.350E-2	1.212E-2	2.927E-3	5.938E-4
	Rate	1.84	2.05	2.30	
	$\|\delta_\nabla^+ e\|_2$	1.940E-1	6.319E-2	1.561E-2	3.191E-3
	Rate	1.62	2.02	2.29	
	$\|e\|_\infty$	1.165E-2	2.748E-3	6.449E-4	1.295E-4
	Rate	2.08	2.09	2.32	
$\Omega = 0.9$	$\|e\|_2$	4.060E-2	1.136E-2	2.741E-3	5.557E-4
	Rate	1.84	2.05	2.30	
	$\|\delta_\nabla^+ e\|_2$	1.863E-1	6.085E-2	1.499E-2	3.062E-3
	Rate	1.61	2.02	2.29	
	$\|e\|_\infty$	1.101E-2	2.726E-3	6.339E-4	1.271E-4
	Rate	2.01	2.10	2.32	

Table 6.2: Error analysis of the SIFD method (6.10) for the GPE (6.1) at time $t = 0.5$ for different Ω, mesh size h and time step τ.

discretized level. It is much cheaper than CNFD method, especially in high dimensions and/or when fast Poisson solver is applied in practical computation.

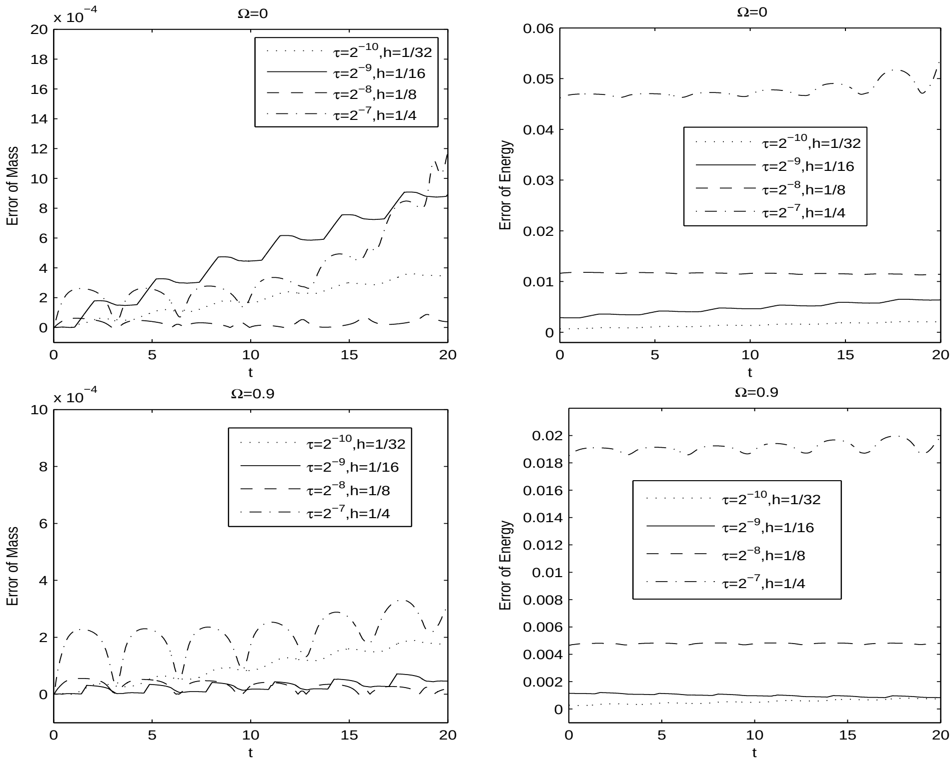

Figure 6.1: Time evolution of the errors between the discretized mass and energy with their continuous counter-parts, i.e. $\big|\|\psi^n\|_2^2 - N(\psi_0)\big|$ and $|E_h(\psi^n) - E(\psi_0)|$, of the SIFD scheme (6.10) for different Ω and $\tau = O(h)$.

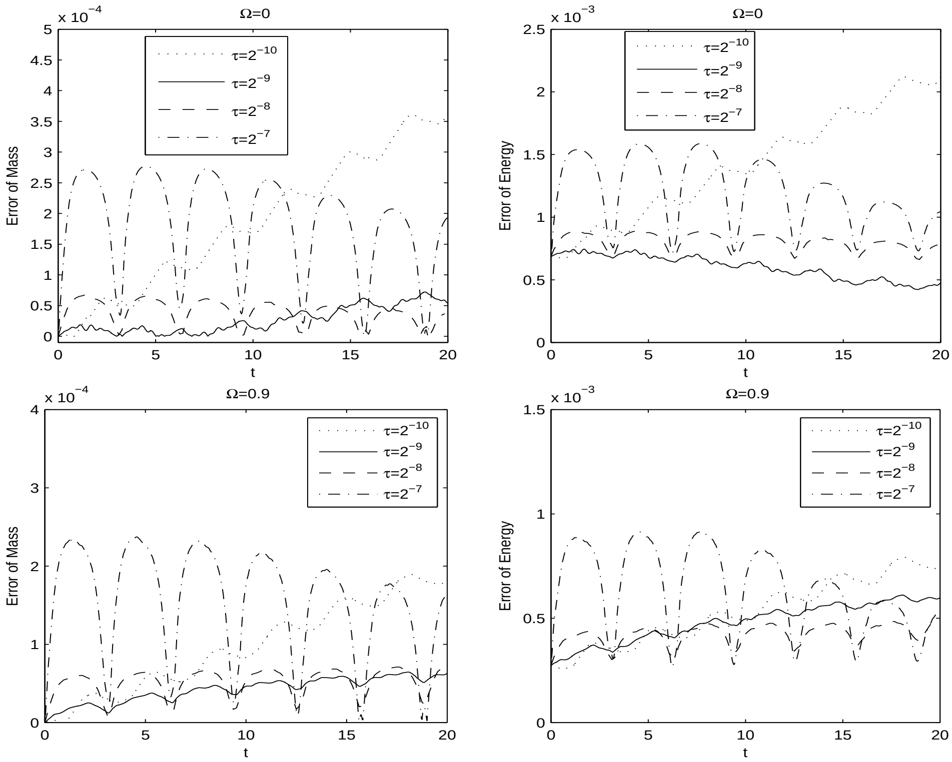

Figure 6.2: Time evolution of the errors between the discretized mass and energy with their continuous counter-parts, i.e. $\big|\,\|\psi^n\|_2^2 - N(\psi_0)\big|$ and $|E_h(\psi^n) - E(\psi_0)|$, of the SIFD scheme (6.10) with $h = 1/32$ for different Ω and time steps τ.

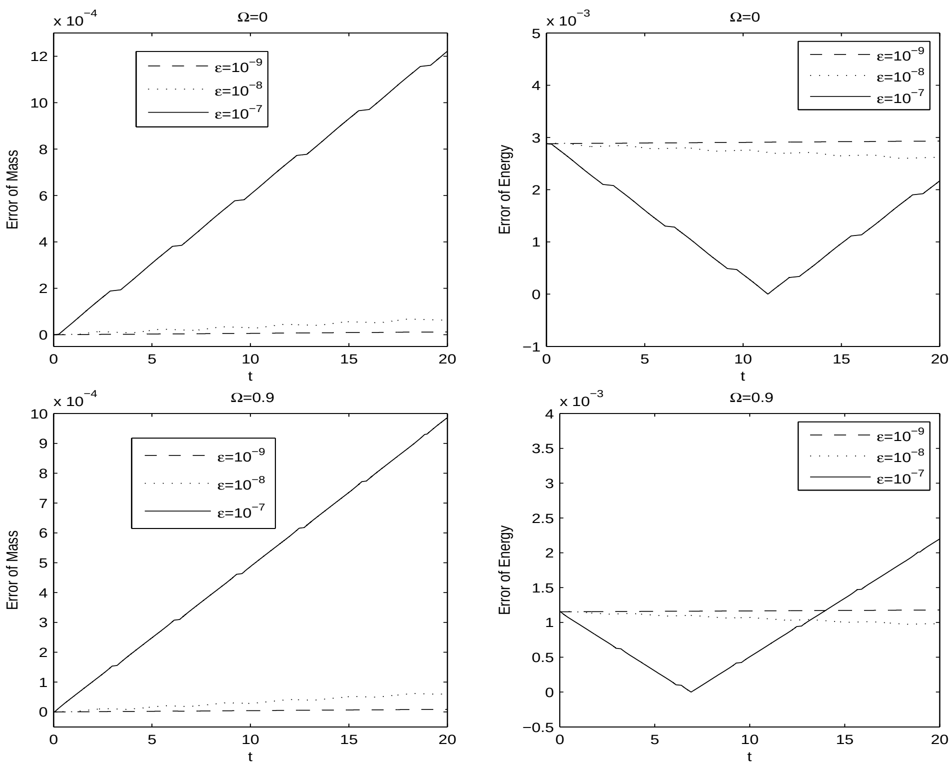

Figure 6.3: Time evolution of the errors between the discretized mass and energy with their continuous counter-parts, i.e. $\big|\, \|\psi^n\|_2^2 - N(\psi_0) \big|$ and $|E_h(\psi^n) - E(\psi_0)|$, of the CNFD scheme (6.7) with mesh $h = 1/16$ and time step $\tau = 2^{-9}$ when the nonlinear system is iteratively solved up to the accuracy ε for different Ω and ε.

Chapter 7

Uniform error estimates of finite difference methods for the nonlinear Schrödinger equation with wave operator

GPE (cubic NLSE) can be obtained by taking the nonrelativistic limit of Klein-Gorden equation (KG), or singular limit of the Zakharov system. In such case, we will need to consider a nonlinear Schrödinger equation perturbed by the wave operator (NLSW) in the case of KG, where the solution highly oscillates in time in small perturbation regime. Here, we are going to analyze the uniform convergence rates of finite difference methods for NLSW, independent of the perturbation.

7.1 Introduction

Let us recall the nonlinear Schrödinger equation with wave operator (NLSW) in d ($d = 1, 2, 3$) dimensions (1.16):

$$\begin{cases} i\partial_t u^\varepsilon(\mathbf{x},t) - \varepsilon^2\partial_{tt}u^\varepsilon(\mathbf{x},t) + \nabla^2 u^\varepsilon(\mathbf{x},t) + f(|u^\varepsilon|^2)u^\varepsilon(\mathbf{x},t) = 0, & \mathbf{x}\in\mathbb{R}^d,\ t>0,\\ u^\varepsilon(\mathbf{x},0) = u_0(\mathbf{x}), \qquad \partial_t u^\varepsilon(\mathbf{x},0) = u_1^\varepsilon(\mathbf{x}), & \mathbf{x}\in\mathbb{R}^d, \end{cases} \tag{7.1}$$

where $0 < \varepsilon \le 1$ is a dimensionless parameter, $f : [0, +\infty) \to \mathbb{R}$ is a real-valued function. It is easy to see that NLSW has the following two important conserved quantities, i.e. the *mass*

$$N^\varepsilon(t) := \int_{\mathbb{R}^d} |u^\varepsilon(\mathbf{x},t)|^2\, d\mathbf{x} - 2\varepsilon^2 \int_{\mathbb{R}^d} \mathrm{Im}\left(\overline{u^\varepsilon(\mathbf{x},t)}\partial_t u^\varepsilon(\mathbf{x},t)\right)\, d\mathbf{x} \equiv N^\varepsilon(0), \quad t \geq 0, \quad (7.2)$$

and the *energy*

$$E^\varepsilon(t) := \int_{\mathbb{R}^d} \left[\varepsilon^2|\partial_t u^\varepsilon(\mathbf{x},t)|^2 + |\nabla u^\varepsilon(\mathbf{x},t)|^2 - F(|u^\varepsilon(\mathbf{x},t)|^2)\right]\, d\mathbf{x} \equiv E^\varepsilon(0), \quad t \geq 0, \quad (7.3)$$

and F is the primitive function of f defined as

$$F(s) = \int_0^s f(\rho)\, d\rho, \qquad s \geq 0. \quad (7.4)$$

In the nonrelativistic limit of the Klein-Gordon equation and the singular limit of the Langmuir wave envelope approximation, i.e. $\varepsilon \to 0^+$, NLSW (7.1) collapses to the standard nonlinear Schrödinger equation (NLSE) [31, 104, 129, 150]

$$\begin{cases} i\partial_t u(\mathbf{x},t) + \nabla^2 u(\mathbf{x},t) + f(|u|^2)u(\mathbf{x},t) = 0, & \mathbf{x} \in \mathbb{R}^d,\ t > 0, \\ u(\mathbf{x},0) = u_0(\mathbf{x}), & \mathbf{x} \in \mathbb{R}^d, \end{cases} \quad (7.5)$$

and the corresponding conservation laws (7.2) and (7.3) hold for NLSE with $\varepsilon = 0$. In particular, it is proved in [31] that, if the nonlinearity satisfies

$$|\partial^k f(\rho)| \leq K\rho^{\sigma-k}, \quad \text{for some constant } K > 0 \text{ and } \sigma \geq 1, \quad k = 0, 1, 2,$$

then for the initial data $(u_0, u_1^\varepsilon) \in H^2 \times H^2$ with $\|u_1^\varepsilon\|_{H^2}$ uniformly bounded, there exists a constant $T > 0$ independent of ε, such that the solution u^ε of NLSW (7.1) and the solution u of NLSE (7.5) exist on $[0, T]$ [104, 129, 150]. Furthermore, the following convergence rate can be obtained (see Appendix D)

$$\|u^\varepsilon - u\|_{L^\infty([0,T];H^2)} \leq C\varepsilon^2. \quad (7.6)$$

Formally, as $\varepsilon \to 0^+$, the solution of NLSW (7.1) exhibits oscillation in time t with wavelength $O(\varepsilon^2)$ due to the wave operator and/or the initial data u_1^ε. Actually, suppose the initial data u_1^ε satisfies the condition

$$u_1^\varepsilon(\mathbf{x}) = i\left(\Delta u_0(\mathbf{x}) + f(|u_0(\mathbf{x})|^2)u_0(\mathbf{x})\right) + \varepsilon^\alpha w(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \qquad \alpha \geq 0, \quad (7.7)$$

we would have the following asymptotic expansion for the solution $u^\varepsilon(\mathbf{x},t)$ of NLSW (7.1) as

$$\begin{aligned} u^\varepsilon(\mathbf{x},t) &= u(\mathbf{x},t) + \varepsilon^2\{\text{terms without oscillation}\} \qquad (7.8)\\ &+\varepsilon^{2+\min\{\alpha,2\}}v(\mathbf{x},t/\varepsilon^2) + \text{higher order terms with oscillation}, \ \mathbf{x}\in\mathbb{R}^d, \quad t\geq 0, \end{aligned}$$

where $u := u(\mathbf{x},t)$ satisfies NLS (7.5). The expansion (7.8) can be verified in the spirit

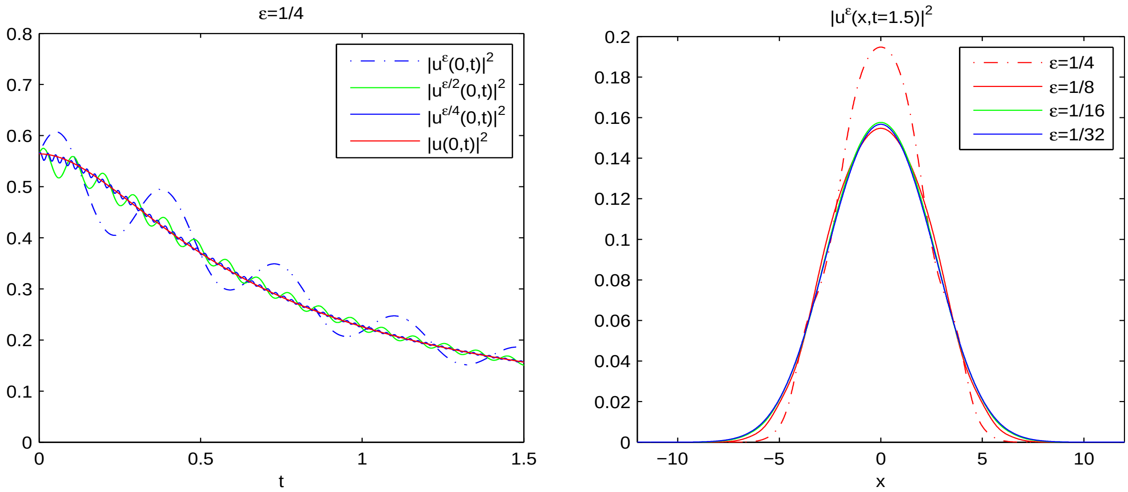

Figure 7.1: Temporal profile of $|u^\varepsilon(0,t)|^2$ and $|u(0,t)|^2$ (left) and spatial profile of $|u^\varepsilon(\mathbf{x},t=1.5)|^2$ (right), for different ε, with $\alpha = 0$ and u_0, w, f being given in section 7.5.

of [31], and we plot the densities $|u^\varepsilon(0,t)|^2$ and $|u^\varepsilon(\mathbf{x},t=1.5)|^2$ in the case of $\alpha=0$ and $d=1$ (cf. Fig. 7.1).

Based on this asymptotic expansion, we can make assumptions (A) and (B) (cf. section 7.2) on the solution of NLSW. Furthermore, from (7.8), we can classify the initial data into ill-prepared ($0\leq\alpha<2$) and well-prepared ($\alpha\geq 2$) cases. In fact, when $0\leq\alpha<2$, the leading order oscillation term comes from the initial data; and resp., when $\alpha>2$, it comes from the perturbation of the wave operator.

As stated in Chapter 1, there have been different kinds of numerical methods proposed for GPE, or for more general NLSE, such as the time-splitting pseudospectral method [18, 78, 121, 142] and the finite difference methods [5]. However, few numerical methods have been considered for NLSW in the literature, and most of them are the conservative finite difference methods [51, 73, 154]. For NLSW in 1D with $\varepsilon = O(1)$, the error estimates of conservative finite difference schemes have been obtained in [154]. However, the proofs in [154] rely strongly on the conservative properties of the schemes and the discrete version of the Sobolev inequality in 1D while the corresponding Sobolev inequality is unavailable in two (2D) and three (3D) dimensions (similar as Chapter 6 for the NLSE case). Thus their proof can not be extended to either higher dimensions (2D or 3D) or nonconservative schemes. Noticing the above asymptotic expansion results for NLSW, there exists high oscillation in time for small ε, which would cause trouble in analyzing the discretizations for NLSW (7.1), especially in the regime $0 < \varepsilon \ll 1$. Our aim is to develop a unified approach for establishing uniform error estimates in terms of $\varepsilon \in (0,1]$, of conservative CNFD and SIFD for NLSW (7.1) in d-dimensions ($d = 1, 2, 3$). Our approach combines the techniques used in Chapter 6, which include the energy method, cut-off technique for dealing with general nonlinearity and the inverse inequality for obtaining a uniform posterior bound of the numerical solution.

Throughout this chapter, we adopt the standard Sobolev spaces and their corresponding norms, let C denote a generic constant independent of ε, mesh size h and time step τ, and use the notation $p \lesssim q$ to mean that there exists a generic constant C which is independent of ε, τ and h such that $|q| \le C\, q$.

7.2 Finite difference schemes and main results

In practical computation, NLSW (7.1) is usually truncated on a bounded interval $U = (a, b)$ in 1D, or a bounded rectangle $U = (a, b) \times (c, d)$ in 2D or a bounded box $U = (a, b) \times (c, d) \times (e, f)$ in 3D, with zero Dirichlet boundary condition. For the simplicity of notation, we only deal with the case in 1D, i.e. $d = 1$ and $U = (a, b)$. Extensions to 2D and 3D are straightforward, and the error estimates in l^2-norm and discrete semi-H^1 norm are the same in 2D and 3D. In 1D, NLSW (7.1) is truncated on an interval $U = (a, b)$ as

$$\begin{cases} i\partial_t u^\varepsilon(x,t) - \varepsilon^2 \partial_{tt} u^\varepsilon + \partial_{xx} u^\varepsilon + f(|u^\varepsilon|^2) u^\varepsilon = 0, & x \in U \subset \mathbb{R},\ t > 0, \\ u^\varepsilon(x,0) = u_0(x), \qquad \partial_t u^\varepsilon(x,0) = u_1^\varepsilon(x), & x \in \overline{U} = [a,b], \\ u^\varepsilon(x,t)\big|_{\partial U} = 0, & t > 0. \end{cases} \tag{7.9}$$

Formally, as $\varepsilon \to 0^+$, the equation (7.9) collapses to the standard NLSE [31, 129, 150]

$$\begin{cases} i\partial_t u(x,t) + \partial_{xx}u(x,t) + f(|u|^2)u(x,t) = 0, & x \in U \subset \mathbb{R},\ t>0, \\ u(x,0) = u_0(x), & x \in \overline{U}, \\ u(x,t)\big|_{\partial U} = 0, & t > 0. \end{cases} \tag{7.10}$$

We assume that the initial data u_1^ε satisfies the condition

$$u_1^\varepsilon(x) = u_1(x) + \varepsilon^\alpha w^\varepsilon(x),\ u_1(x) := \partial_t u(x,t)|_{t=0} = i\left[\partial_{xx}u_0(x) + f(|u_0(x)|^2)u_0(x)\right], \tag{7.11}$$

where $x \in U$, w^ε is uniformly bounded in H^2 (w.r.t. ε) with $\liminf\limits_{\varepsilon\to 0^+} \|w^\varepsilon\|_{H^2} > 0$ and $\alpha \geq 0$ is a parameter describing the consistency of the initial data with respect to NLSE (7.10).

7.2.1 Numerical methods

Choose time step $\tau := \Delta t$ and denote time steps as $t_n := n\,\tau$ for $n = 0, 1, 2, \ldots$; choose mesh size $\Delta x := \frac{b-a}{M}$ with M being a positive integer and denote $h := \Delta x$ and grid points as $x_j := a + j\,\Delta x$, $j = 0, 1, \ldots, M$. Define the index sets

$$\mathcal{T}_M = \{j \mid j = 1, 2, \ldots, M-1\}, \qquad \mathcal{T}_M^0 = \{j \mid j = 0, 1, 2, \ldots, M\}.$$

Let $u_j^{\varepsilon,n}$ and u_j^n be the numerical approximations of $u^\varepsilon(x_j, t_n)$ and $u(x_j, t_n)$, respectively, for $j \in \mathcal{T}_M^0$ and $n \geq 0$, and denote $u^{\varepsilon,n}$, $u^n \in \mathbb{C}^{(M+1)}$ to be the numerical solutions at time $t = t_n$. We adopt notations of the finite difference operators as in Chapter 6.

The *conservative Crank-Nicolson finite difference* (CNFD) discretization of NLSW (7.9) reads as

$$(i\delta_t - \varepsilon^2\delta_t^2)u_j^{\varepsilon,n} = -\frac{1}{2}\left[\delta_x^2 u_j^{\varepsilon,n+1} + \delta_x^2 u_j^{\varepsilon,n-1}\right] - G(u_j^{\varepsilon,n+1}, u_j^{\varepsilon,n-1}), \quad j \in \mathcal{T}_M,\ n \geq 1, \tag{7.12}$$

where $G(z_1, z_2)$ is defined for $z_1, z_2 \in \mathbb{C}$ as

$$G(z_1,z_2) := \int_0^1 f(\theta|z_1|^2 + (1-\theta)|z_2|^2)\,d\theta \cdot \frac{z_1+z_2}{2} = \frac{F(|z_1|^2) - F(|z_2|^2)}{|z_1|^2 - |z_2|^2} \cdot \frac{z_1+z_2}{2}. \tag{7.13}$$

The same as GPE case (Chapter 6), although conservative CNFD type method can keep the mass and energy conservation in the discretized level which are analogous to the conservation in the continuous level, a fully nonlinear system has to be solved very accurately at each time step which may be very time consuming, especially in 2D and 3D. So we also consider the *semi-implicit finite difference* (SIFD) discretization for NLSW analogous to the GPE case (Chapter 6). The SIFD discretization for NLSW (7.9) is to apply Crank-Nicolson/leap-frog schemes for discretizing linear/nonlinear terms, respectively, as

$$i\delta_t u_j^{\varepsilon,n} = \varepsilon^2\delta_t^2 u_j^{\varepsilon,n} - \frac{1}{2}\left[\delta_x^2 u_j^{\varepsilon,n+1} + \delta_x^2 u_j^{\varepsilon,n-1}\right] - f(|u_j^{\varepsilon,n}|^2)u_j^{\varepsilon,n}, \quad j \in \mathcal{T}_M,\ n \geq 1. \tag{7.14}$$

For both schemes, the boundary and initial conditions are discretized as

$$u_0^{\varepsilon,n} = u_M^{\varepsilon,n} = 0, \quad n \geq 0; \qquad\qquad u_j^{\varepsilon,0} = u_0(x_j), \quad j \in \mathcal{T}_M^0. \tag{7.15}$$

Since CNFD (7.12) and SIFD (7.14) are three-level schemes, value at time step $n = 1$ should be assigned.

Choice of the first step value: Under the hypothesis of suitable regularity of $u^\varepsilon(x,t)$, one may use the Taylor expansion to have

$$u_j^{\varepsilon,1} \approx u_0^\varepsilon(x_j) + \tau u_t^\varepsilon(x_j,0) + \frac{\tau^2}{2}u_{tt}^\varepsilon(x_j,0), \qquad u_t^\varepsilon(x_j,0) = u_1^\varepsilon(x_j), \qquad j \in \mathcal{T}_M, \tag{7.16}$$

$$u_{tt}^\varepsilon(x_j,0) = \frac{1}{\varepsilon^2}[iu_1^\varepsilon(x_j) + \partial_{xx}u_0(x_j) + f(|u_0|^2)u_0(x_j)] = i\varepsilon^{\alpha-2}w^\varepsilon(x_j), \quad j \in \mathcal{T}_M. \tag{7.17}$$

Due to the oscillation in time especially for the ill-prepared initial data case ($0 \leq \alpha < 2$), approximation (7.16) is not appropriate if $\varepsilon \ll 1$. In such case, τ has to be very small to resolve the error from the Taylor expansion (7.16). Our aim is to obtain a suitable choice of the first step value $u_j^{\varepsilon,1}$ which is uniformly accurate for all $\varepsilon \in (0,1]$. Denote

$$\Theta(v) = \partial_{xx}v + f(|v|^2)v, \qquad v \in H^2(U), \tag{7.18}$$

then by integrating NLSW (7.9) with respect to t, we can write the solution $u^\varepsilon(x,t)$ as

$$u^\varepsilon(x,t) = u_0(x) - i\varepsilon^2(e^{it/\varepsilon^2} - 1)u_1^\varepsilon(x) - i\int_0^t (e^{i(t-s)/\varepsilon^2} - 1)\Theta(u^\varepsilon(x,s))\,ds. \tag{7.19}$$

Rewriting the integral term as

$$\int_0^t (e^{i(t-s)/\varepsilon^2} - 1)\Theta(u^\varepsilon(s))\,ds = \int_0^t (e^{i(t-s)/\varepsilon^2} - 1)\left[\Theta(u^\varepsilon(s)) - \Theta(u^\varepsilon(0)) + \Theta(u^\varepsilon(0))\right]\,ds$$
$$= \left[-i\varepsilon^2(e^{it/\varepsilon^2} - 1) - t\right]\Theta(u^\varepsilon(0)) + \int_0^t \left(e^{i(t-s)/\varepsilon^2} - 1\right)\left[\Theta(u^\varepsilon(s)) - \Theta(u^\varepsilon(0))\right]\,ds,$$

then applying the trapezoidal rule to the integral in the RHS, we could obtain a second order approximation of $u^\varepsilon(x,\tau)$ as

$$u^\varepsilon(x,\tau) \approx u_0(x) - \varepsilon^2(e^{i\tau/\varepsilon^2} - 1)(iu_1^\varepsilon(x) + \Theta(u^\varepsilon(x,0))) + i\tau\Theta(u^\varepsilon(x,0)). \tag{7.20}$$

Hence, we propose the first step as

$$u_j^{\varepsilon,1} = u_0(x_j) - i\varepsilon^{2+\alpha}(e^{i\tau/\varepsilon^2} - 1)w^\varepsilon(x_j) + i\tau\Theta_j, \quad j \in \mathcal{T}_M. \tag{7.21}$$

where Θ_j is given by

$$\Theta_j = \delta_x^2 u_0(x_j) + f(|u_0(x_j)|^2)u_0(x_j), \quad j \in \mathcal{T}_M. \tag{7.22}$$

Now (7.12) or (7.14), together with (7.15) and (7.21) complete the scheme CNFD or SIFD for NLSW (7.9). For both CNFD and SIFD schemes, we can prove the uniform convergence rates at the order of $O(h^2 + \tau^{2/3})$ and $O(h^2 + \tau)$ for ill-prepared and well-prepared initial data, respectively.

7.2.2 Main results

Before introducing our main results, denote

$$X_M = \left\{ v = (v_j)_{j \in \mathcal{T}_M^0} \mid v_0 = v_M = 0 \right\} \subset \mathbb{C}^{M+1},$$

and define the norms and inner product over X_M analogous to Chapter 6 as

$$\|v\|_2^2 = h\sum_{j=0}^{M-1} |v_j|^2, \ \|\delta_x^+ v\|_2^2 = h\sum_{j=0}^{M-1} \left|\delta_x^+ v_j\right|^2, \ \|\delta_x^2 v\|_2^2 = h\sum_{j=1}^{M-1} \left|\delta_x^2 v_j\right|^2, \ \|v\|_\infty = \sup_{j\in\mathcal{T}_M^0} |v_j|,$$

$$(u, v) = h\sum_{j=0}^{M-1} u_j \bar{v}_j, \quad \langle u, v\rangle = h\sum_{j=1}^{M-1} u_j \bar{v}_j, \qquad \forall u, v \in X_M. \tag{7.23}$$

For simplicity of notations, we also define

$$\alpha^* = \min\{\alpha, 2\}. \tag{7.24}$$

According to the known results in [31, 104, 129, 150] and the asymptotic expansion in section 7.1, we can make the following assumptions, i.e. assumptions on the initial data (7.11) for (7.9)

(A) $\quad 1 \lesssim \|w^\varepsilon(x)\|_{L^\infty(U)} + \|\partial_x w^\varepsilon(x)\|_{L^\infty(U)} + \|\partial_{xx} w^\varepsilon(x)\|_{L^\infty(U)} \lesssim 1;$

and assumptions on $u^\varepsilon(\cdot,t)$ and $u(\cdot,t)$ for $0<T<T_{\max}$ with $T_{\max}$ being the maximal common existing time and $U_T = U\times[0,T]$,

(B) $u, u^\varepsilon \in C^4\left([0,T];W^{1,\infty}(U)\right)\cap C^2\left([0,T];W^{3,\infty}(U)\right)\cap C^0\left([0,T];W^{5,\infty}(U)\cap H_0^1(U)\right)$,

$$\|u^\varepsilon\|_{L^\infty(U_T)} + \|\partial_t u^\varepsilon\|_{L^\infty(U_T)} + \sum_{m=1}^{5}\left\|\frac{\partial^m}{\partial x^m}u^\varepsilon\right\|_{L^\infty(U_T)} \lesssim 1,$$

and $\displaystyle\left\|\frac{\partial^{m+n}}{\partial t^m\partial x^n}u^\varepsilon\right\|_{L^\infty(U_T)} \lesssim \frac{1}{\varepsilon^{2m-2-\alpha^*}}, \qquad 2\le m\le 4,\ m+n\le 5.$

Under assumptions (A) and (B), the following convergence rate holds,

$$\|u(t)-u^\varepsilon(t)\|_{W^{2,\infty}(U)} \lesssim \varepsilon^2, \quad t\in[0,T]. \tag{7.25}$$

Define the 'error' function $e^{\varepsilon,n}\in X_M$ for $n\ge 0$ as

$$e_j^{\varepsilon,n} = u^\varepsilon(x_j,t_n) - u_j^{\varepsilon,n}, \quad j\in\mathcal{T}_M, \tag{7.26}$$

then we have the following estimates:

Theorem 7.1 *(Convergence of CNFD) Assume $f(s)\in C^3([0,+\infty))$, under assumptions (A) and (B), there exist $h_0>0$ and $\tau_0>0$ sufficiently small, when $0<h\le h_0$ and $0<\tau\le\tau_0$, we have the following optimal error estimates for the CNFD method (7.14) with (7.15) and (7.21) for $\varepsilon\in(0,1]$*

$$\|e^{\varepsilon,n}\|_2 + \|\delta_x^+ e^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \quad 0\le n\le\frac{T}{\tau}, \tag{7.27}$$

$$\|e^{\varepsilon,n}\|_2 + \|\delta_x^+ e^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad 0\le n\le\frac{T}{\tau}. \tag{7.28}$$

Thus, by taking the minimum, we have the ε-independent convergence rate as

$$\|e^{\varepsilon,n}\|_2 + \|\delta_x^+ e^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^{4/(6-\alpha^*)}, \quad 0\le n\le\frac{T}{\tau}. \tag{7.29}$$

Similarly, for the SIFD method, we have

Theorem 7.2 *(Convergence of SIFD) Assume $f(s)\in C^2([0,+\infty))$, under assumptions (A) and (B), there exists $h_0>0$ and $\tau_0>0$ sufficiently small, when $0<h\le h_0$ and $0<\tau\le\tau_0$, the discretization (7.14) with (7.15) and (7.21) admits a unique solution $u^{\varepsilon,n}\in X_M$ such that the following optimal error estimates hold,*

$$\|e^{\varepsilon,n}\|_2 + \|\delta_x^+ e^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \qquad 0\le n\le\frac{T}{\tau}, \tag{7.30}$$

$$\|e^{\varepsilon,n}\|_2 + \|\delta_x^+ e^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \qquad 0\le n\le\frac{T}{\tau}. \tag{7.31}$$

Thus, by taking the minimum, we have the ε-independent convergence rate as

$$\|e^{\varepsilon,n}\|_2 + \|\delta_x^+ e^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^{4/(6-\alpha^*)}, \quad 0 \le n \le \frac{T}{\tau}. \tag{7.32}$$

7.3 Convergence of the SIFD scheme

In order to prove Theorem 7.2 for SIFD, we first establish the following lemmas.

Lemma 7.1 *(Solvability of SIFD) For any given $u^{\varepsilon,0}, u^{\varepsilon,1} \in X_M$, there exists a unique solution $u^{\varepsilon,n} \in X_M$ of (7.14) with (7.15) for $n > 1$.*

Proof: Standard fixed point arguments would apply (see [11]) and we omit the proof for brevity. □

Denote the local truncation error $\eta^{\varepsilon,n} \in X_M$ of SIFD (7.14) with (7.15) and (7.21) for $n \ge 1$ and $j \in \mathcal{T}_M$ as

$$\eta_j^{\varepsilon,n} := (i\delta_t - \varepsilon^2\delta_t^2)u^\varepsilon(x_j,t_n) + \frac{1}{2}(\delta_x^2 u^\varepsilon(x_j,t_{n+1}) + \delta_x^2 u^\varepsilon(x_j,t_{n-1})) + f(|u^\varepsilon(x_j,t_n)|^2)u^\varepsilon(x_j,t_n).$$

Lemma 7.2 *(Local truncation error for SIFD) Under assumption (B), assume that $f \in C^1([0,\infty))$, we have*

$$\|\eta^{\varepsilon,n}\|_2 + \|\delta_x^+ \eta^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \quad 1 \le n \le \frac{T}{\tau} - 1. \tag{7.33}$$

Proof: Using the Taylor expansion and NLSW (7.9), we obtain for $j \in \mathcal{T}_M$ and $n \ge 1$,

$$\begin{aligned}
\eta_j^{\varepsilon,n} =& \frac{i\tau^2}{2}\int_0^1\int_0^\theta\int_{-s}^s u_{ttt}^\varepsilon(x_j,\sigma\tau+t_n)\,d\sigma ds d\theta + \frac{\tau^2}{2}\int_0^1\int_{-\theta}^\theta u_{xxtt}^\varepsilon(x_j,s\tau+t_n)ds d\theta \\
&+ \frac{h^2}{2}\int_0^1\int_0^\theta\int_0^s\int_{-\sigma}^\sigma \sum_{k=\pm1} u_{xxxx}^\varepsilon(x_j+s_1 h, t_n+k\tau)ds_1 d\sigma ds d\theta \\
&- \varepsilon^2\tau^2\int_0^1\int_0^\theta\int_0^s\int_{-\sigma}^\sigma u_{tttt}^\varepsilon(x_j,s_1\tau+t_n)\,ds_1 d\sigma ds d\theta.
\end{aligned}$$

Under assumption (B), using the triangle inequality, for $j \in \mathcal{T}_M$ and $n \ge 1$, we get

$$|\eta_j^{\varepsilon,n}| \lesssim h^2\|\partial_{xxxx}u^\varepsilon\|_{L^\infty} + \tau^2\Big(\|\partial_{ttt}u^\varepsilon\|_{L^\infty} + \varepsilon^2\|\partial_{tttt}u^\varepsilon\|_{L^\infty} + \|\partial_{xxtt}u^\varepsilon\|_{L^\infty}\Big) \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}},$$

where the L^∞-norm means $\|u\|_{L^\infty} := \sup_{0\le t\le T}\sup_{x\in U}|u(x,t)|$. The first conclusion of the lemma then follows. For $1 \le j \le M-2$, applying δ_x^+ to $\eta_j^{\varepsilon,n}$ and using the formula above, noticing $f \in C^1([0,\infty))$, it is easy to check that

$$|\delta_x^+\eta_j^{\varepsilon,n}| \lesssim h^2\|\partial_{xxxxx}u^\varepsilon\|_{L^\infty} + \tau^2\Big(\|\partial_{tttx}u^\varepsilon\|_{L^\infty} + \varepsilon^2\|\partial_{ttttx}u^\varepsilon\|_{L^\infty} + \|\partial_{xxxtt}u^\varepsilon\|_{L^\infty}\Big)$$
$$\lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}.$$

For $j = 0$ and $M-1$, we apply the boundary condition to deduce that $\frac{\partial^k}{\partial t^k}u^\varepsilon(x,t)|_{x\in\partial U} = 0$ for $k \ge 0$, and the equation (7.9) shows that $u_{xx}(x,t)|_{x\in\partial U} = 0$ and $u_{xxxx}(x,t)|_{x\in\partial U} = 0$. Similar as above, we can get

$$|\delta_x^+\eta_0^{\varepsilon,n}| \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \qquad |\delta_x^+\eta_{M-1}^{\varepsilon,n}| \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}. \tag{7.34}$$

Thus, we complete the proof. □

Since $u^{\varepsilon,0}$ and $u^{\varepsilon,1}$ are known, we have the error estimates at the first step.

Lemma 7.3 *(Error bounds at $n = 1$) Under assumptions (A) and (B), we have*

$$\|e^{\varepsilon,1}\|_2 + \|\delta_x^+e^{\varepsilon,1}\|_2 + \|\delta_x^2e^{\varepsilon,1}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \quad \|\delta_t^+e^{\varepsilon,0}\|_2 + \|\delta_t^+\delta_x^+e^{\varepsilon,0}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \tag{7.35}$$

and also

$$\|e^{\varepsilon,1}\|_2 + \|\delta_x^+e^{\varepsilon,1}\|_2 + \|\delta_x^2e^{\varepsilon,1}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad \|\delta_t^+e^{\varepsilon,0}\|_2 + \|\delta_t^+\delta_x^+e^{\varepsilon,0}\|_2 \lesssim 1. \tag{7.36}$$

Proof: By definition, $e^{\varepsilon,0} = \mathbf{0} \in \mathbb{C}^{M+1}$. For $n = 1$, recalling NLSW (7.9) and the choice of $u^{\varepsilon,1}$ (7.21), using the Taylor expansion, we see that for $j \in \mathcal{T}_M$

$$\begin{aligned}
u^\varepsilon(x_j,\tau) =& u_0(x_j) + \tau(i\left(\partial_{xx}u_0(x_j) + f(|u_0(x_j)|^2)u_0(x_j)\right) + \varepsilon^\alpha w^\varepsilon(x_j))\\
&+ \frac{i\tau^2}{2}\varepsilon^{\alpha-2}w^\varepsilon(x_j) + \frac{1}{2}\int_0^\tau u_{ttt}^\varepsilon(x_j,s)\cdot(\tau-s)^2\,ds,\\
u_j^{\varepsilon,1} =& u_0(x_j) + \tau\left[i\left(\partial_{xx}u_0(x_j) + f(|u_0(x_j)|^2)u_0(x_j)\right) + \varepsilon^\alpha w^\varepsilon(x_j)\right]\\
&+ \left[-\tau - i\varepsilon^2\left(i\frac{\tau}{\varepsilon^2} - \frac{\tau^2}{2\varepsilon^4} + O(\tau^3\varepsilon^{-6})\right)\right]\varepsilon^\alpha w^\varepsilon(x_j) + \frac{i\tau h^2}{12}\partial_{xxxx}u_0(x_j + \theta_j^{(1)}h),\\
e_j^{\varepsilon,1} =& -\frac{i\tau h^2}{12}\partial_{xxxx}u_0(x_j + \theta_j^{(1)}h) + \frac{\tau^3}{6}\partial_{ttt}u^\varepsilon(x_j,\theta_j^{(2)}\tau) + O(\frac{\tau^3}{\varepsilon^{4-\alpha}})w^\varepsilon(x_j),
\end{aligned}$$

where $\theta_j^{(1)} \in [-1,1]$, $\theta_j^{(2)} \in [0,1]$ are constants. Noticing that for $\varepsilon \in (0,1]$, $\frac{1}{\varepsilon^{4-\alpha}} \leq \frac{1}{\varepsilon^{4-\alpha^*}}$, it is easy to get the conclusion in (7.35) for $\|e^{\varepsilon,1}\|_2 + \|\delta_x^+ e^{\varepsilon,1}\|_2$ (the boundary case is the same as that in Lemma 7.2) and $\|\delta_t^+ e^{\varepsilon,0}\|_2$. For $1 \leq j \leq M-1$, we get

$$\begin{aligned}
|\delta_x^2 e_j^{\varepsilon,1}| &\lesssim O\left(\frac{\tau^3}{\varepsilon^{4-\alpha}}\right) \cdot \|\partial_{xx} w^\varepsilon\|_{L^\infty(U)} + \tau h \|\partial_{xxxxx} u_0\|_{L^\infty(U)} + \int_0^\tau s^2 ds \|\partial_{tttxx} u^\varepsilon\|_{L^\infty(U_T)} \\
&\lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \\
|\delta_t^+ \delta_x^+ e^{\varepsilon,0}| &\lesssim O\left(\frac{\tau^2}{\varepsilon^{4-\alpha}}\right) \|\partial_x w^\varepsilon\|_{L^\infty(U)} + h^2 \|\partial_{xxxxx} u_0\|_{L^\infty(U)} + \tau^2 \|\partial_{tttx} u^\varepsilon\|_{L^\infty(U_T)} \\
&\lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}},
\end{aligned}$$

which implies the results for $\|\delta_t^+ \delta_x^+ e^{\varepsilon,0}\|_2$ (the boundary case is similar as above) and $\|\delta_x^2 e^{\varepsilon,1}\|_2$ in (7.35).

For the assertion (7.36), we use the relation between $u(x,t)$ and $u^\varepsilon(x,t)$. Taylor expansion would give for $1 \leq j \leq M-1$

$$\begin{aligned}
&u(x_j,\tau) - u_j^{\varepsilon,1} \\
&= -\frac{i\tau h^2}{24} \partial_{xxxx} u_0(x_j + \theta_j^2 h) + \int_0^\tau u_{tt}(x_j,s)(\tau - s)\, ds + i\varepsilon^{2+\alpha}(e^{i\tau/\varepsilon^2} - 1) w^\varepsilon(x_j),
\end{aligned}$$

and

$$\begin{aligned}
|\delta_x^+ \left(u(x_j,\tau) - u_j^{\varepsilon,1}\right)| &\lesssim \tau h^2 \|\partial_{xxxxx} u_0\|_{L^\infty} + \tau^2 \|\partial_{ttx} u\|_{L^\infty} + \varepsilon^2 \|\partial_x w^\varepsilon\|_{L^\infty}, \\
|\delta_x^2 \left(u(x_j,\tau) - u_j^{\varepsilon,1}\right)| &\lesssim \tau h \|\partial_{xxxxx} u_0\|_{L^\infty} + \tau^2 \|\partial_{ttxx} u\|_{L^\infty} + \varepsilon^2 \|\partial_{xx} w^\varepsilon\|_{L^\infty},
\end{aligned}$$

it is convenient to use the boundary condition as before to find that

$$\|u(x_j,\tau) - u_j^{\varepsilon,1}\|_2 + \|\delta_x^+ \left(u(x_j,\tau) - u_j^{\varepsilon,1}\right)\|_2 + \|\delta_x^2 \left(u(x_j,\tau) - u_j^{\varepsilon,1}\right)\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2.$$

Recalling the convergence $|u^\varepsilon(x_j,\tau) - u(x_j,\tau)| \lesssim \varepsilon^2$ and

$$\begin{aligned}
\left|\delta_x^+ \left[u^\varepsilon(x_j,\tau) - u(x_j,\tau)\right]\right| &\lesssim \varepsilon^2 + h^2(\|u_{xxx}\|_{L^\infty(U_T)} + \|u_{xxx}^\varepsilon\|_{L^\infty(U_T)}),\ j = 0,1,\ldots,M-1, \\
\left|\delta_x^2 \left[u^\varepsilon(x_j,\tau) - u(x_j,\tau)\right]\right| &\lesssim \varepsilon^2 + h^2(\|u_{xxxx}\|_{L^\infty(U_T)} + \|u_{xxxx}^\varepsilon\|_{L^\infty(U_T)}),\ j = 1,\ldots,M-1,
\end{aligned}$$

the triangular inequality then gives the conclusion for $\|e^{\varepsilon,1}\|_2 + \|\delta_x^+ e^{\varepsilon,1}\|_2 + \|\delta_x^2 e^{\varepsilon,1}\|_2$ in (7.36).

Similarly, for $0 \le j \le M-1$

$$\left|\delta_t^+\left(u(x_j,0)-u_j^{\varepsilon,0}\right)\right| \lesssim h^2\|\partial_{xxxx}u_0\|_{L^\infty(U)}+\tau\|\partial_{tt}u\|_{L^\infty(U_T)}+\varepsilon^\alpha\|w^\varepsilon\|_{L^\infty(U)},$$
$$\left|\delta_t^+\delta_x^+\left(u(x_j,0)-u_j^{\varepsilon,0}\right)\right| \lesssim h^2\|\partial_{xxxxx}u_0\|_{L^\infty(U)}+\tau\|\partial_{ttx}u\|_{L^\infty(U_T)}+\varepsilon^\alpha\|\partial_x w^\varepsilon\|_{L^\infty(U)},$$

combined with the triangle inequality and assumption (B) which implies

$$\left|\delta_t^+u^\varepsilon(x_j,0)-\delta_t^+u(x_j,0)\right|+\left|\delta_t^+\delta_x^+u^\varepsilon(x_j,0)-\delta_t^+\delta_x^+u(x_j,0)\right|\lesssim 1, \tag{7.37}$$

we draw conclusion (7.36) for $\|\delta_t^+e^{\varepsilon,0}\|_2+\|\delta_t^+\delta_x^+e^{\varepsilon,0}\|_2$. □

One main difficulty in deriving error bounds for SIFD and/or in high dimensions is the l^∞ bounds for the finite difference solutions. In [6, 13, 145], this difficulty was overcome by truncating the nonlinearity f to a global Lipschitz function with compact support in d-dimensions ($d = 1, 2, 3$). This is guaranteed if the continuous solution is bounded and the numerical solution is not far away from the analytical solution. Here, we could apply the same idea. Choose a smooth function $\rho(s) \in C^\infty(\mathbb{R}^1)$ such that

$$\rho(s)=\begin{cases}1, & 0\le|s|\le 1\,,\\ \in[0,1], & 1\le|s|\le 2\,,\\ 0, & |s|\ge 2\,.\end{cases} \tag{7.38}$$

By assumption (B), we can define

$$M_0=\max\left\{\|u(x,t)\|_{L^\infty(U_T)},\ \sup_{\varepsilon\in(0,1]}\|u^\varepsilon(x,t)\|_{L^\infty(U_T)}\right\} \tag{7.39}$$

and choose a positive number $B = (M_0 + 1)^2$. For $s \ge 0$ and $z \in \mathbb{C}$, define

$$f_B(s)=f(s)\rho(s/B),\ F_B(s)=\int_0^s f_B(\sigma)d\sigma,\ \rho_{_B}(s)=\rho(s/B),\ g_{_B}(z)=z\rho_{_B}(|z|^2). \tag{7.40}$$

Then $f_B(s)$ and $g_{_B}(z)$ are global Lipschitz and

$$|f_B(s_1)-f_B(s_2)|\le C_B|\sqrt{s_1}-\sqrt{s_2}|,\quad \forall s_1,s_2\ge 0. \tag{7.41}$$

Choose $v^{\varepsilon,0}=u^{\varepsilon,0}$, $v^{\varepsilon,1}=u^{\varepsilon,1}$, and define $v^{\varepsilon,n}\in X_M$ $(n\ge 1)$ for $j\in\mathcal{T}_M$ as

$$\left(i\delta_t-\varepsilon^2\delta_t^2\right)v_j^{\varepsilon,n}+\frac{1}{2}(\delta_x^2v_j^{\varepsilon,n+1}+\delta_x^2v_j^{\varepsilon,n-1})+f_B(|v_j^{\varepsilon,n}|^2)v_j^{\varepsilon,n}=0. \tag{7.42}$$

In fact, $v^{\varepsilon,n}$ can be viewed as another approximation of $u^\varepsilon(x,t_n)$.

Define the 'error' function $\hat{e}^{\varepsilon,n} \in X_M$ as

$$\hat{e}_j^{\varepsilon,n} := u^\varepsilon(x_j,t_n) - v_j^{\varepsilon,n}, \quad j \in \mathcal{T}_M^0,\ n \geq 0, \tag{7.43}$$

and the local truncation error $\hat{\eta}^{\varepsilon,n} \in X_M$ for $n \geq 1$ and $j \in \mathcal{T}_M$ as

$$\hat{\eta}_j^{\varepsilon,n} := (i\delta_t - \varepsilon^2\delta_t^2 + f_B(|u^\varepsilon(x_j,t_n)|^2))u^\varepsilon(x_j,t_n) + \frac{1}{2}(\delta_x^2 u^\varepsilon(x_j,t_{n+1}) + \delta_x^2 u^\varepsilon(x_j,t_{n-1})). \tag{7.44}$$

Similar as Lemma 7.2, we have the bounds for $\hat{\eta}^{\varepsilon,n}$ $(n \geq 1)$ as

$$\|\hat{\eta}^{\varepsilon,n}\|_2 + \|\delta_x^+\hat{\eta}^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}. \tag{7.45}$$

Subtracting (7.42) from (7.44), we obtain the 'error' equation for $\hat{e}^{\varepsilon,n} \in X_M$ as

$$\left(i\delta_t - \varepsilon^2\delta_t^2\right)\hat{e}_j^{\varepsilon,n} + \frac{1}{2}(\delta_x^2\hat{e}_j^{\varepsilon,n+1} + \delta_x^2\hat{e}_j^{\varepsilon,n-1}) - \hat{\eta}_j^{\varepsilon,n} + \xi_j^{\varepsilon,n} = 0, \tag{7.46}$$

where $\xi^{\varepsilon,n} \in X_M$ $(n \geq 1)$ is defined for $j \in \mathcal{T}_M$ as

$$\xi_j^{\varepsilon,n} = f_B(|v_j^{\varepsilon,n}|^2)\hat{e}_j^{\varepsilon,n} + u^\varepsilon(x_j,t_n)\left(f_B(|u^\varepsilon(x_j,t_n)|^2) - f_B(|v_j^{\varepsilon,n}|^2)\right). \tag{7.47}$$

For $\xi^{\varepsilon,n}$, we have the following properties.

Lemma 7.4 *Under the assumptions in Theorem 7.2, for $\xi^{\varepsilon,n} \in X_M$ $(n \geq 1)$ in (7.47), we have*

$$|\xi_j^{\varepsilon,n}| \lesssim |\hat{e}_j^{\varepsilon,n}|, \qquad |\delta_x^+\xi_j^{\varepsilon,n}| \lesssim |\hat{e}_j^{\varepsilon,n}| + |\hat{e}_{j+1}^{\varepsilon,n}| + |\delta_x^+\hat{e}_j^{\varepsilon,n}|, \quad 0 \leq j \leq M-1,\ 1 \leq n \leq \frac{T}{\tau}. \tag{7.48}$$

Proof: Using the properties of $f_B(s)$, it is easy to obtain

$$|\xi_j^{\varepsilon,n}| \lesssim |\hat{e}_j^{\varepsilon,n}|, \quad j \in \mathcal{T}_M^0,\ n \geq 1. \tag{7.49}$$

For $0 \leq j \leq M-1$, $n \geq 1$ and $\theta \in [0,1]$, denote

$$u_{j,\theta}^\varepsilon = \theta u^\varepsilon(x_{j+1},t_n) + (1-\theta)u^\varepsilon(x_j,t_n), \quad v_{j,\theta}^\varepsilon = \theta v_{j+1}^{\varepsilon,n} + (1-\theta)v_j^{\varepsilon,n}, \tag{7.50}$$

then we have

$$\delta_x^+\xi_j^{\varepsilon,n} = \delta_x^+\left(f(|u^\varepsilon(x_j,t_n)|^2)u^\varepsilon(x_j,t_n)\right) - \delta_x^+\left(f(|v_j^{\varepsilon,n}|^2)v_j^{\varepsilon,n}\right) = I_1 - I_2 \qquad \text{with}$$

$$I_1 = \int_0^1 \left[\left(f_B(|u_{j,\theta}^\varepsilon|^2) + f_B'(|u_{j,\theta}^\varepsilon|^2)|u_{j,\theta}^\varepsilon|^2\right)\delta_x^+u^\varepsilon(x_j,t_n) + f_B'(|u_{j,\theta}^\varepsilon|^2)(u_{j,\theta}^\varepsilon)^2\delta_x^+\overline{u^\varepsilon(x_j,t_n)}\right]d\theta,$$

$$I_2 = \int_0^1 \left[\left(f_B(|v_{j,\theta}^\varepsilon|^2) + f_B'(|v_{j,\theta}^\varepsilon|^2)|v_{j,\theta}^\varepsilon|^2\right)\delta_x^+v_j^{\varepsilon,n} + f_B'(|v_{j,\theta}^\varepsilon|^2)(v_{j,\theta}^\varepsilon)^2\overline{\delta_x^+v_j^{\varepsilon,n}}\right]d\theta.$$

Using the definition of f_B, it is easy to see $f_B \in C_0^2(\mathbb{R})$ and the following holds

$$\left| \left[\left(f_B(|u^\varepsilon_{j,\theta}|^2) + f'_B(|u^\varepsilon_{j,\theta}|^2)|u^\varepsilon_{j,\theta}|^2\right) - \left(f_B(|v^\varepsilon_{j,\theta}|^2) + f'_B(|v^\varepsilon_{j,\theta}|^2)|v^\varepsilon_{j,\theta}|^2\right) \right] \delta_x^+ u^\varepsilon(x_j, t_n) \right|$$
$$\lesssim \left| \, |u^\varepsilon_{j,\theta}| - |v^\varepsilon_{j,\theta}| \, \right| \lesssim |\hat{e}^{\varepsilon,n}_j| + |\hat{e}^{\varepsilon,n}_{j+1}|,$$
$$\left| \left[f'_B(|u^\varepsilon_{j,\theta}|^2)(u^\varepsilon_{j,\theta})^2 - f'_B(|v^\varepsilon_{j,\theta}|^2)(v^\varepsilon_{j,\theta})^2 \right] \overline{\delta_x^+ u^\varepsilon(x_j, t_n)} \right| \lesssim \left||u^\varepsilon_{j,\theta}| - |v^\varepsilon_{j,\theta}|\right| \lesssim |\hat{e}^{\varepsilon,n}_j| + |\hat{e}^{\varepsilon,n}_{j+1}|,$$
$$\left| \left[f_B(|v^\varepsilon_{j,\theta}|^2) + f'_B(|v^\varepsilon_{j,\theta}|^2)|v^\varepsilon_{j,\theta}|^2 \right] (\delta_x^+ u^\varepsilon(x_j, t_n) - \delta_x^+ v^{\varepsilon,n}_j) \right| \lesssim |\delta_x^+ \hat{e}^{\varepsilon,n}_j|,$$
$$\left| f'_B(|v^\varepsilon_{j,\theta}|^2)(v^\varepsilon_{j,\theta})^2 \left(\overline{\delta_x^+ u^\varepsilon(x_j, t_n)} - \overline{\delta_x^+ v^{\varepsilon,n}_j} \right) \right| \lesssim |\delta_x^+ \hat{e}^{\varepsilon,n}_j|.$$

Hence, we get

$$|\delta_x^+ \hat{e}^{\varepsilon,n}_j| \lesssim |\hat{e}^{\varepsilon,n}_j| + |\hat{e}^{\varepsilon,n}_{j+1}| + |\delta_x^+ \hat{e}^{\varepsilon,n}_j|, \quad 0 \le j \le M-1, \, n \ge 1. \tag{7.51}$$

The proof is complete. □

Proof of Theorem 7.2: The proof is divided into 3 main steps.

Step 1. To establish (7.30)-type error bound for $\hat{e}^{\varepsilon,n}$. From the 'error' equation (7.46), multiplying both sides of (7.46) by $\overline{\hat{e}^{\varepsilon,n+1}_j + \hat{e}^{\varepsilon,n-1}_j}$ and summing for $j \in \mathcal{T}_M$, using summation by parts formula, taking imaginary parts, we have

$$\|\hat{e}^{\varepsilon,n+1}\|_2^2 + 4\varepsilon^2 \,\mathrm{Im}\left(\hat{e}^{\varepsilon,n}, \delta_t^+ \hat{e}^{\varepsilon,n}\right) - \left\{\|\hat{e}^{\varepsilon,n-1}\|_2^2 + 4\varepsilon^2 \,\mathrm{Im}\left(\hat{e}^{\varepsilon,n-1}, \delta_t^+ \hat{e}^{\varepsilon,n-1}\right)\right\}$$
$$= -2\tau \mathrm{Im}\left(\xi^{\varepsilon,n} - \hat{\eta}^{\varepsilon,n}, \hat{e}^{\varepsilon,n+1} + \hat{e}^{\varepsilon,n-1}\right), \quad n \ge 1. \tag{7.52}$$

Adding (7.52) for $1, 2, \ldots, n$ ($n \le \frac{T}{\tau} - 1$), in view of Lemma 7.4 and the local truncation 'error' (7.44), we have

$$\|\hat{e}^{\varepsilon,n+1}\|_2^2 + \|\hat{e}^{\varepsilon,n}\|_2^2 + 4\varepsilon^2 \mathrm{Im}\left(\hat{e}^{n}, \delta_t^+ \hat{e}^{\varepsilon,n}\right) \lesssim n\tau \left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2 + \tau \sum_{m=1}^{n+1} \|\hat{e}^{\varepsilon,m}\|_2^2. \tag{7.53}$$

Multiplying both sides of (7.46) by $\overline{\hat{e}^{\varepsilon,n+1}_j - \hat{e}^{\varepsilon,n-1}_j}$ and summing for $j \in \mathcal{T}_M$, using summation by parts formula, taking real parts, we have

$$-(\varepsilon^2 \|\delta_t^+ \hat{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^+ \hat{e}^{\varepsilon,n+1}\|_2^2) + (\varepsilon^2 \|\delta_t^+ \hat{e}^{\varepsilon,n-1}\|_2^2 + \frac{1}{2}\|\delta_x^+ \hat{e}^{\varepsilon,n-1}\|_2^2)$$
$$= -\,\mathrm{Re}\left(\xi^{\varepsilon,n} - \hat{\eta}^{\varepsilon,n}, \hat{e}^{\varepsilon,n+1} - \hat{e}^{\varepsilon,n-1}\right). \tag{7.54}$$

Noticing that

$$\begin{aligned}&\left|\mathrm{Re}\left(\xi^{\varepsilon,n}-\hat{\eta}^{\varepsilon,n},\hat{e}^{\varepsilon,n+1}-\hat{e}^{\varepsilon,n-1}\right)\right|=\tau\left|\mathrm{Re}\left(\xi^{\varepsilon,n}-\hat{\eta}^{\varepsilon,n},\delta_t^+\hat{e}^{\varepsilon,n}+\delta_t^+\hat{e}^{\varepsilon,n-1}\right)\right|\\&\leq\frac{C\tau}{\varepsilon^2}\left[\left(h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2+\|\hat{e}^{\varepsilon,n}\|_2^2\right]+\tau\varepsilon^2\left(\|\delta_t^+\hat{e}^{\varepsilon,n-1}\|_2^2+\|\delta_t^+\hat{e}^{\varepsilon,n}\|_2^2\right),\end{aligned}$$

combined with (7.54), taking summation for $1,2,\ldots,n$ and using Lemma 7.3, we find that

$$\begin{aligned}&\varepsilon^2\|\delta_t^+\hat{e}^{\varepsilon,n}\|_2^2+\frac{1}{2}\|\delta_x^+\hat{e}^{\varepsilon,n+1}\|_2^2+\frac{1}{2}\|\delta_x^+e^{\varepsilon,n}\|_2^2\\&\lesssim\frac{n\tau}{\varepsilon^2}\left(h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2+\tau\sum_{m=1}^{n}\varepsilon^2\|\delta_t^+\hat{e}^{\varepsilon,m}\|_2^2+\tau\sum_{m=1}^{n+1}\frac{1}{\varepsilon^2}\|\hat{e}^{\varepsilon,m}\|_2^2,\quad 1\leq n\leq\frac{T}{\tau}-1.\end{aligned}\tag{7.55}$$

For $1\leq n\leq\frac{T}{\tau}-1$, define

$$\mathcal{S}^n=8\left(\varepsilon^2\|\delta_t^+\hat{e}^{\varepsilon,n}\|_2^2+\frac{1}{2}\|\delta_x^+\hat{e}^{\varepsilon,n+1}\|_2^2+\frac{1}{2}\|\delta_x^+\hat{e}^{\varepsilon,n}\|_2^2\right)+\frac{1}{2\varepsilon^2}\left(\|\hat{e}^{\varepsilon,n+1}\|_2^2+\|\hat{e}^{\varepsilon,n}\|_2^2\right).\tag{7.56}$$

In view of the Cauchy inequality which implies

$$8\varepsilon^2\|\delta_t^+\hat{e}^{\varepsilon,n}\|_2^2+\frac{1}{2\varepsilon^2}\|\hat{e}^{\varepsilon,n}\|_2^2\geq 4|\left(\delta_t^+\hat{e}^{\varepsilon,n},\hat{e}^{\varepsilon,n}\right)|,$$

together with $\frac{1}{\varepsilon^2}\times$ (7.53) $+\,16\times$ (7.55), we obtain

$$\mathcal{S}^n\lesssim\frac{n\tau}{\varepsilon^2}(h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}})^2+\tau\sum_{m=1}^{n}\mathcal{S}^m,\quad 1\leq n\leq\frac{T}{\tau}-1.\tag{7.57}$$

Hence, discrete Gronwall inequality [46, 67] implies that for τ small enough,

$$\mathcal{S}^n\lesssim\frac{1}{\varepsilon^2}\left(h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2,\quad 1\leq n\leq\frac{T}{\tau}-1.\tag{7.58}$$

In particular, we have established the l^2 error bounds

$$\|\hat{e}^{\varepsilon,n}\|_2\lesssim h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}},\quad n\leq\frac{T}{\tau}.\tag{7.59}$$

However, the discrete H^1 convergence is not optimal. In order to derive the optimal convergence rate in discrete semi-H^1 norm, multiplying both sides of (7.46) by $\overline{\delta_x^2(\hat{e}_j^{\varepsilon,n+1}+\hat{e}_j^{\varepsilon,n-1})}$, then summing together for $j=1,2,\ldots,M-1$, after taking the imaginary parts of both sides and applying the summation by parts formula, using the l^2 error estimates (7.59), we have

$$
\begin{aligned}
&\|\delta_x^+ \hat{e}^{\varepsilon,n+1}\|_2^2 + 4\varepsilon^2 \,\mathrm{Im}\left(\delta_x^+ \hat{e}^{\varepsilon,n}, \delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n}\right) - \left\{\|\delta_x^+ \hat{e}^{\varepsilon,n-1}\|_2^2 + 4\varepsilon^2 \,\mathrm{Im}\left(\delta_x^+ \hat{e}^{\varepsilon,n-1}, \delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n-1}\right)\right\} \\
&= -2\tau \,\mathrm{Im}\left\langle \xi^{\varepsilon,n} - \hat{\eta}^{\varepsilon,n}, \delta_x^2(\hat{e}^{\varepsilon,n+1} + \hat{e}^{\varepsilon,n-1})\right\rangle = 2\tau \mathrm{Im}\left(\delta_x^+ \xi^{\varepsilon,n} - \delta_x^+ \hat{\eta}^{\varepsilon,n}, \delta_x^+ \hat{e}^{\varepsilon,n+1} + \delta_x^+ \hat{e}^{\varepsilon,n-1}\right) \\
&\leq C\tau \left[\|\delta_x^+ \hat{e}^{\varepsilon,n+1}\|_2^2 + \|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + \|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + \|\hat{e}^{\varepsilon,n}\|_2^2 + \left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2\right] \\
&\leq C\tau \left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2 + C\tau(\|\delta_x^+ \hat{e}^{\varepsilon,n+1}\|_2^2 + \|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + \|\delta_x^+ \hat{e}^{\varepsilon,n-1}\|_2^2), \quad 1 \leq n \leq \frac{T}{\tau} - 1.
\end{aligned}
$$

Summing above inequalities for $1, 2, \ldots, n$ and making use of Lemma 7.3, we then have

$$
\begin{aligned}
&\|\delta_x^+ \hat{e}^{\varepsilon,n+1}\|_2^2 + \|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + 4\varepsilon^2 \,\mathrm{Im}\left(\delta_x^+ \hat{e}^{\varepsilon,n}, \delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n}\right) \\
&\leq n\tau \left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2 + \tau \sum_{m=1}^{n+1} \|\delta_x^+ \hat{e}^{\varepsilon,m}\|_2^2 + \sum_{m=0}^{1} \|\delta_x^+ \hat{e}^{\varepsilon,m}\|_2^2 + 4\varepsilon^2 \,\mathrm{Im}\left(\delta_x^+ \hat{e}^{\varepsilon,0}, \delta_t^+ \delta_x \hat{e}^{\varepsilon,1}\right) \\
&\lesssim \left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2 + \tau \sum_{m=1}^{n+1} \|\delta_x^+ \hat{e}^{\varepsilon,m}\|_2^2, \qquad 1 \leq n \leq \frac{T}{\tau} - 1. \qquad (7.60)
\end{aligned}
$$

Multiplying both sides of (7.46) by $\overline{\delta_x^2(\hat{e}_j^{\varepsilon,n+1} - \hat{e}_j^{\varepsilon,n-1})}$, summing up together for $j = 1, 2, \ldots, M-1$, then taking the real parts both sides and applying the summation by parts formula, using the l^2 error estimates (7.59) and the local truncation error (7.44), we have for $n \geq 1$

$$
\begin{aligned}
&\varepsilon^2 \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^2 \hat{e}^{\varepsilon,n+1}\|_2^2 - \varepsilon^2 \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n-1}\|_2^2 - \frac{1}{2}\|\delta_x^2 \hat{e}^{\varepsilon,n-1}\|_2^2 \\
&= \mathrm{Re}\left\langle \xi^{\varepsilon,n} - \hat{\eta}^{\varepsilon,n}, \delta_x^2(\hat{e}_j^{\varepsilon,n+1} - \hat{e}_j^{\varepsilon,n-1})\right\rangle = -\mathrm{Re}\left(\delta_x^+ \xi^{\varepsilon,n} - \delta_x^+ \hat{\eta}^{\varepsilon,n}, \delta_x^+(\hat{e}_j^{\varepsilon,n+1} - \hat{e}_j^{\varepsilon,n-1})\right) \\
&= -\tau \mathrm{Re}\left(\delta_x^+ \xi^{\varepsilon,n} - \delta_x^+ \hat{\eta}^{\varepsilon,n}, \delta_t^+ \delta_x^+ \hat{e}_j^{\varepsilon,n} + \delta_t^+ \delta_x^+ \hat{e}_j^{\varepsilon,n-1})\right) \\
&\leq \tau \left(\varepsilon^2 \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n-1}\|_2^2 + \varepsilon^2 \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2\right) + \frac{C\tau}{\varepsilon^2}\|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + \frac{C\tau}{\varepsilon^2}\left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2.
\end{aligned}
$$

Summing the above inequalities together for $1, 2, \ldots, n$ and using Lemma 7.3, we find that

$$
\begin{aligned}
&\varepsilon^2 \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^2 \hat{e}^{\varepsilon,n+1}\|_2^2 + \frac{1}{2}\|\delta_x^2 \hat{e}^{\varepsilon,n}\|_2^2 \\
&\lesssim \tau \sum_{m=1}^{n} \varepsilon^2 \|\delta_t^+ \hat{e}^{\varepsilon,m}\|_2^2 + \frac{\tau}{\varepsilon^2} \sum_{m=1}^{n+1} \|\delta_x^+ \hat{e}^{\varepsilon,m}\|_2^2 + \|\delta_x^+ \hat{e}^{\varepsilon,1}\|_2^2 + \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,0}\|_2^2 + \frac{1}{\varepsilon^2}\left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2 \\
&\lesssim \tau \sum_{m=1}^{n} \varepsilon^2 \|\delta_t^+ \delta_x^+ \hat{e}^{\varepsilon,m}\|_2^2 + \frac{\tau}{\varepsilon^2} \sum_{m=1}^{n+1} \|\delta_x^+ \hat{e}^{\varepsilon,m}\|_2^2 + \frac{1}{\varepsilon^2}\left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2, \quad 1 \leq n \leq \frac{T}{\tau} - 1.
\end{aligned}
\qquad (7.61)
$$

In view of (7.60) and (7.61), define $\mathcal{T}^n$ for $n \geq 1$ as

$$\mathcal{T}^n = 8\left(\varepsilon^2\|\delta_t^+\delta_x^+\hat{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^2\hat{e}^{\varepsilon,n+1}\|_2^2 + \frac{1}{2}\|\delta_x^2\hat{e}^{\varepsilon,n}\|_2^2\right) + \frac{1}{2\varepsilon^2}\left(\|\delta_x^+\hat{e}^{\varepsilon,n+1}\|_2^2 + \|\delta_x^+\hat{e}^{\varepsilon,n}\|_2^2\right).$$

Again, Cauchy inequality with $\frac{1}{\varepsilon^2} \times (7.60) + 16 \times (7.61)$ will give that

$$\mathcal{T}^n \lesssim \frac{1}{\varepsilon^2}\left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2 + \tau\sum_{m=1}^{n}\mathcal{T}^m, \quad 1 \leq n \leq \frac{T}{\tau} - 1. \tag{7.62}$$

Then the discrete Gronwall inequality [46,67] will imply that for τ small enough,

$$\mathcal{T}^n \lesssim \frac{1}{\varepsilon^2}\left(h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}\right)^2, \qquad 1 \leq n \leq \frac{T}{\tau} - 1. \tag{7.63}$$

Hence, the discrete-H^1 bounds for the 'error' $\hat{e}^{\varepsilon,n}$ holds as

$$\|\delta_x^+\hat{e}^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \qquad n \leq \frac{T}{\tau}. \tag{7.64}$$

Step 2. To prove (7.31)-type error bound for $\hat{e}^{\varepsilon,n}$. For the approximation $v^{\varepsilon,n} \in X_M$ defined in (7.42), introduce the 'biased error' function $\tilde{e}^{\varepsilon,n} \in X_M$, i.e. the difference between $v^{\varepsilon,n}$ and the solution $u(x,t_n)$ of NLSE (7.10), for $j \in \mathcal{T}_M$ as

$$\tilde{e}_j^{\varepsilon,n} = u(x_j,t_n) - v_j^{\varepsilon,n}, \quad n \geq 0. \tag{7.65}$$

Define the 'local truncation error' $\tilde{\eta}^{\varepsilon,n} \in X_M$ for $n \geq 1$ and $j \in \mathcal{T}_M$ as

$$\tilde{\eta}_j^{\varepsilon,n} := (i\delta_t - \varepsilon^2\delta_t^2 + f_B(|u(x_j,t_n)|^2))u(x_j,t_n) + \frac{1}{2}(\delta_x^2 u(x_j,t_{n+1}) + \delta_x^2 u(x_j,t_{n-1})). \tag{7.66}$$

Similar as Lemma 7.2, we can prove that under the assumptions in Theorem 7.2,

$$\|\tilde{\eta}^{\varepsilon,n}\|_2 + \|\delta_x^+\tilde{\eta}^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad 1 \leq n \leq \frac{T}{\tau} - 1. \tag{7.67}$$

Subtracting (7.42) from (7.66), we obtain the 'error' equation for $\tilde{e}^{\varepsilon,n} \in X_M$ as

$$\left(i\delta_t - \varepsilon^2\delta_t^2\right)\tilde{e}_j^{\varepsilon,n} + \frac{1}{2}(\delta_x^2\tilde{e}_j^{\varepsilon,n+1} + \delta_x^2\tilde{e}_j^{\varepsilon,n-1}) - \tilde{\eta}_j^{\varepsilon,n} + \tilde{\xi}_j^{\varepsilon,n} = 0, \tag{7.68}$$

where $\tilde{\xi}^{\varepsilon,n} \in X_M$ $(n \geq 1)$ is defined for $j \in \mathcal{T}_M$ as

$$\tilde{\xi}_j^{\varepsilon,n} = f_B(|v_j^{\varepsilon,n}|^2)\tilde{e}_j^{\varepsilon,n} + u(x_j,t_n)\left(f_B(|u(x_j,t_n)|^2) - f_B(|v_j^{\varepsilon,n}|^2)\right). \tag{7.69}$$

Then we have the following properties on $\tilde{\xi}^{\varepsilon,n}$ similar as Lemma 7.4,

$$|\tilde{\xi}_j^{\varepsilon,n}| \lesssim |\tilde{e}_j^{\varepsilon,n}|, \qquad |\delta_x^+\tilde{\xi}_j^{\varepsilon,n}| \lesssim |\tilde{e}_j^{\varepsilon,n}| + |\tilde{e}_{j+1}^{\varepsilon,n}| + |\delta_x^+\tilde{e}_j^{\varepsilon,n}|, \quad 0 \leq j \leq M-1,\ n \geq 1. \tag{7.70}$$

As shown in Lemma 7.3, we have $\tilde{e}^{\varepsilon,0} = 0$ and

$$\|\tilde{e}^{\varepsilon,1}\|_2 + \|\delta_x^+ \tilde{e}^{\varepsilon,1}\|_2 + \|\delta_x^2 \tilde{e}^{\varepsilon,1}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad \|\delta_t^+ \tilde{e}^{\varepsilon,0}\|_2 + \|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,0}\|_2 \lesssim 1. \quad (7.71)$$

From 'error' equation (7.68), multiplying both sides of (7.68) by $\overline{\tilde{e}_j^{\varepsilon,n+1} + \tilde{e}_j^{\varepsilon,n-1}}$ and summing for $j \in \mathcal{T}_M$, using summation by parts formula, taking imaginary parts, we have

$$\begin{aligned} &\|\tilde{e}^{\varepsilon,n+1}\|_2^2 + 4\varepsilon^2 \operatorname{Im}\left(\tilde{e}^{\varepsilon,n}, \delta_t^+ \tilde{e}^{\varepsilon,n}\right) - \left\{\|\tilde{e}^{\varepsilon,n-1}\|_2^2 + 4\varepsilon^2 \operatorname{Im}\left(\tilde{e}^{\varepsilon,n-1}, \delta_t^+ \tilde{e}^{\varepsilon,n-1}\right)\right\} \\ &= -2\tau \operatorname{Im}\left(\tilde{\xi}^{\varepsilon,n} - \tilde{\eta}^{\varepsilon,n}, \tilde{e}^{\varepsilon,n+1} + \tilde{e}^{\varepsilon,n-1}\right), \quad n \geq 1. \end{aligned} \quad (7.72)$$

Adding (7.72) for $1, 2, \ldots, n$ ($n \leq \frac{T}{\tau} - 1$), similar as the proof of (7.27) for $\hat{e}^{\varepsilon,n}$, we have

$$\|\tilde{e}^{\varepsilon,n+1}\|_2^2 + \|\tilde{e}^{\varepsilon,n}\|_2^2 + 4\varepsilon^2 \operatorname{Im}\left(\tilde{e}^{n}, \delta_t^+ \tilde{e}^{\varepsilon,n}\right) \lesssim n\tau \left(h^2 + \tau^2 + \varepsilon^2\right)^2 + \tau \sum_{m=1}^{n+1} \|\tilde{e}^{\varepsilon,m}\|_2^2. \quad (7.73)$$

Multiplying both sides of (7.117) by $\overline{\hat{e}_j^{\varepsilon,n+1} - \hat{e}_j^{\varepsilon,n-1}}$ and summing for $j \in \mathcal{T}_M$, using summation by parts formula, taking real parts, we have

$$\begin{aligned} &-(\varepsilon^2 \|\delta_t^+ \tilde{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^+ \tilde{e}^{\varepsilon,n+1}\|_2^2) + (\varepsilon^2 \|\delta_t^+ \tilde{e}^{\varepsilon,n-1}\|_2^2 + \frac{1}{2}\|\delta_x^+ \tilde{e}^{\varepsilon,n-1}\|_2^2) \\ &= -\operatorname{Re}\left(\tilde{\xi}^{\varepsilon,n} - \tilde{\eta}^{\varepsilon,n}, \tilde{e}^{\varepsilon,n+1} - \tilde{e}^{\varepsilon,n-1}\right), \qquad n \geq 1. \end{aligned} \quad (7.74)$$

Noticing that

$$\begin{aligned} &\left|\operatorname{Re}\left(\tilde{\xi}^{\varepsilon,n} - \tilde{\eta}^{\varepsilon,n}, \tilde{e}^{\varepsilon,n+1} - \tilde{e}^{\varepsilon,n-1}\right)\right| = \tau\left|\operatorname{Re}\left(\tilde{\xi}^{\varepsilon,n} - \tilde{\eta}^{\varepsilon,n}, \delta_t^+ \tilde{e}^{\varepsilon,n} + \delta_t^+ \tilde{e}^{\varepsilon,n-1}\right)\right| \\ &\leq \frac{C\tau}{\varepsilon^2}\left((h^2 + \tau^2 + \varepsilon^2)^2 + \|\tilde{e}^{\varepsilon,n}\|_2^2\right) + \frac{1}{2}\tau\varepsilon^2\left(\|\delta_t^+ \tilde{e}^{\varepsilon,n-1}\|_2^2 + \|\delta_t^+ \tilde{e}^{\varepsilon,n}\|_2^2\right), \end{aligned}$$

summing (7.74) for $1, 2, \ldots, n$ and making use of (7.71), we have

$$\begin{aligned} \varepsilon^2 \|\delta_t^+ \tilde{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^+ \tilde{e}^{\varepsilon,n+1}\|_2^2 + \frac{1}{2}\|\delta_x^+ \tilde{e}^{\varepsilon,n}\|_2^2 &\leq \tau \sum_{m=1}^{n} \varepsilon^2 \|\delta_t^+ \tilde{e}^{\varepsilon,m}\|_2^2 + \tau \sum_{m=1}^{n+1} \frac{1}{\varepsilon^2}\|\tilde{e}^{\varepsilon,m}\|_2^2 \\ &+ n\tau \frac{C}{\varepsilon^2}(h^2 + \tau^2 + \varepsilon^2)^2 + C\varepsilon^2 + C(h^2 + \tau^2 + \varepsilon^2)^2, \quad 1 \leq n \leq \frac{T}{\tau} - 1. \end{aligned} \quad (7.75)$$

Let

$$\mathcal{E}^n = 8(\varepsilon^2 \|\delta_t^+ \tilde{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^+ \tilde{e}^{\varepsilon,n+1}\|_2^2 + \frac{1}{2}\|\delta_x^+ \tilde{e}^{\varepsilon,n}\|_2^2) + \frac{1}{2\varepsilon^2}\left(\|\tilde{e}^{\varepsilon,n+1}\|_2^2 + \|\tilde{e}^{\varepsilon,n}\|_2^2\right), \; n \geq 1, \quad (7.76)$$

then similar as the case of $\hat{e}^{\varepsilon,n}$, using the Cauchy inequality together with (7.75) and (7.73), we have

$$\mathcal{E}^n \lesssim \frac{1}{\varepsilon^2}(h^2 + \tau^2 + \varepsilon^2)^2 + \tau \sum_{m=1}^{n} \mathcal{E}^m, \quad (7.77)$$

and the discrete Gronwall inequality [46, 67] will imply for small τ

$$\mathcal{E}^n \lesssim \frac{1}{\varepsilon^2}(h^2+\tau^2+\varepsilon^2)^2, \quad 1\le n\le \frac{T}{\tau}-1. \tag{7.78}$$

Hence the l^2 estimate holds

$$\|\tilde{e}^{\varepsilon,n}\|_2 \lesssim h^2+\tau^2+\varepsilon^2, \quad n\le \frac{T}{\tau}. \tag{7.79}$$

To prove the corresponding discrete H^1 error estimates, multiplying both sides of (7.68) by $\delta_x^2(\overline{\tilde{e}_j^{\varepsilon,n+1}}+\overline{\tilde{e}_j^{\varepsilon,n-1}})$, summing together for $j=1,2,\ldots,M-1$, summation by parts, taking imaginary parts of both sides and making use of the l^2 estimates and (7.67), we then have

$$\begin{aligned}
&\|\delta_x^+\tilde{e}^{\varepsilon,n+1}\|_2^2+4\varepsilon^2\mathrm{Im}\left(\delta_x^+\tilde{e}^{\varepsilon,n},\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n}\right)-\|\delta_x^+\tilde{e}^{\varepsilon,n-1}\|_2^2-4\varepsilon^2\mathrm{Im}\left(\delta_x^+\tilde{e}^{\varepsilon,n-1},\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n-1}\right)\\
&=-2\tau\,\mathrm{Im}\left\langle\tilde{\xi}^{\varepsilon,n}-\tilde{\eta}^{\varepsilon,n},\delta_x^2(\tilde{e}^{\varepsilon,n+1}+\tilde{e}^{\varepsilon,n-1})\right\rangle=2\tau\,\mathrm{Im}\left(\delta_x^+(\tilde{\xi}^{\varepsilon,n}-\tilde{\eta}^{\varepsilon,n}),\delta_x^+(\tilde{e}^{\varepsilon,n+1}+\tilde{e}^{\varepsilon,n-1})\right)\\
&\le C\tau(\|\delta_x^+\tilde{e}^{\varepsilon,n+1}\|_2^2+\|\delta_x^+\tilde{e}^{\varepsilon,n}\|_2^2+\|\delta_x^+\tilde{e}^{\varepsilon,n-1}\|_2^2+\|\tilde{e}^{\varepsilon,n}\|_2^2)+C\tau(h^2+\tau^2+\varepsilon^2)^2\\
&\le C\tau\left(\|\delta_x^+\tilde{e}^{\varepsilon,n+1}\|_2^2+\|\delta_x^+\tilde{e}^{\varepsilon,n}\|_2^2+\|\delta_x^+\tilde{e}^{\varepsilon,n-1}\|_2^2\right)+C\tau(h^2+\tau^2+\varepsilon^2)^2, \quad 1\le n\le\frac{T}{\tau}-1.
\end{aligned}$$

Adding the above inequalities together for time steps $1,2,\ldots,n$, using Lemma 7.3, we have

$$\|\delta_x^+\tilde{e}^{\varepsilon,n+1}\|_2^2+\|\delta_x^+\tilde{e}^{\varepsilon,n}\|_2^2+4\varepsilon^2\,\mathrm{Im}\left(\delta_x^+\tilde{e}^{\varepsilon,n},\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n}\right)\lesssim(h^2+\tau^2+\varepsilon^2)^2+\tau\sum_{m=1}^{n+1}\|\delta_x^+\tilde{e}^{\varepsilon,m}\|_2^2. \tag{7.80}$$

Multiplying both sides of (7.68) by $\overline{\delta_x^2(\tilde{e}_j^{\varepsilon,n+1}-\tilde{e}_j^{\varepsilon,n-1})}$, summing together for $j=1,2,\ldots,M-1$, summation by parts, taking real parts of both sides and making use of the l^2 estimates and (7.67), we get for $1\le n\le\frac{T}{\tau}-1$

$$\begin{aligned}
&\varepsilon^2\|\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n}\|_2^2+\frac{1}{2}\|\delta_x^2\tilde{e}^{\varepsilon,n+1}\|_2^2-\varepsilon^2\|\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n-1}\|_2^2-\frac{1}{2}\|\delta_x^2\tilde{e}^{\varepsilon,n-1}\|_2^2\\
&=\mathrm{Re}\left\langle\tilde{\xi}^{\varepsilon,n}-\tilde{\eta}^{\varepsilon,n},\delta_x^2(\tilde{e}^{\varepsilon,n+1}-\tilde{e}^{\varepsilon,n-1})\right\rangle=-\mathrm{Re}\left(\delta_x^+\tilde{\xi}^{\varepsilon,n}-\delta_x^+\tilde{\eta}^{\varepsilon,n},\delta_x^+(\tilde{e}^{\varepsilon,n+1}-\tilde{e}^{\varepsilon,n-1})\right)\\
&=-\tau\mathrm{Re}\left(\delta_x^+\tilde{\xi}^{\varepsilon,n}-\delta_x^+\tilde{\eta}^{\varepsilon,n},\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n+1}+\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n-1}\right)\\
&\le C\tau\left(\varepsilon^2\|\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n+1}\|_2^2+\varepsilon^2\|\delta_t^+\delta_x^+\tilde{e}^{\varepsilon,n-1}\|_2^2\right)+\frac{C\tau}{\varepsilon^2}\left[\|\delta_x^+\tilde{e}^{\varepsilon,n}\|_2^2+\|\tilde{e}^{\varepsilon,n}\|_2^2\right]\\
&\qquad+\frac{C\tau}{\varepsilon^2}(h^2+\tau^2+\varepsilon^2)^2.
\end{aligned}$$

Summing the above inequalities for time steps $1, 2, \ldots, n$, using Lemma 7.3 on the error of $\|\delta_x^2 \tilde{e}^{\varepsilon,1}\|_2$ and $\|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,0}\|_2$, we have for $1 \le n \le \frac{T}{\tau} - 1$

$$
\begin{aligned}
&\varepsilon^2 \|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^2 \tilde{e}^{\varepsilon,n+1}\|_2^2 + \frac{1}{2}\|\delta_x^2 \tilde{e}^{\varepsilon,n}\|_2^2 \le \varepsilon^2 \|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,0}\|_2^2 + \|\delta_x^2 \tilde{e}^{\varepsilon,1}\|_2^2 \\
&+ C\varepsilon^2 \tau \sum_{m=1}^{n} \|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,m}\|_2^2 + \frac{1}{\varepsilon^2}\left(\tau \sum_{m=1}^{n+1} \|\delta_x^+ \tilde{e}^{\varepsilon,m}\|_2^2 + n\tau C(h^2 + \tau^2 + \varepsilon^2)^2\right) \\
&\lesssim \varepsilon^2 \tau \sum_{m=1}^{n} \|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,m}\|_2^2 + \frac{\tau}{\varepsilon^2} \sum_{m=1}^{n+1} \|\delta_x^+ \tilde{e}^{\varepsilon,m}\|_2^2 + \frac{1}{\varepsilon^2}(h^2 + \tau^2 + \varepsilon^2)^2. \qquad (7.81)
\end{aligned}
$$

Similar as before, define $\tilde{\mathcal{E}}^n$ for $n \ge 1$ as

$$
\tilde{\mathcal{E}}^n = 8(\varepsilon^2 \|\delta_t^+ \delta_x^+ \tilde{e}^{\varepsilon,n}\|_2^2 + \frac{1}{2}\|\delta_x^2 \tilde{e}^{\varepsilon,n+1}\|_2^2 + \frac{1}{2}\|\delta_x^2 \tilde{e}^{\varepsilon,n}\|_2^2) + \frac{1}{2\varepsilon^2}\left(\|\delta_x^+ \tilde{e}^{\varepsilon,n+1}\|_2^2 + \|\delta_x^+ \tilde{e}^{\varepsilon,n}\|_2^2\right), \tag{7.82}
$$

combining (7.80) and (7.81), applying the Cauchy inequality, we get

$$
\tilde{\mathcal{E}}^n \lesssim \frac{1}{\varepsilon^2}(h^2 + \tau^2 + \varepsilon^2)^2 + \tau \sum_{m=1}^{n} \tilde{\mathcal{E}}^m, \quad 1 \le n \le \frac{T}{\tau} - 1. \tag{7.83}
$$

The discrete Gronwall inequality [46, 67] implies that for small enough τ

$$
\tilde{\mathcal{E}}^n \lesssim \frac{1}{\varepsilon^2}(h^2 + \tau^2 + \varepsilon^2)^2, \quad 1 \le n \le \frac{T}{\tau} - 1. \tag{7.84}
$$

Hence

$$
\|\delta_x^+ \tilde{e}^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad 1 \le n \le \frac{T}{\tau}. \tag{7.85}
$$

Noticing

$$
\hat{e}_j^{\varepsilon,n} = \tilde{e}_j^{\varepsilon,n} + (u^\varepsilon(x_j, t_n) - u(x_j, t_n)), \quad j \in \mathcal{T}_M,\ n \ge 0, \tag{7.86}
$$

and assumption (B) which implies

$$
\|u^\varepsilon(x_j, t_n) - u(x_j, t_n)\|_2 + \|\delta_x^+ u^\varepsilon(x_j, t_n) - \delta_x^+ u(x_j, t_n)\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad n \ge 0, \tag{7.87}
$$

combining (7.79) and (7.85) together, we then conclude that

$$
\|\hat{e}^{\varepsilon,n}\|_2 + \|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad 0 \le n \le \frac{T}{\tau}. \tag{7.88}
$$

Step 3. To obtain ε-uniform estimate (7.59). From (7.59), (7.64) and (7.88), taking the minimum of ε^2 and $\frac{\varepsilon^2}{\varepsilon^{4-\alpha^*}}$, we get

$$
\|\hat{e}^{\varepsilon,n}\|_2 + \|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^{\frac{4}{6-\alpha^*}}, \quad 0 \le n \le \frac{T}{\tau}. \tag{7.89}
$$

Noticing that $4/(6-\alpha^*) \geq \frac{2}{3}$, using the discrete Sobolev inequality [145]

$$\|\hat{e}^{\varepsilon,n}\|_\infty \leq C\|\delta_x^+ \hat{e}^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^{\frac{4}{6-\alpha^*}}. \tag{7.90}$$

When τ and h become sufficiently small, we have $\|\hat{e}^{\varepsilon,n}\|_\infty \leq 1$, and

$$\|v^{\varepsilon,n}\|_\infty \leq \|u^\varepsilon\|_{L^\infty(U_T)} + \|\hat{e}^{\varepsilon,n}\|_\infty \leq \|u^\varepsilon\|_{L^\infty(U_T)} + 1 \leq \sqrt{B}, \quad n \leq \frac{T}{\tau}. \tag{7.91}$$

Thus, using the properties of $f_B(s)$, scheme (7.42) collapses to SIFD (7.14), and $v^{\varepsilon,n}$ is the solution of SIFD (7.14). In other words, we have proved the results in Theorem 7.2 for SIFD (7.14). □

Remark 7.1 *Here we emphasis that our approach can be extended to the higher dimensions, e.g. 2D and 3D directly. The key point is the discrete Sobolev inequality in 2D and 3D as*

$$\|u_h\|_\infty \leq C|\ln h|\,\|u_h\|_{H_s^1}, \qquad \|v_h\|_\infty \leq Ch^{-1/2}\|v_h\|_{H^1}, \tag{7.92}$$

where u_h and v_h are 2D and 3D mesh functions with zero at the boundary, respectively, and the discrete norms $\|\cdot\|_{H_s^1}$ and $\|\cdot\|_\infty$ can be defined similarly as the discrete semi-H^1 norm and the l^∞ norm in (7.23) or in Chapter 6. The same proof in 2D and 3D will lead to (7.89), and the above Sobolev inequalities will imply (7.91) by noticing that $4/(6-\alpha^*) \geq \frac{2}{3} > \frac{1}{2}$ and the assumption $\tau \lesssim h$.

7.4 Convergence of the CNFD scheme

In order to prove Theorem 7.1 for CNFD, again we first establish the following lemmas.

Lemma 7.5 *(Conservation properties of CNFD) For CNFD scheme (7.12) with (7.15) and (7.21), for any mesh size $h > 0$, time step $\tau > 0$ and initial data (u_0, u_1^ε), it satisfies the mass and energy conservation laws in the discretized level, i.e.,*

$$N_h^\varepsilon(u^{\varepsilon,n}) := \frac{1}{2}\left(\|u^{\varepsilon,n}\|_2^2 + \|u^{\varepsilon,n+1}\|_2^2\right) - 2\varepsilon^2\, Im(\delta_t^+ u^{\varepsilon,n}, u^{\varepsilon,n}) \equiv N_h^\varepsilon(u^{\varepsilon,0}), \qquad n \geq 0, \tag{7.93}$$

$$\begin{aligned} E_h^\varepsilon(u^{\varepsilon,n}) :=& \varepsilon^2\|\delta_t^+ u^{\varepsilon,n}\|_2^2 + \frac{1}{2}\sum_{m=n}^{n+1}\|\delta_x^+ u^{\varepsilon,m}\|_2^2 - \frac{1}{2}h\sum_{j=0}^{M-1}\left(F(|u_j^{\varepsilon,n}|^2) + F(|u_j^{\varepsilon,n+1}|^2)\right) \\ \equiv& E_h^\varepsilon(u^{\varepsilon,0}), \qquad n \geq 0. \end{aligned} \tag{7.94}$$

Proof: Follow the analogous arguments of the CNFD method for NLSE [46, 67] and NLSW [73, 154] and we omit the details here for brevity. □

Lemma 7.6 *(Solvability of the difference equations) For any given $u^{\varepsilon,n-1}$ and $u^{\varepsilon,n}$, there exists a solution $u^{\varepsilon,n+1}$ of the CNFD discretization (7.12) with (7.15). In addition, if the nonlinear term $f(|z|^2)z$ ($z \in \mathbb{C}$) is global Lipschitz, i.e. there exists a constant $C > 0$ such that*

$$\left|f(|z_1|^2)z_1 - f(|z_2|^2)z_2\right| \le C|z_1 - z_2|, \quad \forall z_1, z_2 \in \mathbb{C}, \tag{7.95}$$

then there exists $\tau_0 > 0$ such that the solution is unique when $\tau < \tau_0$.

Proof: The proof is standard for NLSW [73, 154] and we omit it here for brevity. □

Denote the local truncation error $\zeta^{\varepsilon,n} \in X_M$ for CNFD (7.12) with (7.15) and (7.21) for $n \ge 1$ and $j \in \mathcal{T}_M$ as

$$\zeta_j^{\varepsilon,n} := (i\delta_t - \varepsilon^2\delta_t^2)u^\varepsilon(x_j, t_n) + \frac{1}{2}(\delta_x^2 u^\varepsilon(x_j, t_{n+1}) + \delta_x^2 u^\varepsilon(x_j, t_{n-1}) + G(u^\varepsilon(x_j, t_{n+1}), u^\varepsilon(x_j, t_{n-1})).$$

Similar as Lemma 7.2, we can have the following results.

Lemma 7.7 *(Local truncation error for CNFD) Under assumption (B), assume $f \in C^3([0,\infty))$, we have*

$$\|\zeta^{\varepsilon,n}\|_2 + \|\delta_x^+\zeta^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \quad 1 \le n \le \frac{T}{\tau} - 1. \tag{7.96}$$

Proof: For $n \ge 1$ and $j \in \mathcal{T}_M$, expanding Taylor series for nonlinear part G at $|u^\varepsilon(x_j, t_n)|^2$, and noticing (7.13) and the following

$$\begin{aligned}
\Gamma_j^n &:= \frac{1}{\tau}\left(|u^\varepsilon(x_j, t_{n+1})|^2 - |u^\varepsilon(x_j, t_n)|^2\right) = \int_0^1 \partial_t(|u^\varepsilon|^2)(x_j, t_n + s\tau)\,ds, \\
\widetilde{\Gamma}_j^n &:= \frac{2}{\tau^2}\left(\frac{1}{2}\left(|u^\varepsilon(x_j, t_{n+1})|^2 + |u^\varepsilon(x_j, t_{n-1})|^2\right) - |u^\varepsilon(x_j, t_n)|^2\right) \\
&= \int_0^1 \int_{-\theta}^{\theta} \partial_{tt}(|u^\varepsilon|^2)(x_j, t_n + s\tau)\,ds d\theta,
\end{aligned}$$

then applying the Taylor expansion and NLSW (7.9), we obtain

$$\begin{aligned}
\zeta_j^{\varepsilon,n} = & \frac{i\tau^2}{2}\int_0^1\int_0^\theta\int_{-s}^{s} u_{ttt}^\varepsilon(x_j,\sigma\tau+t_n)\,d\sigma ds d\theta + \frac{\tau^2}{2}\int_0^1\int_{-\theta}^{\theta} u_{xxtt}^\varepsilon(x_j,s\tau+t_n)dsd\theta \\
& + \frac{h^2}{2}\int_0^1\int_0^\theta\int_0^s\int_{-\sigma}^{\sigma}\sum_{k=\pm 1} u_{xxxx}^\varepsilon(x_j+s_1h,t_n+k\tau)ds_1 d\sigma ds d\theta \\
& + \left(\tau^2\int_0^1\int_0^1(1-\sigma)(\theta\Gamma_j^n-(1-\theta)\Gamma_j^{n-1})^2 f''(\xi_j(\theta,\sigma))\,d\sigma d\theta + \frac{\tau^2}{2}f'(|u^\varepsilon(x_j,t_n)|^2)\widetilde{\Gamma}_j^n\right) \\
& \cdot\frac{1}{2}\left(u^\varepsilon(x_j,t_{n+1})+u^\varepsilon(x_j,t_{n-1})\right) + \frac{\tau^2}{2}f(|u^\varepsilon(x_j,t_n)|^2)\int_0^1\int_{-\theta}^{\theta} u_{tt}^\varepsilon(x_j,t_n+s\tau)\,dsd\theta \\
& - \varepsilon^2\tau^2\int_0^1\int_0^\theta\int_0^s\int_{-\sigma}^{\sigma} u_{tttt}^\varepsilon(x_j,s_1\tau+t_n)\,ds_1 d\sigma ds d\theta,
\end{aligned}$$

where $\xi_j(\theta,\sigma)=\sigma(\theta|u^\varepsilon(x_j,t_{n+1})|^2+(1-\theta)|u^\varepsilon(x_j,t_{n-1})|^2)+(1-\sigma)|u^\varepsilon(x_j,t_n)|^2$. Under assumption (B), using the triangle inequality, noticing that $f\in C^2([0,\infty))$, for $j\in\mathcal{T}_M$ and $n\geq 1$, we get

$$\begin{aligned}
|\zeta_j^{\varepsilon,n}| \lesssim & h^2\|\partial_{xxxx}u^\varepsilon\|_{L^\infty}+\tau^2\big(\|\partial_{ttt}u^\varepsilon\|_{L^\infty}+\varepsilon^2\|\partial_{tttt}u^\varepsilon\|_{L^\infty}+\|\partial_{tt}u^\varepsilon\|_{L^\infty}\|f(|u^\varepsilon|^2)\|_{L^\infty} \\
& +\|\partial_{xxtt}u^\varepsilon\|_{L^\infty}+\big(\|\partial_t|u^\varepsilon|^2\|_{L^\infty}^2\|f''(|u^\varepsilon|^2)\|_{L^\infty}+\|f'(|u^\varepsilon|^2)\|_{L^\infty}\|\partial_{tt}|u^\varepsilon|^2\|_{L^\infty}\big)\,\|u^\varepsilon\|_{L^\infty}\big) \\
\lesssim & h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}}.
\end{aligned}$$

The first part of the Lemma is proven. For $1\leq j\leq M-1$, in view of the above representation of $\zeta_j^{\varepsilon,n}$ and a similar calculation as above, noticing $f\in C^3([0,\infty))$ when dealing with the nonlinear term G, for $1\leq j\leq M-1$, it is easy to check that

$$\begin{aligned}
|\delta_x^+\zeta_j^{\varepsilon,n}| \lesssim & h^2\|\partial_{xxxxx}u^\varepsilon\|_{L^\infty}+\tau^2\Bigg(\|\partial_{tttx}u^\varepsilon\|_{L^\infty}+\varepsilon^2\|\partial_{ttttx}u^\varepsilon\|_{L^\infty}+\Big[\|\partial_{tt}u^\varepsilon\|_{L^\infty}\|f'(|u^\varepsilon|^2)\|_{L^\infty} \\
& +\big(\|\partial_t|u^\varepsilon|^2\|_{L^\infty}^2\|f'''(|u^\varepsilon|^2)\|_{L^\infty}+\|f''(|u^\varepsilon|^2)\|_{L^\infty}\|\partial_{tt}|u^\varepsilon|^2\|_{L^\infty}\big)\cdot\|u^\varepsilon\|_{L^\infty}\Big] \\
& \cdot\|\partial_x|u^\varepsilon|^2\|_{L^\infty}+\big(\|\partial_x(\partial_t|u^\varepsilon|^2)^2\|_{L^\infty}\|f''(|u^\varepsilon|^2)\|_{L^\infty}+\|f'(|u^\varepsilon|^2)\|_{L^\infty}\|\partial_{ttx}|u^\varepsilon|^2\|_{L^\infty}\big) \\
& \cdot\|u^\varepsilon\|_{L^\infty}+\big(\|\partial_t|u^\varepsilon|^2\|_{L^\infty}^2\|f''(|u^\varepsilon|^2)\|_{L^\infty}+\|f'(|u^\varepsilon|^2)\|_{L^\infty}\|\partial_{tt}|u^\varepsilon|^2\|_{L^\infty}\big)\,\|\partial_x u^\varepsilon\|_{L^\infty} \\
& +\|\partial_{ttx}u^\varepsilon\|_{L^\infty}\|f(|u^\varepsilon|^2)\|_{L^\infty}+\|\partial_{xxxtt}u^\varepsilon\|_{L^\infty}\Bigg)\lesssim h^2+\frac{\tau^2}{\varepsilon^{4-\alpha^*}}.
\end{aligned}$$

For $j=0$ and $M-1$, we apply the boundary condition to deduce that $\frac{\partial^k}{\partial t^k}u^\varepsilon(x,t)|_{x\in\partial\Omega}=0$ for $k\geq 0$, and the equation (7.9) shows that $u_{xx}(x,t)|_{x\in\partial\Omega}=0$ and $u_{xxxx}(x,t)|_{x\in\partial\Omega}=0$. Similarly as above, we can get the above estimates for $j=0,M-1$. Thus, we complete the proof.

□

The error bounds for $e^{\varepsilon,n}$ at $n = 0, 1$ are the same as Lemma 7.3 since the boundary and initial conditions for CNFD (7.12) and SIFD (7.14) are the same.

The proof for the CNFD scheme (7.12) is quite similar to that of the SIFD scheme, and we outline the schedule below, i.e. we prove the key lemmas.

Let $\hat{u}^{\varepsilon,0} = u^{\varepsilon,0}$, $\hat{u}^{\varepsilon,1} = u^{\varepsilon,1}$ and $\hat{u}^{\varepsilon,n} \in X_M$ $(n \geq 1)$ be given by

$$(i\delta_t - \varepsilon^2\delta_t^2)\hat{u}_j^{\varepsilon,n} + \frac{1}{2}\delta_x^2(\hat{u}_j^{\varepsilon,n+1} + \hat{u}_j^{\varepsilon,n-1}) + G_B(\hat{u}_j^{\varepsilon,n+1}, \hat{u}_j^{\varepsilon,n-1}) = 0, \quad j \in \mathcal{T}_M, \tag{7.97}$$

where $G_B(z_1, z_2)$ for $z_1, z_2 \in \mathbb{C}$ is given by

$$\begin{aligned} G_B(z_1, z_2) &= \int_0^1 f_B(\theta|z_1|^2 + (1-\theta)|z_2|^2)\, d\theta \cdot g_{_B}\left(\frac{z_1 + z_2}{2}\right) \\ &= \frac{F_B(|z_1|^2) - F_B(|z_2|^2)}{|z_1|^2 - |z_2|^2} \cdot g_{_B}\left(\frac{z_1 + z_2}{2}\right), \end{aligned}$$

with $g_{_B}(z)$, $f_B(\cdot)$ and $F_B(\cdot)$ being defined in (7.40). Actually $\hat{u}_j^{\varepsilon,n}$ can be viewed as another approximation of $u^\varepsilon(x_j, t_n)$. From Lemma 7.6, (7.97) is uniquely solvable for small τ. Define the 'error' $\chi^{\varepsilon,n} \in X_M$ for $n \geq 1$ as

$$\chi_j^{\varepsilon,n} = u^\varepsilon(x_j, t_n) - \hat{u}_j^{\varepsilon,n}, \quad j \in \mathcal{T}_M, \tag{7.98}$$

and the local truncation error $\hat{\zeta}^{\varepsilon,n} \in X_M$ for $j \in \mathcal{T}_M$ and $n \geq 1$ as

$$\hat{\zeta}_j^{\varepsilon,n} := (i\delta_t - \varepsilon^2\delta_t^2)u^\varepsilon(x_j, t_n) + \frac{1}{2}\delta_x^2\left(u^\varepsilon(x_j, t_{n+1}) + u^\varepsilon(x_j, t_{n-1})\right) + G_B\left(u^\varepsilon(x_j, t_{n+1}), u^\varepsilon(x_j, t_{n-1})\right). \tag{7.99}$$

Similar as Lemma 7.2, we can prove that under the assumptions in Theorem 7.1,

$$\|\hat{\zeta}^{\varepsilon,n}\|_2 + \|\delta_x^+\hat{\zeta}^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \quad 1 \leq n \leq \frac{T}{\tau} - 1, \tag{7.100}$$

and the estimate for $\|\hat{e}^{\varepsilon,1}\|_2 + \|\delta_x^+\hat{e}^{\varepsilon,1}\|_2$ is proved in Lemma 7.3.

Subtracting (7.97) from (7.99), we obtain

$$i\delta_t\chi_j^{\varepsilon,n} - \varepsilon^2\delta_t^2\chi_j^{\varepsilon,n} + \frac{1}{2}\delta_x^2\left(\chi_j^{\varepsilon,n+1} + \chi_j^{\varepsilon,n-1}\right) + \vartheta_j^{\varepsilon,n} - \hat{\zeta}_j^{\varepsilon,n} = 0, \quad j \in \mathcal{T}_M, \tag{7.101}$$

where $\vartheta^{\varepsilon,n} \in X_M$ is defined for $j \in \mathcal{T}_M$ and $n \geq 1$ as

$$\vartheta_j^{\varepsilon,n} \quad = \quad G_B\left(u^\varepsilon(x_j, t_{n+1}), u^\varepsilon(x_j, t_{n-1})\right) - G_B(\hat{u}_j^{\varepsilon,n+1}, \hat{u}_j^{\varepsilon,n-1}). \tag{7.102}$$

Then we have the following properties on $\vartheta^{\varepsilon,n}$.

Lemma 7.8 *Under the assumptions in Theorem 7.1, for $\vartheta^{\varepsilon,n} \in X_M$ $(n \ge 1)$ in (7.102), we have for* $0 \le j \le M-1$, $n \ge 1$

$$|\vartheta_j^{\varepsilon,n}| \lesssim |\chi_j^{\varepsilon,n+1}| + |\chi_j^{\varepsilon,n-1}|, \quad |\delta_x^+ \vartheta_j^{\varepsilon,n}| \lesssim \sum_{m=n-1,n+1} \left(|\chi_j^{\varepsilon,m}| + |\delta_x^+ \chi_j^{\varepsilon,m}| + |\chi_{j+1}^{\varepsilon,m}|\right).$$

Proof: For $j \in \mathcal{T}_M^0$, $n \ge 1$ and $\theta \in [0,1]$, denote

$$\rho_j^{\varepsilon,n}(\theta) = \theta|u^\varepsilon(x_j,t_{n+1})|^2 + (1-\theta)|u^\varepsilon(x_j,t_{n-1})|^2,\ \hat{\rho}_j^{\varepsilon,n}(\theta) = \theta|\hat{u}_j^{\varepsilon,n+1}|^2 + (1-\theta)|\hat{u}_j^{\varepsilon,n-1}|^2,$$
$$\mu_j^{\varepsilon,n} = \frac{1}{2}\left[u^\varepsilon(x_j,t_{n+1}) + u^\varepsilon(x_j,t_{n-1})\right],\ \hat{\mu}_j^{\varepsilon,n} = \frac{\hat{u}_j^{\varepsilon,n+1} + \hat{u}_j^{\varepsilon,n-1}}{2},\ \pi_j^{\varepsilon,n} = |u^\varepsilon(x_j,t_n)| + |\hat{u}_j^{\varepsilon,n}|,$$

using the definition of G_B, F_B and g_B, it is easy to get

$$\vartheta_j^{\varepsilon,n} = \mu_j^{\varepsilon,n} \int_0^1 [f_B(\rho_j^{\varepsilon,n}(\theta)) - f_B(\hat{\rho}_j^{\varepsilon,n}(\theta))]d\theta + [g_B(\mu_j^{\varepsilon,n}) - g_B(\hat{\mu}_j^{\varepsilon,n})] \int_0^1 f_B(\hat{\rho}_j^{\varepsilon,n}(\theta))\, d\theta.$$

Noticing the Lipschitz property of $f_B(s^2)$ and

$$\left|\sqrt{\rho_j^{\varepsilon,n}(\theta)} - \sqrt{\hat{\rho}_j^{\varepsilon,n}(\theta)}\right| \le \frac{\theta\pi_j^{\varepsilon,n+1}|\chi_j^{\varepsilon,n+1}| + (1-\theta)\pi_j^{\varepsilon,n-1}|\chi_j^{\varepsilon,n-1}|}{\sqrt{\rho_j^{\varepsilon,n}(\theta)} + \sqrt{\hat{\rho}_j^{\varepsilon,n}(\theta)}} \le |\chi_j^{\varepsilon,n+1}| + |\chi_j^{\varepsilon,n-1}|,$$

combined with the Lipschitz property of $g_B(z)$, we can obtain

$$|\vartheta_j^{\varepsilon,n}| \lesssim |\chi_j^{\varepsilon,n+1}| + |\chi_j^{\varepsilon,n-1}|, \quad j \in \mathcal{T}_M^0. \tag{7.103}$$

Rewriting $\vartheta_j^{\varepsilon,n}$ as

$$\vartheta_j^{\varepsilon,n} = g_B(\hat{\mu}_j^{\varepsilon,n}) \int_0^1 [f_B(\rho_j^{\varepsilon,n}(\theta) - f_B(\hat{\rho}_j^{\varepsilon,n}(\theta))]\, d\theta + [g_B(\mu_j^{\varepsilon,n}) - g_B(\hat{\mu}_j^{\varepsilon,n})] \int_0^1 f_B(\rho_j^{\varepsilon,n}(\theta))\, d\theta, \tag{7.104}$$

and applying δ_x^+ to $\vartheta_j^{\varepsilon,n}$, we have

$$\begin{aligned}\delta_x^+ \vartheta_j^{\varepsilon,n} =\ & g_B(\hat{\mu}_j^{\varepsilon,n}) \int_0^1 \delta_x^+[f_B(\rho_j^{\varepsilon,n}(\theta)) - f_B(\hat{\rho}_j^{\varepsilon,n}(\theta))]\, d\theta \\ & + [g_B(\mu_j^{\varepsilon,n}) - g_B(\hat{\mu}_j^{\varepsilon,n})] \int_0^1 \delta_x^+ f_B(\rho_j^{\varepsilon,n}(\theta))\, d\theta + \delta_x^+[g_B(\mu_j^{\varepsilon,n}) - g_B(\hat{\mu}_j^{\varepsilon,n})] \int_0^1 f_B(\rho_{j+1}^{\varepsilon,n}(\theta))\, d\theta \\ & + \delta_x^+ g_B(\hat{\mu}_j^{\varepsilon,n}) \int_0^1 [f_B(\rho_{j+1}^{\varepsilon,n}(\theta)) - f_B(\hat{\rho}_{j+1}^{\varepsilon,n}(\theta))]\, d\theta.\end{aligned}$$

Firstly, for $\theta, s \in [0,1]$, and $n \ge 1$, we denote $\kappa_j^{\varepsilon,n}(\theta,s), \hat{\kappa}_j^{\varepsilon,n}(\theta,s)$ for $0 \le j \le M-1$ as

$$\kappa_j^{\varepsilon,n}(\theta,s) = s\rho_{j+1}^{\varepsilon,n}(\theta) + (1-s)\rho_j^{\varepsilon,n}(\theta), \quad \hat{\kappa}_j^{\varepsilon,n}(\theta,s) = s\hat{\rho}_{j+1}^{\varepsilon,n}(\theta) + (1-s)\hat{\rho}_j^{\varepsilon,n}(\theta). \tag{7.105}$$

Noticing that for $1 \le j \le M-1$

$$\begin{aligned}
&\delta_x^+ \left[f_B\left(\rho_j^{\varepsilon,n}(\theta)\right) - f_B\left(\hat{\rho}_j^{\varepsilon,n}(\theta)\right)\right] \\
&= \left[\delta_x^+ \rho_j^{\varepsilon,n}(\theta) \int_0^1 f_B'\left(\kappa_j^{\varepsilon,n}(\theta,s)\right) ds - \delta_x^+ \hat{\rho}_j^{\varepsilon,n}(\theta) \int_0^1 f_B'(\hat{\kappa}_j^{\varepsilon,n}(\theta,s))\, ds\right] \\
&= \int_0^1 \left[f_B'\left(\kappa_j^{\varepsilon,n}(\theta,s)\right) - f_B'\left(\hat{\kappa}_j^{\varepsilon,n}(\theta,s)\right)\right] \delta_x \rho_j^{\varepsilon,n}(\theta)\, ds \\
&\quad + \int_0^1 f_B'(\hat{\kappa}_j^{\varepsilon,n}(\theta,s)) \left[\delta_x^+ (\rho_j^{\varepsilon,n}(\theta) - \hat{\rho}_j^{\varepsilon,n}(\theta))\right] ds,
\end{aligned}$$

a careful calculation shows that

$$\begin{aligned}
&\delta_x^+ \left[\rho_j^{\varepsilon,n}(\theta) - \hat{\rho}_j^{\varepsilon,n}(\theta)\right] = \theta\Bigg[2\,\mathrm{Re}\left(u^\varepsilon(x_j,t_{n+1})\delta_x^+ \overline{\chi_j^{\varepsilon,n+1}} + \overline{\chi_{j+1}^{\varepsilon,n+1}} \delta_x^+ u^\varepsilon(x_j,t_{n+1})\right) \\
&- \chi_j^{\varepsilon,n+1} \delta_x^+ \overline{\chi_j^{\varepsilon,n+1}} - \overline{\chi_{j+1}^{\varepsilon,n+1}} \delta_x^+ \chi_j^{\varepsilon,n+1}\Bigg] + (1-\theta)\Bigg[-\chi_j^{\varepsilon,n-1}\delta_x^+ \overline{\chi_j^{\varepsilon,n-1}} - \overline{\chi_{j+1}^{\varepsilon,n-1}} \delta_x^+ \chi_j^{\varepsilon,n-1} \\
&+ 2\,\mathrm{Re}\left(u^\varepsilon(x_j,t_{n-1})\delta_x^+ \overline{\chi_j^{\varepsilon,n-1}} + \overline{\chi_{j+1}^{\varepsilon,n-1}} \delta_x^+ u^\varepsilon(x_j,t_{n-1})\right)\Bigg],
\end{aligned}$$

and $\sqrt{1-\theta}|\chi_{j+1}^{\varepsilon,n-1}| \le \sqrt{\hat{\rho}_{j+1}^{\varepsilon,n}(\theta)} + |u^\varepsilon(x_{j+1},t_{n-1})|$, $\sqrt{1-\theta}|\chi_j^{\varepsilon,n-1}| \le \sqrt{\hat{\rho}_j^{\varepsilon,n}(\theta)} + |u^\varepsilon(x_j,t_{n-1})|$, $\sqrt{\theta}|\chi_{j+1}^{\varepsilon,n+1}| \le \sqrt{\hat{\rho}_{j+1}^{\varepsilon,n}(\theta)} + |u^\varepsilon(x_{j+1},t_{n+1})|$, $\sqrt{\theta}|\chi_j^{\varepsilon,n+1}| \le \sqrt{\hat{\rho}_j^{\varepsilon,n}(\theta)} + |u^\varepsilon(x_j,t_{n+1})|$. Moreover, from the Lipschitz property of f_B (7.41), we have

$$\left|\int_0^1 f_B'(\hat{\kappa}_j^{\varepsilon,n}(\theta,s))\, ds\right| = \left|\frac{f_B\left(\hat{\rho}_{j+1}^{\varepsilon,n}(\theta)\right) - f_B\left(\hat{\rho}_j^{\varepsilon,n}(\theta)\right)}{\hat{\rho}_{j+1}^{\varepsilon,n}(\theta) - \hat{\rho}_j^{\varepsilon,n}(\theta)}\right| \le \frac{C}{\sqrt{\hat{\rho}_{j+1}^{\varepsilon,n}(\theta)} + \sqrt{\hat{\rho}_j^{\varepsilon,n}(\theta)}}. \quad (7.106)$$

Recalling the boundedness of $\delta_x^+ \rho_j^{\varepsilon,n}(\theta)$, $g_B(\cdot)$ and $f_B'(\cdot)$ as well as the Lipschitz property of $f_B'(s^2)$, i.e. $|f_B'(s_1) - f_B'(s_2)| \le C|\sqrt{s_1} - \sqrt{s_2}|$, combining the proof for (7.103), we arrive at

$$\left|\int_0^1 \delta_x^+ \left[f_B(\rho_j^{\varepsilon,n}(\theta)) - f_B(\hat{\rho}_j^{\varepsilon,n}(\theta))\right] d\theta \cdot g_B(\hat{\mu}_j^{\varepsilon,n})\right| \lesssim \sum_{m=n+1,n-1} (|\chi_j^{\varepsilon,m}| + |\chi_{j+1}^{\varepsilon,m}| + |\delta_x^+ \chi_j^{\varepsilon,m}|). \quad (7.107)$$

Secondly, from the property $g_B(\cdot) \in C_0^\infty$, we know

$$|\delta_x^+ g_B(\hat{\mu}_j^{\varepsilon,n})| \le C\left|\delta_x^+ \hat{\mu}_j^{\varepsilon,n}\right| \le C\left|\delta_x^+ \chi_j^{\varepsilon,n+1} + \delta_x^+ \chi_j^{\varepsilon,n+1} - \delta_x^+ u^\varepsilon(x_j,t_{n+1}) - \delta_x^+ u^\varepsilon(x_j,t_{n-1})\right|.$$

In view of the boundedness of $f_B(s)$ as well as the proof for (7.103), we get

$$\left|\int_0^1 \left[f_B(\rho_{j+1}^{\varepsilon,n}(\theta)) - f_B(\hat{\rho}_{j+1}^{\varepsilon,n}(\theta))\right] d\theta \cdot \delta_x^+ g_B(\hat{\mu}_j^{\varepsilon,n})\right| \lesssim \sum_{m=n-1,n+1} (|\chi_{j+1}^{\varepsilon,m}| + |\chi_j^{\varepsilon,m}| + |\delta_x^+ \chi_j^{\varepsilon,m}|). \quad (7.108)$$

Thirdly, noticing $\delta_x^+ f_B\left(\rho_j^{\varepsilon,n}(\theta)\right)$ is bounded and $g_B(z)$ is Lipschitz, we have

$$\left|\int_0^1 \delta_x^+ f_B\left(\rho_j^{\varepsilon,n}(\theta)\right)\,d\theta\cdot\left[g_B(\mu_j^{\varepsilon,n})-g_B(\hat{\mu}_j^{\varepsilon,n})\right]\right|\lesssim|\chi_j^{\varepsilon,n+1}|+|\chi_j^{\varepsilon,n-1}|. \tag{7.109}$$

Lastly, denoting $\sigma_j^n(\theta)$, $\hat{\sigma}_j^n(\theta)$ for $\theta\in[0,1]$ and $0\le j\le M-1$ as

$$\sigma_j^n(\theta)=\theta\mu_{j+1}^{\varepsilon,n}+(1-\theta)\mu_j^{\varepsilon,n},\quad \hat{\sigma}_j^n(\theta)=\theta\hat{\mu}_{j+1}^{\varepsilon,n}+(1-\theta)\hat{\mu}_j^{\varepsilon,n},$$

recalling the definition of $\rho_B(s)$ and $g_B(z)$, we find that

$$\delta_x^+\left(g_B(\mu_j^{\varepsilon,n})-g_B(\hat{\mu}_j^{\varepsilon,n})\right)=\delta_x^+\left[\rho_B(|\mu_j^{\varepsilon,n}|^2)\mu_j^{\varepsilon,n}-\rho_B(|\hat{\mu}_j^{\varepsilon,n}|^2)\hat{\mu}_j^{\varepsilon,n}\right]=I_1+I_2,$$

where

$$I_1=\int_0^1\left[\delta_x^+\mu_j^{\varepsilon,n}\partial_z g_B(\sigma_j^n(\theta))-\delta_x^+\hat{\mu}_j^{\varepsilon,n}\partial_z g_B\left(\hat{\sigma}_j^n(\theta)\right)\right]d\theta,\ \partial_z g_B(z)=\rho_B(|z|^2)+|z|^2\rho_B'(|z|^2),$$
$$I_2=\int_0^1\left[\delta_x^+\overline{\mu_j^{\varepsilon,n}}\partial_{\bar z} g_B(\sigma_j^n(\theta))-\delta_x^+\overline{\hat{\mu}_j^{\varepsilon,n}}\partial_{\bar z} g_B\left(\hat{\sigma}_j^n(\theta)\right)\right]d\theta,\ \partial_{\bar z} g_B(z)=z^2\rho_B'(|z|^2).$$

Noticing $\delta_x^+\mu_j^{\varepsilon,n}$ is bounded and the C_0^∞ property of $\rho_B(s)$, we know $\partial_z g_B(z)$ is Lipschitz and

$$\begin{aligned}|I_1|&\le\left|\int_0^1\left(\partial_z g_B(\sigma_j^n(\theta))-\partial_z g_B(\hat{\sigma}_j^n(\theta))\right)\delta_x^+\mu_j^{\varepsilon,n}\,d\theta\right|+\left|\int_0^1[\delta_x^+(\mu_j^{\varepsilon,n}-\hat{\mu}_j^{\varepsilon,n})]\,\partial_z g_B(\hat{\sigma}_j^n(\theta))\,d\theta\right|\\&\lesssim\max_{\theta\in[0,1]}\left\{\left|\,|\sigma_j^n(\theta)|-|\hat{\sigma}_j^n(\theta)|\right|\right\}+\left|\delta_x^+(\chi_j^{\varepsilon,n+1}+\chi_j^{\varepsilon,n-1})\right|\\&\lesssim\sum_{m=n+1,n-1}\left(|\chi_j^{\varepsilon,m}|+|\chi_{j+1}^{\varepsilon,m}|+|\delta_x^+\chi_j^{\varepsilon,m}|\right).\end{aligned}$$

In the same spirit, we have

$$|I_2|\lesssim|\chi_j^{\varepsilon,n+1}|+|\chi_{j+1}^{\varepsilon,n+1}|+|\chi_j^{\varepsilon,n-1}|+|\chi_{j+1}^{\varepsilon,n-1}|+|\delta_x^+\chi_j^{\varepsilon,n+1}|+|\delta_x^+\chi_j^{\varepsilon,n-1}|. \tag{7.110}$$

Hence, we obtain

$$\left|\int_0^1 f_B\left(\rho_{j+1}^{\varepsilon,n}(\theta)\right)\,d\theta\cdot\delta_x^+\left[g_B(\mu_j^{\varepsilon,n})-g_B(\hat{\mu}_j^{\varepsilon,n})\right]\right|\lesssim\sum_{m=n-1,n+1}\left(|\chi_j^{\varepsilon,m}|+|\delta_x^+\chi_j^{\varepsilon,m}|+|\chi_{j+1}^{\varepsilon,m}|\right). \tag{7.111}$$

Combining (7.107), (7.108), (7.109) and (7.111) together, we finally prove that

$$\left|\delta_x^+\vartheta_j^{\varepsilon,n}\right|\lesssim\sum_{m=n-1,n+1}\left(|\chi_j^{\varepsilon,m}|+|\delta_x^+\chi_j^{\varepsilon,m}|+|\chi_{j+1}^{\varepsilon,m}|\right),\quad 0\le j\le M-1,\ n\ge 1. \tag{7.112}$$

The proof is complete. $\square$

Having Lemma 7.8, local truncation error (7.100) and the initial error Lemma 7.3, following the analogous proof for SIFD, we could obtain

$$\|\chi^{\varepsilon,n}\|_2 + \|\delta_x^+\chi^{\varepsilon,n}\|_2 \lesssim h^2 + \frac{\tau^2}{\varepsilon^{4-\alpha^*}}, \quad n \le \frac{T}{\tau}. \tag{7.113}$$

To complete the proof, we have to prove (7.28) type estimate for $\chi^{\varepsilon,n}$. It is a straight forward extension of the proof for SIFD and the proof for Lemma 7.8. More precisely, define

$$\tilde{\chi}_j^{\varepsilon,n} = u(x_j,t_n) - \hat{u}_j^{\varepsilon,n} = \chi_j^{\varepsilon,n} + u(x_j,t_n) - u^\varepsilon(x_j,t_n), \quad j \in \mathcal{T}_M^0, \quad n \ge 0. \tag{7.114}$$

and the 'local truncation error' $\tilde{\zeta}^{\varepsilon,n} \in X_M$ for $n \ge 1$ and $j \in \mathcal{T}_M$ as

$$\tilde{\zeta}_j^{\varepsilon,n} := (i\delta_t - \varepsilon^2\delta_t^2)u(x_j,t_n) + \frac{1}{2}\delta_x^2\left(u(x_j,t_{n+1}) + u(x_j,t_{n-1})\right) + G_B(u(x_j,t_{n+1}),u(x_j,t_{n-1})). \tag{7.115}$$

then we have

$$\|\tilde{\zeta}^{\varepsilon,n}\|_2 + \|\delta_x^+\tilde{\zeta}^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad n \ge 1. \tag{7.116}$$

Subtracting (7.97) from (7.115), we obtain for $n \ge 1$

$$i\delta_t\tilde{\chi}_j^{\varepsilon,n} - \varepsilon^2\delta_t^2\tilde{\chi}_j^{\varepsilon,n} + \frac{1}{2}\delta_x^2\left(\tilde{\chi}_j^{\varepsilon,n+1} + \tilde{\chi}_j^{\varepsilon,n-1}\right) + \tilde{\vartheta}_j^{\varepsilon,n} - \tilde{\zeta}_j^{\varepsilon,n} = 0, \quad j \in \mathcal{T}_M, \tag{7.117}$$

where $\tilde{\vartheta}^{\varepsilon,n} \in X_M$ is given for $j \in \mathcal{T}_M$ and $n \ge 1$ as

$$\tilde{\vartheta}_j^{\varepsilon,n} = G_B\left(u(x_j,t_{n+1}),u(x_j,t_{n-1})\right) - G_B\left(\hat{u}_j^{\varepsilon,n+1},\hat{u}_j^{\varepsilon,n-1}\right). \tag{7.118}$$

Then the following lemma holds and we omit the proof here.

Lemma 7.9 *Under the assumptions in Theorem 7.1, for* $\tilde{\vartheta}^{\varepsilon,n} \in X_M$ $(n \ge 1)$ *in (7.118), we have for* $0 \le j \le M-1$ *and* $n \ge 1$,

$$|\tilde{\vartheta}_j^{\varepsilon,n}| \lesssim |\tilde{\chi}_j^{\varepsilon,n+1}| + |\tilde{\chi}_j^{\varepsilon,n-1}|, \; |\delta_x^+\tilde{\vartheta}_j^{\varepsilon,n}| \lesssim \sum_{m=n-1,n+1}\left(|\tilde{\chi}_j^{\varepsilon,m}| + |\delta_x^+\tilde{\chi}_j^{\varepsilon,m}| + |\tilde{\chi}_{j+1}^{\varepsilon,m}|\right).$$

Following the analogous proof for the SIFD, in view of Lemma 7.9, local error (7.116) and initial error Lemma 7.3, recalling assumption (B), we can derive that

$$\|\chi^{\varepsilon,n}\|_2 + \|\delta_x^+\chi^{\varepsilon,n}\|_2 \lesssim h^2 + \tau^2 + \varepsilon^2, \quad n \le \frac{T}{\tau}. \tag{7.119}$$

Proof of Theorem 7.1: Combining (7.113) and (7.119) together, analogous proof for SIFD applies and the conclusion follows. $\square$

7.5 Numerical results

In this section, we report numerical results for both SIFD (7.14) and CNFD (7.12) schemes applied to NLSW (7.9) with $f(|u^\varepsilon|^2) = -|u^\varepsilon|^2$. The corresponding limiting NLSE is the defocusing cubic NLSE.

For the numerical tests, we choose $u_0(x) = \pi^{-1/4}e^{-x^2/2}$ and $w^\varepsilon(x) = e^{-x^2/2}$ in (7.9). The computational domain is chosen as $[a, b] = [-16, 16]$. The 'exact' solution is computed with a very fine mesh $h = 1/512$ and time step $\tau = 10^{-6}$. We study the following two cases of initial data:

Case I. $\alpha = 2$, i.e. the well-prepared case.

Case II. $\alpha = 0$, i.e. the ill-prepared case.

We measure the error e_h at time $t = 1$ with the discrete H^1 norm $\|e_h\|_{H^1} = \|e_h\|_2 + \|\delta_x^+ e_h\|_2$.

Tab. 7.1 depicts spatial errors of SIFD for Cases I and II, for different h and ε, with fixed $\tau = 10^{-6}$, where the time step τ is so small such that the temporal error can be neglected. From the Table, we can conclude that, SIFD is uniformly second order accurate in h for all ε. Tabs. 7.2 and 7.3 list temporal errors of SIFD for Cases I and II, for different ε and τ, with fixed $h = 1/512$. With this very fine mesh $h = 1/512$, the spatial error can be ignored. Tab. 7.2 shows that, when τ is small (upper triangle part), the temporal error is of second order for each ε; when ε is small (lower triangle part), the temporal error is also of second order; near the diagonal part (for $\alpha = 2$, slightly upper), the degeneracy of the second order accuracy is observed. This confirms our error estimates (7.30) and (7.31) for SIFD. Tab. 7.3 presents the errors of SIFD at the degeneracy regime for $\alpha = 2$ in the regime $\tau \sim \varepsilon^2$, and resp., for $\alpha = 0$ in the regime $\tau \sim \varepsilon^3$, predicted by our error estimates. The results clearly demonstrate that SIFD converges at $O(h^2 + \tau)$ and $O(h^2 + \tau^{2/3})$ for $\alpha = 2$ and $\alpha = 0$, respectively. Similar tests were also carried out for CNFD and we obtain similar conclusion, thus they are omitted here for brevity.

$\alpha=2$	$h=1/2$	$h=1/2^2$	$h=1/2^3$	$h=1/2^4$	$h=1/2^5$	$h=1/2^6$	$h=1/2^7$
$\varepsilon=1/2^2$	1.51E-1	4.05E-2	1.03E-2	2.57E-3	6.45E-4	1.60E-4	3.90E-5
		1.90	1.98	2.00	1.99	2.01	2.04
$\varepsilon=1/2^3$	1.94E-1	5.35E-2	1.36E-2	3.41E-3	8.51E-4	2.10E-4	4.92E-5
		1.89	1.98	2.00	2.00	2.02	2.09
$\varepsilon=1/2^4$	2.15E-1	6.05E-2	1.55E-2	3.88E-3	9.67E-4	2.39E-4	5.68E-5
		1.83	1.96	2.00	2.00	2.02	2.07
$\varepsilon=1/2^5$	2.22E-1	6.29E-2	1.61E-2	4.04E-3	1.01E-3	2.49E-4	5.93E-5
		1.82	1.97	1.99	2.00	2.02	2.07
$\varepsilon=1/2^6$	2.23E-1	6.36E-2	1.63E-2	4.08E-3	1.02E-3	2.52E-4	6.00E-5
		1.81	1.96	2.00	2.00	2.02	2.07
$\varepsilon=1/2^7$	2.24E-1	6.37E-2	1.63E-2	4.10E-3	1.02E-3	2.52E-4	6.01E-5
		1.81	1.97	1.99	2.01	2.02	2.07
$\varepsilon=1/2^{10}$	2.24E-1	6.38E-2	1.63E-2	4.10E-3	1.02E-3	2.53E-4	6.02E-5
		1.81	1.97	1.99	2.01	2.01	2.07
$\varepsilon=1/2^{20}$	2.24E-1	6.38E-2	1.63E-2	4.10E-3	1.02E-3	2.53E-4	6.02E-5
		1.81	1.97	1.99	2.01	2.01	2.07

Table 7.1: Spatial error analysis for SIFD scheme (7.14) with different ε and h for *Case I*, i.e. $\alpha=2$, with norm $\|e\|_{H^1}=\|e\|_2+\|\delta_x^+ e\|_2$. The convergence rate is calculated as $\log_2(\|e(2h)\|_{H^1}/\|e(h)\|_{H^1})$.

$\alpha=0$	$h=1/2$	$h=1/2^2$	$h=1/2^3$	$h=1/2^4$	$h=1/2^5$	$h=1/2^6$	$h=1/2^7$
$\varepsilon=1/2^2$	1.52E-1	4.09E-2	1.04E-2	2.60E-3	6.53E-4	1.62E-4	3.94E-5
		1.89	1.98	2.00	1.99	2.01	2.04
$\varepsilon=1/2^3$	1.95E-1	5.36E-2	1.36E-2	3.41E-3	8.52E-4	2.10E-4	4.93E-5
		1.86	1.98	2.00	2.00	2.02	2.09
$\varepsilon=1/2^4$	2.15E-1	6.05E-2	1.55E-2	3.88E-3	9.67E-4	2.39E-4	5.68E-5
		1.83	1.96	2.00	2.00	2.02	2.07
$\varepsilon=1/2^5$	2.22E-1	6.29E-2	1.61E-2	4.04E-3	1.01E-3	2.49E-4	5.93E-5
		1.82	1.97	1.99	2.00	2.02	2.07
$\varepsilon=1/2^6$	2.23E-1	6.36E-2	1.63E-2	4.08E-3	1.02E-3	2.52E-4	6.00E-5
		1.81	1.96	2.00	2.00	2.02	2.07
$\varepsilon=1/2^7$	2.24E-1	6.37E-2	1.63E-2	4.10E-3	1.02E-3	2.52E-4	6.01E-5
		1.81	1.97	1.99	2.01	2.02	2.07
$\varepsilon=1/2^{10}$	2.24E-1	6.38E-2	1.63E-2	4.10E-3	1.02E-3	2.53E-4	6.02E-5
		1.81	1.97	1.99	2.01	2.01	2.07
$\varepsilon=1/2^{20}$	2.24E-1	6.38E-2	1.63E-2	4.10E-3	1.02E-3	2.53E-4	6.02E-5
		1.81	1.97	1.99	2.01	2.01	2.07

Table 7.1: (con't) For *Case II*, i.e. $\alpha=0$.

$\alpha = 2$	$\tau = 0.1$	$\tau = \frac{0.1}{2}$	$\tau = \frac{0.1}{2^2}$	$\tau = \frac{0.1}{2^3}$	$\tau = \frac{0.1}{2^4}$	$\tau = \frac{0.1}{2^5}$	$\tau = \frac{0.1}{2^6}$	$\tau = \frac{0.1}{2^7}$
$\varepsilon = \frac{1}{2^2}$	1.10E-1	4.75E-2	1.49E-2	3.86E-3	9.70E-4	2.43E-4	6.10E-5	1.56E-5
		1.21	1.67	1.95	1.99	2.00	1.99	1.97
$\varepsilon = \frac{1}{2^3}$	1.60E-1	5.06E-2	1.46E-2	5.45E-3	3.07E-3	8.27E-4	2.08E-4	5.21E-5
		1.66	1.79	1.42	0.83	1.89	1.99	2.00
$\varepsilon = \frac{1}{2^4}$	1.98E-1	6.02E-2	1.85E-2	4.78E-3	1.25E-3	4.14E-4	3.74E-4	1.81E-4
		1.72	1.70	1.95	1.94	1.59	0.15	1.05
$\varepsilon = \frac{1}{2^5}$	1.90E-1	7.30E-2	1.92E-2	5.00E-3	1.39E-3	3.49E-4	8.75E-5	2.74E-5
		1.38	1.93	1.94	1.85	1.99	2.00	1.68
$\varepsilon = \frac{1}{2^6}$	1.89E-1	6.87E-2	2.18E-2	5.28E-3	1.32E-3	3.34E-4	9.09E-5	2.17E-5
		1.46	1.66	2.06	2.00	1.98	1.88	2.07
$\varepsilon = \frac{1}{2^7}$	1.89E-1	6.79E-2	2.06E-2	5.81E-3	1.36E-3	3.38E-4	8.26E-5	2.20E-5
		1.48	1.72	1.83	2.09	2.01	2.03	1.91
$\varepsilon = \frac{1}{2^{10}}$	1.89E-1	6.76E-2	2.01E-2	5.37E-3	1.37E-3	3.50E-4	9.27E-5	2.14E-5
		1.48	1.75	1.90	1.97	1.97	1.92	2.11
$\varepsilon = \frac{1}{2^{20}}$	1.89E-1	6.76E-2	2.01E-2	5.37E-3	1.36E-3	3.42E-4	8.56E-5	2.14E-5
		1.48	1.75	1.90	1.98	1.99	2.00	2.00

Table 7.2: Temporal error analysis for SIFD scheme (7.14) with different ε and τ for *Case I*, i.e. $\alpha = 2$, with norm $\|e\|_{H^1}$.

$\alpha = 0$	$\tau = 0.1$	$\tau = \frac{0.1}{2}$	$\tau = \frac{0.1}{2^2}$	$\tau = \frac{0.1}{2^3}$	$\tau = \frac{0.1}{2^4}$	$\tau = \frac{0.1}{2^5}$	$\tau = \frac{0.1}{2^6}$	$\tau = \frac{0.1}{2^7}$
$\varepsilon = \frac{1}{2^2}$	2.91E-1	1.39E-1	4.05E-2	1.04E-2	2.63E-3	6.59E-4	1.66E-4	4.54E-5
		1.07	1.78	1.96	1.98	2.00	1.99	1.87
$\varepsilon = \frac{1}{2^3}$	1.76E-1	9.04E-2	6.52E-2	7.35E-2	3.30E-2	8.71E-3	2.19E-3	5.50E-4
		0.96	0.47	-0.17	1.16	1.92	1.99	1.99
$\varepsilon = \frac{1}{2^4}$	1.96E-1	6.02E-2	2.10E-2	1.01E-2	1.98E-2	3.81E-3	1.92E-2	8.16E-3
		1.70	1.52	1.06	-0.97	2.38	-2.33	1.23
$\varepsilon = \frac{1}{2^5}$	1.90E-1	7.26E-2	1.94E-2	6.11E-3	3.36E-3	3.61E-3	4.69E-3	1.01E-3
		1.39	1.90	1.67	0.86	-0.10	-0.38	2.22
$\varepsilon = \frac{1}{2^6}$	1.89E-1	6.87E-2	2.17E-2	5.32E-3	1.55E-3	8.15E-4	7.31E-4	1.39E-3
		1.46	1.66	2.03	1.78	0.93	0.16	-0.93
$\varepsilon = \frac{1}{2^7}$	1.89E-1	6.78E-2	2.05E-2	5.81E-3	1.39E-3	4.37E-4	2.50E-4	2.03E-4
		1.48	1.73	1.82	2.06	1.67	0.81	0.30
$\varepsilon = \frac{1}{2^8}$	1.89E-1	6.77E-2	2.02E-2	5.48E-3	1.47E-3	3.46E-4	1.08E-4	6.21E-5
		1.48	1.74	1.88	1.90	2.09	1.68	0.80
$\varepsilon = \frac{1}{2^9}$	1.89E-1	6.76E-2	2.02E-2	5.39E-3	1.39E-3	3.70E-4	8.70E-5	2.35E-5
		1.48	1.74	1.91	1.96	1.91	2.09	1.89
$\varepsilon = \frac{1}{2^{10}}$	1.89E-1	6.76E-2	2.01E-2	5.37E-3	1.37E-3	3.50E-4	9.28E-5	2.22E-5
		1.48	1.75	1.90	1.97	1.97	1.92	2.06
$\varepsilon = \frac{1}{2^{20}}$	1.89E-1	6.76E-2	2.01E-2	5.37E-3	1.36E-3	3.42E-4	8.56E-5	2.14E-5
		1.48	1.75	1.90	1.98	1.99	2.00	2.00

Table 7.2: (con't) For *Case II*, i.e. $\alpha = 0$.

$\alpha = 2$	$\varepsilon = 1$ $\tau = 0.2$	$\varepsilon = 1/2$ $\tau = 0.2/2^2$	$\varepsilon = 1/2^2$ $\tau = 0.2/2^4$	$\varepsilon = 1/2^3$ $\tau = 0.2/2^6$	$\varepsilon = 1/2^4$ $\tau = 0.2/2^8$
$\|e\|_{H^1}$	1.07E-1	1.77E-2	3.86E-3	8.27E-4	1.81E-4
		1.30	1.10	1.11	1.10
$\alpha = 0$	$\varepsilon = 1/2^2$ $\tau = 0.1$	$\varepsilon = 1/2^3$ $\tau = 0.1/2^3$	$\varepsilon = 1/2^4$ $\tau = 0.1/2^6$	$\varepsilon = 1/2^5$ $\tau = 0.1/2^9$	$\varepsilon = 1/2^6$ $\tau = 0.1/2^{12}$
$\|e\|_{H^1}$	2.91E-1	7.35E-2	1.92E-2	4.83E-3	1.21E-3
		1.99/3	1.94/3	1.99/3	2.00/3

Table 7.3: Degeneracy of convergence rates for SIFD with $h = 1/512$, *Case I* and *Case II*. The convergence rate is calculated as $\log_2(\|e(2^2\tau, 2\varepsilon)\|_{H^1}/\|e(\tau,\varepsilon)\|_{H^1})/2$ for $\alpha = 2$ (Case I), and $\log_2(\|e(2^3\tau, 2\varepsilon)\|_{H^1}/\|e(\tau,\varepsilon)\|_{H^1})/3$ for $\alpha = 0$ (Case II).

Chapter 8

Concluding remarks and future work

This thesis is devoted to mathematical analysis and numerical simulation for the Gross-Pitaevskii equation (GPE), focusing on the ground state and dynamical properties as well as their efficient computation.

We payed special attention to the dipolar GPE (2.5) involving a highly singular kernel. Upon reformulating dipolar GPE (2.5) into a Gross-Pitaevskii-Poisson system (GPPS) (2.19)-(2.20), we analyzed the ground sates and well-posedness of dipolar GPE (2.5). The new formulation allowed us to develop a time-splitting sine pseudospectral method for simulating the dynamics of dipolar GPE, and a backward Euler sine pseudospectral method for computing the ground states of (2.5), based on the gradient flow with discrete normalization method. Then, starting from GPPS, effective 1D and 2D equations were derived for dipolar GPE with highly anisotropic confining potential. Subsequently, we considered the ground sates and well-posedness of the 1D and 2D equations. Furthermore, efficient and accurate numerical methods were proposed for finding the corresponding ground states.

The second part was to investigate the ground states of coupled GPEs, modeling a binary BEC with an atomic internal Josephson junction in optical resonators. For analytical results, the existence and uniqueness of the ground states were proved in different parameter regimes. On the other hand, for numerical implementation, we developed a backward Euler finite difference method for the computation. In addition, numerical examples were shown to confirm our analytical results.

The remaining part was related to numerical analysis. Firstly, we presented the analysis for finite difference discretizations for rotational GPE in 2D and 3D. In literature, the results for GPE were only available in one dimension (1D) case for conservative schemes. Using new technique, we proved the optimal convergence results in 2D and 3D cases, for both conservative and non-conservative schemes, confirmed by numerical results. Then, we worked on the uniform convergence analysis of finite difference methods for nonlinear Schrödinger equation perturbed by the wave operator (NLSW). The difficulty was that the solution exhibited high oscillation in time when the small perturbation strength ε was considered. Due to the oscillation, it would be expected to choose the time step corresponding to ε, so that the difference schemes could capture the true solution. We proved rigorously that the convergence rates of the finite difference schemes were independent of ε. Hence, it is not necessary to reduce the time step when ε decreases. Again, our approach works for 1D, 2D and 3D, and for both conservative and non-conservation schemes. Numerical examples confirmed our uniform convergence results.

The present work on dipolar GPE was focusing on the non-rotational case. For the rotational frame, it is important to understand how the dipolar interaction affects the quantized vortices. The 2D equation can be used to study the rotational dipolar GPE, instead of analyzing the full 3D model, which is very complicated. Extensive mathematical analysis and numerical experiments are needed to be done for the corresponding 2D model in future. Of course, it is also desirable to study the full 3D rotational dipolar GPE directly. We propose to do numerical experiments for the 2D model first in future. Another issue is the convergence between the 3D model and the 2D model, which is proved in the weak regime. It would therefore be quite interesting to prove the convergence in the strong $O(1)$ regime. To achieve this aim, new technique needs to be involved.

As shown in the coupled GPEs case, the ground state properties of the system depend on the coupling among the equations. In the more general cases, we may consider the spin-F BEC, which can be described by $2F + 1$ coupled GPEs. Both ground states and dynamical behavior will be analyzed.

In the numerical analysis part, error estimates have been proved for the finite difference approximations of GPE, for 1D, 2D and 3D. In practical computation, the time-splitting pseudospectral method has shown its efficiency especially for the GPE. Thus, it is favorable to study the error estimates for the time-splitting methods. Convergence has been obtained for the semi-discretization [32, 103]. To go further, we shall understand the full discretization case. For NLSW, we have proved the uniform convergence of the finite difference methods. In future, we will investigate the numerical methods particularly suitable for the highly oscillating dispersive equations, especially for NLSW. It is expected that the new methods would achieve higher resolution on the oscillation and the uniform convergence rates would be improved.

Appendix A

Proof of the equality (2.15)

Let

$$\phi(\mathbf{x}) = \frac{1}{r^3}\left(1 - \frac{3(\mathbf{x}\cdot\mathbf{n})^2}{r^2}\right), \qquad r = |\mathbf{x}|, \qquad \mathbf{x} \in \mathbb{R}^3. \tag{A.1}$$

For any $\mathbf{n} \in \mathbb{R}^3$ satisfies $|\mathbf{n}| = 1$, in order to prove (2.15) holds in the distribution sense, it is equivalent to prove the following:

$$\int_{\mathbb{R}^3} \phi(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} = -\frac{4\pi}{3} f(\mathbf{0}) - \int_{\mathbb{R}^3} f(\mathbf{x})\, \partial_{\mathbf{nn}} \left(\frac{1}{r}\right) d\mathbf{x}, \qquad \forall f(\mathbf{x}) \in C_0^\infty(\mathbb{R}^3). \tag{A.2}$$

For any fixed $\varepsilon > 0$, let $B_\varepsilon = \{\mathbf{x} \in \mathbb{R}^3 \mid |\mathbf{x}| < \varepsilon\}$ and $B_\varepsilon^c = \{\mathbf{x} \in \mathbb{R}^3 \mid |\mathbf{x}| \geq \varepsilon\}$. It is straightforward to check that

$$\phi(\mathbf{x}) = -\partial_{\mathbf{nn}} \left(\frac{1}{r}\right), \qquad 0 \neq \mathbf{x} \in \mathbb{R}^3. \tag{A.3}$$

Using integration by parts and noticing (A.3), we get

$$\begin{aligned}
\int_{B_\varepsilon^c} \phi(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} &= -\int_{B_\varepsilon^c} f(\mathbf{x})\, \partial_{\mathbf{nn}} \left(\frac{1}{r}\right)\, d\mathbf{x} \\
&= \int_{B_\varepsilon^c} \partial_{\mathbf{n}} \left(\frac{1}{r}\right)\, \partial_{\mathbf{n}}(f(\mathbf{x}))\, d\mathbf{x} + \int_{\partial B_\varepsilon} f(\mathbf{x})\, \frac{\mathbf{n}\cdot\mathbf{x}}{r}\, \partial_{\mathbf{n}} \left(\frac{1}{r}\right)\, dS \\
&= -\int_{B_\varepsilon^c} \frac{1}{r}\, \partial_{\mathbf{nn}}(f(\mathbf{x}))\, d\mathbf{x} + I_1^\varepsilon + I_2^\varepsilon,
\end{aligned} \tag{A.4}$$

where

$$I_1^\varepsilon := \int_{\partial B_\varepsilon} f(\mathbf{x})\, \frac{\mathbf{n}\cdot\mathbf{x}}{r}\, \partial_{\mathbf{n}} \left(\frac{1}{r}\right)\, dS, \qquad I_2^\varepsilon := -\int_{\partial B_\varepsilon} \frac{\mathbf{n}\cdot\mathbf{x}}{r^2}\, \partial_{\mathbf{n}}\,(f(\mathbf{x}))\, dS. \tag{A.5}$$

From (A.5), changing of variables, we get

$$\begin{aligned} I_1^\varepsilon &= -\int_{\partial B_\varepsilon} \frac{(\mathbf{n}\cdot\mathbf{x})^2}{r^4} f(\mathbf{x})\,dS = -\int_{\partial B_1} \frac{(\mathbf{n}\cdot\mathbf{x})^2}{\varepsilon^2} f(\varepsilon\mathbf{x})\,\varepsilon^2 dS \\ &= -\int_{\partial B_1} (\mathbf{n}\cdot\mathbf{x})^2 f(\mathbf{0})\,dS - \int_{\partial B_1} (\mathbf{n}\cdot\mathbf{x})^2 \left[f(\varepsilon\mathbf{x}) - f(\mathbf{0})\right]\,dS. \end{aligned} \tag{A.6}$$

Choosing $0 \neq \mathbf{n}_1 \in \mathbb{R}^3$ and $0 \neq \mathbf{n}_2 \in \mathbb{R}^3$ such that $\{\mathbf{n_1},\, \mathbf{n_2},\, \mathbf{n}\}$ forms an orthornormal basis of $\mathbb{R}^3$, by symmetry, we obtain

$$\begin{aligned} A &:= \int_{\partial B_1} (\mathbf{n}\cdot\mathbf{x})^2\,dS = \frac{1}{3}\int_{\partial B_1} \left[(\mathbf{n}\cdot\mathbf{x})^2 + (\mathbf{n_1}\cdot\mathbf{x})^2 + (\mathbf{n_2}\cdot\mathbf{x})^2\right]\,dS \\ &= \frac{1}{3}\int_{\partial B_1} |\mathbf{x}|^2 dS = \frac{1}{3}\int_{\partial B_1} dS = \frac{4\pi}{3}, \end{aligned} \tag{A.7}$$

$$\begin{aligned} &\left|\int_{\partial B_1} (\mathbf{n}\cdot\mathbf{x})^2 \left(f(\varepsilon\mathbf{x}) - f(\mathbf{0})\right)\,dS\right| = \left|\int_{\partial B_1} (\mathbf{n}\cdot\mathbf{x})^2 \varepsilon\ \left[\mathbf{x}\cdot\nabla f(\theta\varepsilon\mathbf{x})\right]\,dS\right| \\ &\quad \le \varepsilon\,\|\nabla f\|_{L^\infty(B_\varepsilon)} \int_{\partial B_1} dS \le 4\pi\varepsilon\,\|\nabla f\|_{L^\infty(B_\varepsilon)}, \end{aligned} \tag{A.8}$$

where $0 \le \theta \le 1$. Plugging (A.7) and (A.8) into (A.6), we have

$$I_1^\varepsilon \to -\frac{4\pi}{3} f(\mathbf{0}), \qquad \varepsilon \to 0^+. \tag{A.9}$$

Similarly, for $\varepsilon \to 0^+$, we get

$$|I_2^\varepsilon| \le \|\nabla f\|_{L^\infty(B_\varepsilon)} \int_{\partial B_\varepsilon} \frac{1}{\varepsilon}\,dS = 4\pi\varepsilon\,\|\nabla f\|_{L^\infty(B_\varepsilon)} \to 0, \tag{A.10}$$

$$\left|\int_{B_\varepsilon} \frac{1}{r}\,\partial_{\mathbf{nn}}(f(\mathbf{x}))\,d\mathbf{x}\right| \le \|D^2 f\|_{L^\infty(B_\varepsilon)} \int_{B_\varepsilon} \frac{1}{r}\,d\mathbf{x} \le 2\pi\varepsilon^2\,\|D^2 f\|_{L^\infty(B_\varepsilon)} \to 0. \tag{A.11}$$

Combining (A.9), (A.10) and (A.11), taking $\varepsilon \to 0^+$ in (A.4), we obtain

$$\int_{\mathbb{R}^3} \phi(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} = -\frac{4\pi}{3} f(\mathbf{0}) - \int_{\mathbb{R}^3} \frac{1}{r}\,\partial_{\mathbf{nn}}(f(\mathbf{x}))\,d\mathbf{x}, \qquad \forall f(\mathbf{x}) \in C_0^\infty(\mathbb{R}^3). \tag{A.12}$$

Thus (A.2) follows from (A.12) and the definition of the derivative in the distribution sense, i.e.

$$\int_{\mathbb{R}^3} f(\mathbf{x})\,\partial_{\mathbf{nn}}\left(\frac{1}{r}\right)\,d\mathbf{x} = \int_{\mathbb{R}^3} \frac{1}{r}\,\partial_{\mathbf{nn}}(f(\mathbf{x}))\,d\mathbf{x}, \qquad \forall f(\mathbf{x}) \in C_0^\infty(\mathbb{R}^3), \tag{A.13}$$

and the equality (2.15) is proved. □

Appendix **B**

Derivation of quasi-2D equation I (3.4)

Here, we derive the 2D approximation of GPPS (2.19)-(2.20). Taking ansatz (3.3), multiplying both sides of GPPS (2.19) by $\varepsilon^{-1/2}w_0(z/\varepsilon)$, integrating over z variable, we get

$$\partial_t\phi(x,y,t) = [-\frac{1}{2}(\partial_{xx}+\partial_{yy}) + V_2 + \frac{\beta-\lambda}{\varepsilon\sqrt{2\pi}}|\phi|^2]\phi - 3\lambda\varepsilon^{-1}\phi\int_{\mathbb{R}}\partial_{\mathbf{nn}}\varphi(x,y,z,t)w_0^2(z/\varepsilon)dz.$$

Hence, we only need to evaluate $\varepsilon^{-1}\int_{\mathbb{R}}\partial_{\mathbf{nn}}\varphi(x,y,z,t)w_0^2(z/\varepsilon)dz$ term. Making use of the Poisson equation (2.20) $-\nabla^2\varphi = \varepsilon^{-1}|\phi|^2w_0^2(z/\varepsilon)$, we can have

$$\partial_{\mathbf{nn}}\varphi(x,y,z,t) = \partial_{\mathbf{n}_\perp\mathbf{n}_\perp}\varphi + 2n_1n_3\partial_{xz}\varphi + 2n_2n_3\partial_{yz}\varphi - n_3^2\varphi - n_3^2\varepsilon^{-1}|\phi|^2w_0^2(z/\varepsilon).$$

By the ansatz assumption, we know that $\varphi = U_{\text{dip}} * |\psi|^2$ is symmetric in z, and we can derive that by noticing the odd function's integral is 0 in the whole space,

$$\begin{aligned}&\int_{\mathbb{R}}\partial_{\mathbf{nn}}\varphi(x,y,z,t)w_0^2(z/\varepsilon)dz\\ &= \left(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2(\partial_{xx}+\partial_{yy})\right)\int_{\mathbb{R}}\varphi(x,y,z,t)w_0^2(z/\varepsilon)dz + \frac{-n_3^2}{\sqrt{2\pi}}|\phi(x,y,t)|^2. \qquad \text{(B.1)}\end{aligned}$$

Further calculations show that

$$
\begin{aligned}
&\varepsilon^{-1}\int_{\mathbb{R}}\varphi(x,y,z,t)w_0^2(z/\varepsilon)dz\\
&=\frac{1}{4\pi\varepsilon^2}\int_{\mathbb{R}^4}\frac{|\phi(x',y',t)|^2 w_0^2(z'/\varepsilon)w_0^2(z/\varepsilon)}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}dx'\,dy'\,dz'\,dz\\
&=\frac{1}{4\pi^2\varepsilon}\int_{\mathbb{R}^2}|\phi(x',y',t)|^2\left\{\int_{\mathbb{R}^2}\frac{e^{-(z^2+(z')^2)/\varepsilon^2}}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\,dz\,dz'\right\}dx'\,dy'\\
&\overset{z-z'=\alpha,z+z'=\alpha'}{=\!=\!=\!=\!=\!=\!=}\frac{1}{8\pi^2\varepsilon^2}\int_{\mathbb{R}^2}|\phi(x',y',t)|^2\left\{\int_{\mathbb{R}^2}\frac{e^{-\frac{1}{2\varepsilon^2}(\alpha^2+(\alpha')^2)}}{\sqrt{(x-x')^2+(y-y')^2+\alpha^2}}\,d\alpha\,d\alpha'\right\}dx'\,dy'\\
&=\frac{1}{4\sqrt{2}\pi^{3/2}\varepsilon^2}\int_{\mathbb{R}^2}|\phi(x',y',t)|^2\left\{\int_{\mathbb{R}}\frac{e^{-\frac{1}{2\varepsilon^2}\alpha^2}}{\sqrt{(x-x')^2+(y-y')^2+\alpha^2}}\,d\alpha\right\}dx'\,dy'\\
&\overset{s=\varepsilon^{-1}\alpha}{=\!=\!=\!=}\frac{1}{4\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}^2}|\phi(x',y',t)|^2\left\{\int_{\mathbb{R}}\frac{e^{-\frac{s^2}{2}}}{\sqrt{(x-x')^2+(y-y')^2+\varepsilon^2 s^2}}\,ds\right\}dx'\,dy'\\
&=U_\varepsilon^{2D}*|\phi|^2.
\end{aligned}
\tag{B.2}
$$

Combining the above results together, we then arrive at the quasi-2D I equation (3.4)-(3.5).

Appendix C

Derivation of quasi-1D equation (3.10)

Here, we derive the 1D approximation of GPPS (2.19)-(2.20). Taking ansatz (3.9), multiplying both sides of GPPS (2.19) by $\varepsilon^{-1}w_0^{\perp}(x/\varepsilon, y/\varepsilon)$, integrating over x, y variables, we get

$$\partial_t\phi(z,t) = [-\frac{1}{2}\partial_{zz} + V_1 + \frac{\beta-\lambda}{2\pi\varepsilon^2}|\phi|^2]\phi - 3\lambda\varepsilon^{-2}\phi\int_{\mathbb{R}^2}\partial_{\mathbf{nn}}\varphi(x,y,z,t)\left(w_0^{\perp}(x/\varepsilon,y/\varepsilon)\right)^2 dxdy.$$

Hence, we only need to evaluate $\varepsilon^{-2}\int_{\mathbb{R}^2}\partial_{\mathbf{nn}}\varphi(x,y,z,t)\left(w_0^{\perp}(x/\varepsilon,y/\varepsilon)\right)^2 dxdy$ term. Making use of the Poisson equation (2.20) $-\nabla^2\varphi = \varepsilon^{-2}|\phi|^2\left(w_0^{\perp}(x/\varepsilon,y/\varepsilon)\right)^2$, we can have

$$\partial_{\mathbf{nn}}\varphi(x,y,z,t) = \partial_{zz}\varphi + 2n_1n_3\partial_{xz}\varphi + 2n_2n_3\partial_{yz}\varphi + (n_1^2\partial_{xx} + n_2^2\partial_{yy})\varphi - (n_1^2+n_2^2)\varepsilon^{-1}|\phi|^2\left(w_0^{\perp}\right)^2.$$

By the ansatz assumption (3.9), we know that $\varphi = U_{\text{dip}} * |\psi|^2$ is symmetric in x and y, and we can derive that by noticing the odd function's integral is 0,

$$\begin{aligned}
&\varepsilon^{-2}\int_{\mathbb{R}^2}\partial_{\mathbf{nn}}\varphi(x,y,z,t)\left(w_0^{\perp}(x/\varepsilon,y/\varepsilon)\right)^2 dxdy \\
&= \varepsilon^{-2}\int_{\mathbb{R}^2}(n_3^2 - \frac{1-n_3^2}{2})\partial_{zz}\varphi(x,y,z,t)\left(w_0^{\perp}(x/\varepsilon,y/\varepsilon)\right)^2 dxdy - \frac{3(1-n_3^2)}{4\pi\varepsilon^2}|\phi|^2,
\end{aligned}$$

and consequently

$$
\begin{aligned}
&\varepsilon^{-2}\int_{\mathbb{R}^2}\varphi(x,y,z,t)\left(w_0^{\perp}(y/\varepsilon,z/\varepsilon)\right)^2\,dydz\\
&=\frac{1}{4\pi\varepsilon^2}\int_{\mathbb{R}^5}\frac{|\phi(x',t)|^2\left(w_0^{\perp}(y'/\varepsilon,z'/\varepsilon)\right)^2\left(w_0^{\perp}(y/\varepsilon,z/\varepsilon)\right)^2}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}dx'\,dy'\,dz'\,dy\,dz,\\
&=\frac{1}{4\pi^3\varepsilon^4}\int_{\mathbb{R}}|\phi(x',t)|^2\left\{\int_{\mathbb{R}^4}\frac{e^{-(y^2+(y')^2+z^2+(z')^2)/2\varepsilon^2}}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\,dy\,dy'\,dz\,dz'\right\}dx'\\
&\overset{\substack{y-y'=\alpha,y+y'=\alpha'\\ z-z'=s,z+z'=s'}}{=}\frac{1}{16\pi^3\varepsilon^4}\int_{\mathbb{R}^2}|\phi(x',t)|^2\left\{\int_{\mathbb{R}^2}\frac{e^{-\frac{1}{2\varepsilon^2}(\alpha^2+(\alpha')^2+s^2+(s')^2)}}{\sqrt{(x-x')^2+\alpha^2+\beta^2}}\,d\alpha\,d\alpha'\,d\beta\,d\beta'\right\}dx'\\
&=\frac{1}{8\pi^2\varepsilon^2}\int_{\mathbb{R}}|\phi(x',t)|^2\left\{\int_{\mathbb{R}^2}\frac{e^{-\frac{1}{2\varepsilon^2}(\alpha^2+s^2)}}{\sqrt{(x-x')^2+\alpha^2+s^2}}\,d\alpha\,ds\right\}dx'\\
&\overset{\substack{\alpha=\rho\cos\theta\\ s=\rho\sin\theta}}{=}\frac{\gamma}{4\pi}\int_{\mathbb{R}}|\phi(x',t)|^2\left\{\int_{\mathbb{R}+}\frac{\rho e^{-\frac{\rho^2}{2\varepsilon^2}}}{\sqrt{(x-x')^2+\rho^2}}\,d\rho\right\}dx'\\
&\overset{r=\rho^2/\varepsilon^2}{=}\frac{1}{8\pi}\int_{\mathbb{R}}|\phi(x',t)|^2\left\{\int_{\mathbb{R}+}\frac{e^{-\frac{r}{2}}}{\sqrt{(x-x')^2+\varepsilon^2 r}}dr\right\}dx'\\
&=\frac{1}{4\sqrt{2\pi}\varepsilon}U_\varepsilon^{1D}*|\phi|^2. \qquad\qquad (C.1)
\end{aligned}
$$

Combining the above results together, we can obtain quasi-1D I equation (3.10).

Appendix D

Outline of the convergence between NLSW and NLSE

Here, we outline the convergence rate between the solutions of NLSW and NLSE in $\mathbb{R}^d$ ($d = 1, 2, 3$). Let $S_0^\varepsilon(t)$, $S_1^\varepsilon(t)$ be the semi-groups associated with the linear part of equation (7.1), i.e. $S_0^\varepsilon(t)u_0$ is the solution of

$$\begin{cases} i\partial_t u(\mathbf{x},t) - \varepsilon^2\partial_{tt}u(\mathbf{x},t) + \nabla^2 u(\mathbf{x},t) = 0, & \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \\ u(\mathbf{x},0) = u_0(\mathbf{x}), \qquad \partial_t u(\mathbf{x},0) = 0, & \mathbf{x} \in \mathbb{R}^d, \end{cases} \tag{D.1}$$

and $S_1^\varepsilon(t)u_1$ is the solution of

$$\begin{cases} i\partial_t u(\mathbf{x},t) - \varepsilon^2\partial_{tt}u(\mathbf{x},t) + \nabla^2 u(\mathbf{x},t) = 0, & \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \\ u(\mathbf{x},0) = 0, \qquad \partial_t u(\mathbf{x},0) = u_1(\mathbf{x}), & \mathbf{x} \in \mathbb{R}^d. \end{cases} \tag{D.2}$$

There hold the estimates, for some constant $C > 0$,

$$\forall\phi,\, \forall s, \qquad \|S_0^\varepsilon(t)\phi\|_{H^s} \le C\|\phi\|_{H^s}, \qquad \|S_1^\varepsilon(t)\phi\|_{H^s} \le C\varepsilon^2\|\phi\|_{H^s}. \tag{D.3}$$

Then $u^\varepsilon := u^\varepsilon(\mathbf{x},t)$ solves equation (7.1) if and only if u^ε satisfies the integral equation

$$u^\varepsilon(t) = S_0^\varepsilon(t)u^\varepsilon(0) + S_1^\varepsilon(t)\partial_t u^\varepsilon(0) - \frac{1}{\varepsilon^2}\int_0^t S_1^\varepsilon(t-s) f(|u^\varepsilon(s)|^2)u^\varepsilon(s)\, ds. \tag{D.4}$$

By rewriting the NLSE (7.5) as

$$i\partial_t u - \varepsilon^2\partial_{tt}u + \nabla^2 u + f(|u|^2)u + \varepsilon^2 u_{tt} = 0, \tag{D.5}$$

we can see that the solution $u := u(\mathbf{x}, t)$ of NLSE (7.5) satisfies the integral equation,

$$u(t) = S_0^\varepsilon(t)u(0) + S_1^\varepsilon(t)\partial_t u(0) - \frac{1}{\varepsilon^2}\int_0^t S_1^\varepsilon(t-s)\left(f(|u(s)|^2)u(s) + \varepsilon^2 u_{tt}(s)\right) ds. \quad \text{(D.6)}$$

Subtracting (D.6) from (D.4), and using the properties (D.3), in spirit of [31,51], we could obtain for appropriate initial data, $f(\cdot)$ and $T > 0$

$$\|u^\varepsilon(t) - u(t)\|_{H^s} \le C_T\varepsilon^2, \quad t \in [0, T], \quad s \ge 0. \quad \text{(D.7)}$$

For the behavior of $\partial_t u^\varepsilon(\mathbf{x}, t)$, we look at the case $f = 0$ in NLSW (7.1), then

$$\widehat{u^\varepsilon}(\xi, t) = C_1(\xi)e^{i\frac{1+\sqrt{1+4\varepsilon^2|\xi|^2}}{2\varepsilon^2}t} + C_2(\xi)e^{i\frac{1-\sqrt{1+4\varepsilon^2|\xi|^2}}{2\varepsilon^2}t}, \quad \xi \in \mathbb{R}^d, \quad t \ge 0, \quad \text{(D.8)}$$

where

$$C_1(\xi) = \frac{1}{2}\left[\widehat{u}_0(\xi) - \frac{\hat{u}_0(\xi) + 2\varepsilon^2 i\hat{u}_1(\xi)}{\sqrt{1+4\varepsilon^2|\xi|^2}}\right], \quad C_2(\xi) = \frac{1}{2}\left[\widehat{u}_0(\xi) + \frac{\hat{u}_0(\xi) + 2\varepsilon^2 i\hat{u}_1(\xi)}{\sqrt{1+4\varepsilon^2|\xi|^2}}\right].$$

Hence it is natural to make assumption (B) for the well-prepared and ill-prepared initial data.

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List of Publications

[1] "Second order averaging for the nonlinear Schrodinger equation with strong anisotropic potential" (with Naoufel Ben Abdallah, Francois Castella and Florian Méhats), *Kinet. Relat. Models., Vol. 4, no. 4, pp. 831-856, 2011.*

[2] "Mean-field regime of trapped dipolar Bose-Einstein condensates in one and two dimensions" (with Weizhu Bao, Matthias Rosenkranz and Zhen Lei), *Phys. Rev. A, Vol. 82, 2010, article 043623.*

[3] "Ground states of two-component Bose-Einstein condensates with an internal atomic Josephson junction" (with Weizhu Bao), *East Asia Journal on Applied Mathematics, Vol. 1, pp. 49–81, 2010.*

[4] "Efficient numerical methods for computing ground states and dynamics of dipolar Bose-Einstein condensates" (with Weizhu Bao and Hanquan Wang), *J. Comput. Phys., Vol. 229, pp. 7874–7892, 2010.*

[5] "Existence and uniqueness of weak solutions for a non-uniformly parabolic equation" (with Shulin Zhou), *J. Funct. Anal., 257, no. 10, pp. 3021–3042, 2009.*

[6] "L^q interior estimates of the gradient for weak solutions of quasilinear elliptic equations" (with Fengping Yao), *Acta Math. Sin. (Engl. Ser.), 23, no. 12, pp. 2225–2234, 2007.*

[7] "A note on harmonic functions" (with Feng Li), *Beijing Daxue Xuebao Ziran Kexue Ban, 43, no. 3, pp. 296–298, 2007.*

[8] "Optimal error estimates of finite difference methods for the Gross-Pitaevskii equation with angular momentum rotation" (with Weizhu Bao), *Math. Comp.*, to appear.

[9] " Uniform error estimates of finite difference methods for the nonlinear Schrödinger equation with wave operator" (with Weizhu Bao), *SIAM J Numer. Anal.*, to appear.

[10] "Gross-Pitaevskii-Poisson equation for dipolar Bose-Einstein condensate with anisotropic confinement" (with Weizhu Bao and Naoufel Ben Abdallah), preprint.

[11] "Effective dipole-dipole interactions in multilayered dipolar Bose-Einstein condensates" (with Weizhu Bao and Matthias Rosenkranz), preprint.

[12] "Breathing oscillations of a trapped impurity in a Bose gas" (with T. H. Johnson, M. Bruderer, S. R. Clark, W. Bao, and D. Jaksch), preprint.

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