



SEOUL ICM 2014
INTERNATIONAL
CONGRESS OF
MATHEMATICIANS

Proceedings of the International Congress of Mathematicians

Seoul 2014

VOLUME IV Invited Lectures

Editors

Sun Young Jang

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Dae-Woong Lee

Ikkwon Yie

Mathematical models and numerical methods for Bose-Einstein condensation

Weizhu Bao

Abstract. The achievement of Bose-Einstein condensation (BEC) in ultracold vapors of alkali atoms has given enormous impulse to the theoretical and experimental study of dilute atomic gases in condensed quantum states inside magnetic traps and optical lattices. This article offers a short survey on mathematical models and theories as well as numerical methods for BEC based on the mean field theory. We start with the Gross-Pitaevskii equation (GPE) in three dimensions (3D) for modeling one-component BEC of the weakly interacting bosons, scale it to obtain a three-parameter model and show how to reduce it to two dimensions (2D) and one dimension (1D) GPEs in certain limiting regimes. Mathematical theories and numerical methods for ground states and dynamics of BEC are provided. Extensions to GPE with an angular momentum rotation term for a rotating BEC, to GPE with long-range anisotropic dipole-dipole interaction for a dipolar BEC and to coupled GPEs for spin-orbit coupled BECs are discussed. Finally, some conclusions are drawn and future research perspectives are discussed.

Mathematics Subject Classification (2010). Primary 35Q55; Secondary 70F10.

Keywords. Bose-Einstein condensation, Gross-Pitaevskii equation, nonlinear Schrödinger equation, ground state, dynamics, numerical methods.

1. Introduction

The achievement of Bose-Einstein condensation (BEC) of dilute gases in 1995 [3, 28, 39] marked the beginning of a new era in atomic, molecular and optical (AMO) physics and quantum optics. In fact, the phenomenon known as BEC was predicted by Einstein in 1924 [40, 41] based on the ideas of Bose [27] concerning photons: In a system of bosons obeying Bose statistics under the assumption that it is in equilibrium at temperature T and chemical potential μ , Einstein [40, 41] derived the so-called Bose-Einstein distribution (or Bose-Einstein statistics), in the grand canonical ensemble, for the mean occupation of the j th energy state as

$$n_j = \frac{1}{e^{(\varepsilon_j - \mu)/k_B T} - 1} := f(\varepsilon_j), \quad j = 0, 1, \dots, \quad (1.1)$$

where $\varepsilon_j > \mu$ is the energy of the j th state, n_j is the number of particles in state j , k_B is the Boltzmann constant. The mean total number of particles is given as $N(T, \mu) = \sum_{j=0}^{\infty} f(\varepsilon_j)$,

and the mean total energy is given as $E(T, \mu) = \sum_{j=0}^{\infty} \varepsilon_j f(\varepsilon_j)$. From the above distribution, Einstein [40, 41] predicted that there should be a critical temperature T_c below which a finite fraction of all the particles “condense” into the same one-particle state.

Einstein’s original prediction was for a noninteracting gas and did not receive much attention in a long time. After the observation of superfluidity in liquid ^4He below the λ temperature (2.17K) in 1938, London [61] suggested that despite the strong interatomic interactions BEC was indeed occurring in this system and was responsible for the superfluid properties. This suggestion has stood the test of time and is the basis for our modern understanding of the properties of the superfluid phase. By combining laser cooling and evaporative cooling, in 1995 BEC was realized in a system that is about as different as possible from ^4He , namely, dilute atomic alkali gases trapped by magnetic fields and over the last two decades these systems have been the subject of an explosion of research, both experimentally and theoretically. Perhaps the single aspect of BEC systems that makes them most fascinating is best illustrated by the cover of *Science* magazine of December 22, 1995, in which the Bose condensate is declared “**molecule of the year**” and pictured as a platoon of soldiers marching in lock-step: every atom in the condensate must behave in exactly the same way, and this has the consequence, *inter alia*, that effects which are so small as to be essentially invisible at the level of single atom may be spectacularly amplified. Most BEC experiments reach quantum degeneracy between 50 nK and 2 μK , at densities between 10^{11} and 10^{15} cm^{-3} . The largest condensates are of 100 million atoms for sodium, and a billion for hydrogen; the smallest are just a few hundred atoms. Depending on the magnetic trap, the shape of the condensate is either approximately round, with a diameter of 10–15 μm , or cigar-shaped with about 15 μm in diameter and 300 μm in length. The full cooling cycle that produce a condensate may take from a few seconds to as long as several minutes [37, 52]. For better understanding of the long history towards the BEC and its physical study, we refer to the Nobel lectures [37, 52] and several review papers in physics [38, 56, 65, 67].

The experimental advances in BEC [3, 28, 39] have spurred great excitement in the AMO community and condense matter community as well as computational and applied mathematics community. Since 1995, numerous efforts have been devoted to the studies of ultracold atomic gases and various kinds of condensates of dilute gases have been produced for both bosonic particles and fermionic particles [38, 43, 56]. In this rapidly growing research area, mathematical models and analysis as well as numerical simulation have been playing an important role in understanding the theoretical part of BEC and predicting and guiding the experiments. The goal of this paper is to offer a short survey on mathematical models and theories as well as numerical methods for BEC based on the Gross-Pitaevskii equation (GPE) [7, 46, 65–67]. The paper is organized as follows. In section 2, we present the GPE for BEC based on the mean field approximation. Ground states and their computations are discussed in section 3, and dynamics and its computation are presented in section 4. Extensions to rotating BEC, dipolar BEC and spin-orbit-coupled BEC are presented in section 5. Finally, some conclusions and perspectives are drawn in section 6.

2. The Gross-Pitaevskii equation

In this section, we will present the GPE for modeling BEC based on the mean field approximation [7, 46, 65–67], its nondimensionalization and dimension reduction to lower

dimensions.

2.1. Mean field approximation. For a BEC of ultracold dilute gas with N identical bosons confined in an external trap, only binary interaction is important, then the many-body Hamiltonian for it can be written as [56, 58]

$$H_N = \sum_{j=1}^N \left(-\frac{\hbar^2}{2m} \Delta_j + V(\mathbf{x}_j) \right) + \sum_{1 \leq j < k \leq N} V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k), \quad (2.1)$$

where $\mathbf{x}_j \in \mathbb{R}^3$ denotes the position of the j th particle for $j = 1, \dots, N$, m is the mass of a boson, \hbar is the Planck constant, $\Delta_j = \nabla_j^2$ is the Laplace operator with respect to \mathbf{x}_j , $V(\mathbf{x}_j)$ is the external trapping potential, and $V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k)$ denotes the inter-atomic two body interaction. Denote the complex-valued wave function $\Psi_N := \Psi_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t) \in L^2(\mathbb{R}^{3N} \times \mathbb{R})$ for the N particles in the BEC, which is symmetric with respect to any permutation of the positions \mathbf{x}_j ($1 \leq j \leq N$), then the total energy is given as

$$E_{\text{total}}(\Psi_N) = (\Psi_N, H_N \Psi_N) := \int_{\mathbb{R}^{3N}} \bar{\Psi}_N H_N \Psi_N d\mathbf{x}_1 \dots d\mathbf{x}_N, \quad (2.2)$$

where \bar{f} , $\text{Re}(f)$ and $\text{Im}(f)$ denote the complex conjugate, real part and imaginary part of f , respectively, and the evolution of the system is described by the time-dependent linear Schrödinger equation

$$i\hbar \partial_t \Psi_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t) = \frac{\delta E_{\text{total}}(\Psi_N)}{\delta \bar{\Psi}_N} = H_N \Psi_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t), \quad (2.3)$$

where $i = \sqrt{-1}$ denotes the imaginary unit and t is time.

For a BEC, all particles are in the same quantum state and we can formally take the Hartree ansatz [7, 42, 46, 58, 59, 65–67]

$$\Psi_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t) \approx \prod_{j=1}^N \psi(\mathbf{x}_j, t), \quad (2.4)$$

with the normalization for the single-particle wave function $\psi := \psi(\mathbf{x}, t)$ as

$$\|\psi(\cdot, t)\|^2 := \int_{\mathbb{R}^3} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} = 1, \quad (2.5)$$

where $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ is the Cartesian coordinate in three dimensions (3D). Due to that the BEC gas is dilute and the temperature is below the critical temperature T_c , i.e. a weakly interacting gas, the binary interaction V_{int} is well approximated by the effective contact interacting potential [65–67]:

$$V_{\text{int}}(\mathbf{x}_j - \mathbf{x}_k) = g \delta(\mathbf{x}_j - \mathbf{x}_k), \quad (2.6)$$

where $\delta(\cdot)$ is the Dirac distribution and the constant $g = \frac{4\pi\hbar^2 a_s}{m}$ with a_s the s -wave scattering length of the bosons (positive for repulsive interaction and negative for attractive interaction, which is much smaller than the average distance between the particles). Plugging

(2.4) into (2.2), noticing (2.1) and (2.6), and keeping only the two-body interaction, we obtain $E_{\text{total}}(\Psi_N) \approx N E(\psi)$ with the Gross-Pitaevskii (GP) energy (or energy per particle) defined as [46, 58, 59, 65–67]

$$E(\psi) = \int_{\mathbb{R}^3} \left[\frac{\hbar^2}{2m} |\nabla\psi(\mathbf{x}, t)|^2 + V(\mathbf{x})|\psi(\mathbf{x}, t)|^2 + \frac{Ng}{2} |\psi(\mathbf{x}, t)|^4 \right] d\mathbf{x}. \quad (2.7)$$

The dynamics of the BEC will be governed by the following nonlinear Schrödinger equation (NLSE) with cubic nonlinearity, known as the Gross-Pitaevskii equation (GPE) [7, 42, 46, 58, 59, 65–67]:

$$i\hbar\partial_t\psi = \frac{\delta E(\psi)}{\delta\psi} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + Ng|\psi|^2 \right] \psi, \quad \mathbf{x} \in \mathbb{R}^3, \quad t > 0. \quad (2.8)$$

In most BEC experiments, the trapping potential has been taken as the harmonic oscillator potential [3, 7, 28, 39, 67]

$$V(\mathbf{x}) = \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \quad \mathbf{x} = (x, y, z)^T \in \mathbb{R}^3, \quad (2.9)$$

where ω_x, ω_y and ω_z are the trap frequencies in x -, y - and z -direction, respectively. Without loss of generality, we assume that $\omega_x \leq \omega_y \leq \omega_z$ throughout the paper. For other trapping potentials used in BEC experiments, such as box potential, double-well potential and optical lattice potential, we refer to [7, 26, 65–68] and references therein.

The derivation of the GPE (2.8) from the linear Schrödinger equation (2.3) for a BEC (or a system of N identical particles) based on mean field approximation – dimension reduction – was formally obtained by Pitaevskii [66] and Gross [46] independently in 1960s. Since the first experimental observation of BEC in 1995, much attention has been paid to provide mathematical justification for the derivation when N is large enough: For ground states, Lieb et al. [58, 59] proved rigorously that the GP energy (2.7) approximates the energy of the many-body system correctly in the mean field regime; and for dynamics, Yau et al. [42] established the validity of the GPE (2.8) as an approximation for (2.3), which inspired great interests in the study on dynamics for such many body system recently [35, 36, 54]. The above GPE (2.8) is a very simple equation, which is very convenient for mathematical analysis and numerical calculations, and in the case of the BEC alkali gases, appears to give a rather good quantitative description of the behavior in a large variety of experiments [7, 65–67]. It has become the fundamental mathematical model for studying theoretically the ground states and dynamics of BECs [7, 65–67].

2.2. Nondimensionalization. In order to study theoretically BECs, we nondimensionalize the GPE (2.8) with the harmonic trapping potential (2.9) under the normalization (2.5) and introduce [7, 65–67]

$$\tilde{t} = \frac{t}{t_s}, \quad \tilde{\mathbf{x}} = \frac{\mathbf{x}}{x_s}, \quad \tilde{\psi}(\tilde{\mathbf{x}}, \tilde{t}) = x_s^{3/2} \psi(\mathbf{x}, t), \quad \tilde{E}(\tilde{\psi}) = \frac{E(\psi)}{E_s}, \quad (2.10)$$

where $t_s = \frac{1}{\omega_x}$, $x_s = \sqrt{\frac{\hbar}{m\omega_x}}$ and $E_s = \hbar\omega_x$ are the scaling parameters of dimensionless time, length and energy units, respectively. Plugging (2.10) into (2.8), multiplying by $t_s^2/mx_s^{1/2}$, and then removing all $\tilde{}$, we obtain the following dimensionless GPE under the

normalization (2.5) in 3D [7, 65–67]:

$$i\partial_t\psi(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \kappa|\psi(\mathbf{x}, t)|^2 \right] \psi(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^3, \quad t > 0, \quad (2.11)$$

where $\kappa = \frac{4\pi N a_s}{x_s}$ is the dimensionless interaction constant, the dimensionless trapping potential is given as [7, 65–67]

$$V(\mathbf{x}) = \frac{1}{2} (x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), \quad \mathbf{x} \in \mathbb{R}^3, \quad \text{with } \gamma_y = \frac{\omega_y}{\omega_x} \geq 1, \quad \gamma_z = \frac{\omega_z}{\omega_x} \geq 1, \quad (2.12)$$

and dimensionless energy functional $E(\psi)$ is defined as [7, 65–67]

$$E(\psi) = \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla\psi(\mathbf{x}, t)|^2 + V(\mathbf{x})|\psi(\mathbf{x}, t)|^2 + \frac{\kappa}{2} |\psi(\mathbf{x}, t)|^4 \right] dx. \quad (2.13)$$

2.3. Dimension reduction. In many BEC experiments [3, 28, 39, 65–67], the trapping potential (2.12) is anisotropic, i.e. $\gamma_z \gg 1$ and/or $\gamma_y \gg 1$, and then the GPE in 3D can be further reduced to a GPE in two dimensions (2D) or one dimension (1D). Assume the initial data for the 3D GPE (2.11) is given as

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \quad (2.14)$$

and define the linear operator H as

$$H = -\frac{1}{2}\Delta + V(\mathbf{x}) = -\frac{1}{2}\nabla^2 + V(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \quad (2.15)$$

When $\gamma_z \gg 1$ and $\gamma_y = O(1)$ ($\Leftrightarrow \omega_z \gg \omega_x$ and $\omega_y = O(\omega_x)$), i.e. disk-shaped condensate with strong confinement in the z -direction [3, 28, 39, 65, 67], then the linear operator H can be split as

$$H = -\frac{1}{2}\Delta_{\perp} + V_2(\mathbf{x}_{\perp}) - \frac{1}{2}\partial_{zz} + \frac{z^2}{2\varepsilon^4} := H_{\perp} + H_z^{\varepsilon} = H_{\perp} + \frac{1}{\varepsilon^2}H_{\tilde{z}}, \quad \mathbf{x} \in \mathbb{R}^3, \quad (2.16)$$

where $\mathbf{x}_{\perp} = (x, y)^T \in \mathbb{R}^2$, $\Delta_{\perp} = \partial_{xx} + \partial_{yy}$, $V_2(\mathbf{x}_{\perp}) = \frac{1}{2}(x^2 + \gamma_y^2 y^2)$, $H_{\perp} := -\frac{1}{2}\Delta_{\perp} + V_2(\mathbf{x}_{\perp})$, $\varepsilon = 1/\sqrt{\gamma_z}$, $z = \varepsilon\tilde{z}$ and

$$H_z^{\varepsilon} := -\frac{1}{2}\partial_{zz} + \frac{z^2}{2\varepsilon^4} = \frac{1}{\varepsilon^2} \left[-\frac{1}{2}\partial_{\tilde{z}\tilde{z}} + \frac{\tilde{z}^2}{2} \right] := \frac{1}{\varepsilon^2}H_{\tilde{z}}, \quad z, \tilde{z} \in \mathbb{R}. \quad (2.17)$$

For $H_{\tilde{z}}$ in (2.17), we know that the following linear eigenvalue problem

$$H_{\tilde{z}}\chi(\tilde{z}) = \left[-\frac{1}{2}\partial_{\tilde{z}\tilde{z}} + \frac{\tilde{z}^2}{2} \right] \chi(\tilde{z}) = \mu\chi(\tilde{z}), \quad \tilde{z} \in \mathbb{R}, \quad (2.18)$$

with $\|\chi\|^2 := \int_{\mathbb{R}} |\chi(\tilde{z})|^2 d\tilde{z} = 1$ admits distinct orthonormal eigenfunctions $\chi_k(\tilde{z})$ with corresponding eigenvalues μ_k for $k = 0, 1, \dots$. In fact, they form an orthonormal basis of $L^2(\mathbb{R})$ and can be chosen as [7, 14, 25, 65–67]

$$\mu_k = \frac{k+1}{2}, \quad \chi_k(\tilde{z}) = \frac{1}{\pi^{1/4}\sqrt{2^k k!}} e^{-\tilde{z}^2/2} H_k(\tilde{z}), \quad \tilde{z} \in \mathbb{R}, \quad k = 0, 1, 2, \dots, \quad (2.19)$$

with $H_k(\tilde{z})$ the standard Hermite polynomial of degree k . Thus $(\chi_k^\varepsilon(z), \mu_k^\varepsilon)$ for $k \geq 0$ are orthonormal eigenpairs to the operator H_z^ε with

$$\mu_k^\varepsilon = \frac{\mu_k}{\varepsilon^2} = \frac{k+1}{2\varepsilon^2}, \quad \chi_k^\varepsilon(z) = \frac{1}{\sqrt{\varepsilon}} \chi_k(\tilde{z}) = \frac{1}{\sqrt{\varepsilon}} \chi_k\left(\frac{z}{\varepsilon}\right), \quad z \in \mathbb{R}. \tag{2.20}$$

For simplicity of notation, here we only consider “pure state” case in the strong confinement direction, especially the “ground state” case [7, 14, 25, 65–67]. Assuming that the initial data ψ_0 in (2.14) satisfies

$$\psi_0(\mathbf{x}) \approx \psi_2(\mathbf{x}_\perp) \chi_0^\varepsilon(z), \quad \mathbf{x} \in \mathbb{R}^3, \quad 0 < \varepsilon \ll 1, \tag{2.21}$$

noting the scale separation in (2.16), when $\varepsilon \rightarrow 0^+$, the solution ψ to the 3D GPE (2.11) can be well approximated as [7, 14, 25, 65–67]

$$\psi(\mathbf{x}, t) \approx \psi_2(\mathbf{x}_\perp, t) \chi_0^\varepsilon(z) e^{-i\mu_0^\varepsilon t}, \quad \mathbf{x} \in \mathbb{R}^3, \quad t \geq 0. \tag{2.22}$$

Plugging (2.22) into (2.11) and then multiplying by $\chi_0^\varepsilon(z) e^{i\mu_0^\varepsilon t}$, integrating for z over \mathbb{R} , we obtain formally the GPE in 2D with $\psi_2 := \psi_2(\mathbf{x}_\perp, t)$ as [7, 14, 25, 65–67]

$$i\partial_t \psi_2 = \left[-\frac{1}{2} \Delta_\perp + V_2(\mathbf{x}_\perp) + \kappa \sqrt{\frac{\gamma_z}{2\pi}} |\psi_2|^2 \right] \psi_2, \quad \mathbf{x}_\perp \in \mathbb{R}^2, \quad t > 0. \tag{2.23}$$

The above dimension reduction from 3D to 2D is mathematically and rigorously justified in the very weak interaction regime [6, 25], i.e. $\kappa = O(\varepsilon) = O(1/\sqrt{\gamma_z})$ as $\varepsilon \rightarrow 0^+$. However, for the strong interaction regime, i.e. $\kappa = O(1)$ and $\varepsilon \rightarrow 0^+$, it is very challenging. The key difficulty is due to that the energy associated to the 2D GPE (2.23) is unbounded in this regime. Recently, by using a proper re-scaling, the dimension reduction is justified in this regime too [16].

Similarly, when $\gamma_z \gg 1$ and $\gamma_y \gg 1$ ($\Leftrightarrow \omega_z \gg \omega_x$ and $\omega_y \gg \omega_x$), i.e. cigar-shaped condensate with strong confinement in the (y, z) -plane [3, 28, 39, 65, 67], the 3D GPE (2.11) can be reduced to the following GPE in 1D as [7, 14, 65–67]

$$i\partial_t \psi_1(x, t) = \left[-\frac{1}{2} \partial_{xx} + \frac{x^2}{2} + \kappa \frac{\sqrt{\gamma_y \gamma_z}}{2\pi} |\psi_1(x, t)|^2 \right] \psi_1(x, t), \quad x \in \mathbb{R}, \quad t > 0. \tag{2.24}$$

Then the 3D GPE (2.11), 2D GPE (2.23) and 1D GPE (2.24) can be written in a unified way [7, 14, 65–67]

$$i\partial_t \psi(\mathbf{x}, t) = \left[-\frac{1}{2} \nabla^2 + V(\mathbf{x}) + \beta |\psi(\mathbf{x}, t)|^2 \right] \psi(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \tag{2.25}$$

where $\beta = \kappa, \kappa \sqrt{\gamma_z/2\pi}$ and $\kappa \sqrt{\gamma_y \gamma_z}/2\pi$ when $d = 3, 2$ and 1 , respectively, and

$$V(\mathbf{x}) = \frac{1}{2} \begin{cases} x^2, & d = 1, \\ x^2 + \gamma_y^2 y^2, & d = 2, \\ x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2, & d = 3, \end{cases} \quad \mathbf{x} \in \mathbb{R}^d. \tag{2.26}$$

This GPE conserves the normalization (or mass)

$$N(\psi(\cdot, t)) = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} \equiv \int_{\mathbb{R}^d} |\psi(\mathbf{x}, 0)|^2 d\mathbf{x} = 1, \quad t \geq 0, \tag{2.27}$$

and the energy per particle

$$E(\psi(\cdot, t)) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \psi|^2 + V(\mathbf{x}) |\psi|^2 + \frac{\beta}{2} |\psi|^4 \right] d\mathbf{x} \equiv E(\psi(\cdot, 0)), \quad t \geq 0. \quad (2.28)$$

In fact, the energy functional $E(\psi)$ can be split into three parts as $E(\psi) = E_{\text{kin}}(\psi) + E_{\text{pot}}(\psi) + E_{\text{int}}(\psi)$ with the kinetic energy $E_{\text{kin}}(\psi)$, potential energy $E_{\text{pot}}(\psi)$ and interaction energy $E_{\text{int}}(\psi)$ defined as

$$E_{\text{kin}}(\psi) = \int_{\mathbb{R}^d} \frac{1}{2} |\nabla \psi|^2 d\mathbf{x}, \quad E_{\text{int}}(\psi) = \int_{\mathbb{R}^d} \frac{\beta}{2} |\psi|^4 d\mathbf{x}, \quad E_{\text{pot}}(\psi) = \int_{\mathbb{R}^d} V(\mathbf{x}) |\psi|^2 d\mathbf{x}.$$

3. Ground states

To find the stationary state of the GPE (2.25) for a BEC, we write [7, 12, 65–67]

$$\psi(\mathbf{x}, t) = \phi(\mathbf{x}) e^{-i\mu t}, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0, \quad (3.1)$$

where μ is the chemical potential of the condensate and $\phi(\mathbf{x})$ is a function independent of time. Substituting (3.1) into (2.25) gives the following for (μ, ϕ) :

$$\mu \phi(\mathbf{x}) = -\frac{1}{2} \nabla^2 \phi(\mathbf{x}) + V(\mathbf{x}) \phi(\mathbf{x}) + \beta |\phi(\mathbf{x})|^2 \phi(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad (3.2)$$

under the normalization condition

$$\|\phi\|^2 := \int_{\mathbb{R}^d} |\phi(\mathbf{x})|^2 d\mathbf{x} = 1. \quad (3.3)$$

This is a nonlinear eigenvalue problem with a constraint and any eigenvalue μ can be computed from its corresponding eigenfunction $\phi(\mathbf{x})$ by [7, 12, 65–67]

$$\mu = \mu(\phi) = E(\phi) + \int_{\mathbb{R}^d} \frac{\beta}{2} |\phi(\mathbf{x})|^4 d\mathbf{x} = E(\phi) + E_{\text{int}}(\phi). \quad (3.4)$$

The ground state of a BEC is usually defined as the minimizer of the following nonconvex (or constrained) minimization problem [7, 12]: Find $\phi_g \in S$ such that

$$E_g := E(\phi_g) = \min_{\phi \in S} E(\phi), \quad \text{with } \mu_g := \mu(\phi_g) = E(\phi_g) + E_{\text{int}}(\phi_g), \quad (3.5)$$

where $S = \{\phi \mid \|\phi\| = 1, E(\phi) < \infty\}$ is the unit sphere and μ_g is the corresponding chemical potential. It is easy to show that the ground state ϕ_g is an eigenfunction of the nonlinear eigenvalue problem (3.2) under the constraint (3.3), which is the Euler-Lagrangian equation of constrained minimization problem (3.5). Any eigenfunction of (3.2) whose energy is larger than that of the ground state is usually called excited states in the physics literatures.

3.1. Existence and uniqueness. Denote the best Sobolev constant C_b in 2D as

$$C_b := \inf_{0 \neq f \in H^1(\mathbb{R}^2)} \frac{\|\nabla f\|_{L^2(\mathbb{R}^2)}^2 \|f\|_{L^2(\mathbb{R}^2)}^2}{\|f\|_{L^4(\mathbb{R}^2)}^4}. \quad (3.6)$$

The best constant C_b can be attained at some H^1 function [7] and it is crucial in considering the existence of ground states in 2D. For existence and uniqueness of the ground state to (3.5), we have the following results.

Theorem 3.1 (Existence and uniqueness [7, 59]). *Suppose $V(\mathbf{x}) \geq 0$ ($\mathbf{x} \in \mathbb{R}^d$) in the energy functional (2.28) satisfies the confining condition $\lim_{|\mathbf{x}| \rightarrow \infty} V(\mathbf{x}) = \infty$, then there exists a ground state $\phi_g \in S$ for (3.5) if one of the following holds: (i) $d = 3, \beta \geq 0$; (ii) $d = 2, \beta > -C_b$; (iii) $d = 1$, for all $\beta \in \mathbb{R}$. Moreover, the ground state can be chosen as nonnegative $|\phi_g|$, and $\phi_g(\mathbf{x}) = e^{i\theta_0} |\phi_g(\mathbf{x})|$ for some constant $\theta_0 \in \mathbb{R}$. For $\beta \geq 0$, the nonnegative ground state ϕ_g is unique. If the potential $V(\mathbf{x}) \in L^2_{loc}$, the nonnegative ground state is strictly positive. In contrast, there exists no ground state if one of the following holds: (i') $d = 3, \beta < 0$; (ii') $d = 2, \beta \leq -C_b$.*

For the ground state $\phi_g \in S$ of (3.5) with the harmonic potential (2.26), we have the following properties.

Theorem 3.2 (Virial identity [7, 67]). *The ground state $\phi_g \in S$ of (3.5) satisfies the following virial identity*

$$2E_{\text{kin}}(\phi_g) - 2E_{\text{pot}}(\phi_g) + dE_{\text{int}}(\phi_g) = 0. \tag{3.7}$$

Theorem 3.3 (Symmetry [7, 59]). *Suppose $\gamma_y = \gamma_z = 1$ in (2.26), i.e. the harmonic trapping potential $V(\mathbf{x})$ is radially/spherically symmetric in 2D/3D and monotone increasing, then the positive ground state $\phi_g \in S$ of (3.5) must be radially/spherically symmetric in 2D/3D and monotonically decreasing, i.e. $\phi_g(\mathbf{x}) = \phi_g(r)$ with $r = |\mathbf{x}|$ for $\mathbf{x} \in \mathbb{R}^d$.*

Theorem 3.4 (Decay at far-field [7]). *When $\beta \geq 0$, for any $\nu > 0$, there exists a constant $C_\nu > 0$ such that*

$$|\phi_g(\mathbf{x})| \leq C_\nu e^{-\nu|\mathbf{x}|}, \quad \mathbf{x} \in \mathbb{R}^d, \quad d = 1, 2, 3. \tag{3.8}$$

3.2. Approximations under the harmonic potential. For any fixed $\beta \geq 0$ in (2.28), we denote the positive ground state of (3.5) with (2.26) as $\phi_g := \phi_g^\beta$ and the corresponding energy and chemical potential as $E_g := E_g^\beta = E(\phi_g^\beta)$ and $\mu_g := \mu_g^\beta = \mu(\phi_g^\beta)$, respectively. When $\beta = 0$, i.e. linear case, the exact ground state ϕ_g^0 can be found as [7, 12, 65–67]

$$E_g^0 = \mu_g^0 = \frac{1}{2} \begin{cases} 1, & d = 1, \\ 1 + \gamma_y, & d = 2, \\ 1 + \gamma_y + \gamma_z, & d = 3, \end{cases} \quad \phi_g^0(\mathbf{x}) = \begin{cases} \frac{1}{\pi^{1/4}} e^{-x^2/2}, & d = 1, \\ \frac{\gamma_y^{1/4}}{\pi^{1/2}} e^{-(x^2 + \gamma_y y^2)/2}, & d = 2, \\ \frac{(\gamma_y \gamma_z)^{1/4}}{\pi^{3/4}} e^{-(x^2 + \gamma_y y^2 + \gamma_z z^2)/2}, & d = 3. \end{cases}$$

When $|\beta| = o(1)$ in (2.28), i.e. weak interaction case, the ground state ϕ_g^β can be approximated by $\phi_g^\beta(\mathbf{x}) \approx \phi_g^0(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^d$, and the corresponding energy E_g^β and chemical potential μ_g^β can be approximated with $C_d = \int_{\mathbb{R}^d} |\phi_g^0(\mathbf{x})|^4 dx$ as

$$E_g^\beta \approx E(\phi_g^0) = E_g^0 + \frac{\beta}{2} C_d = E_g^0 + O(\beta), \quad \mu_g^\beta \approx \mu(\phi_g^0) = \mu_g^0 + \beta C_d = \mu_g^0 + O(\beta),$$

where $C_1 = \sqrt{\pi}/2, C_2 = \sqrt{\gamma_y}/2\pi$ and $C_3 = \sqrt{\gamma_y \gamma_z}/(2\pi)^{3/2}$.

When $\beta \gg 1$, the ground state ϕ_g^β can be well approximated by the Thomas-Fermi (TF) approximation $\phi_g^\beta \approx \phi_g^{\text{TF}}$ [7, 67], i.e. by dropping the diffusion term (e.g. the first term on the right hand side of (3.2)), we obtain

$$\mu_g^{\text{TF}} \phi_g^{\text{TF}}(\mathbf{x}) = V(\mathbf{x}) \phi_g^{\text{TF}}(\mathbf{x}) + \beta |\phi_g^{\text{TF}}(\mathbf{x})|^2 \phi_g^{\text{TF}}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad (3.9)$$

with $\mu_g^{\text{TF}} \approx \mu_g^\beta$. Solving the above equation, we get

$$\phi_g^\beta(\mathbf{x}) \approx \phi_g^{\text{TF}}(\mathbf{x}) = \begin{cases} \sqrt{(\mu_g^{\text{TF}} - V(\mathbf{x})) / \beta}, & V(\mathbf{x}) < \mu_g^{\text{TF}}, \\ 0, & \text{otherwise,} \end{cases} \quad (3.10)$$

where μ_g^{TF} is chosen to satisfy the normalization $\|\phi_g^{\text{TF}}\| = 1$, which can be computed as [7, 12, 65–67]

$$\mu_g^\beta \approx \mu_g^{\text{TF}} = \begin{cases} \frac{1}{2} \left(\frac{3\beta}{2}\right)^{2/3}, \\ \left(\frac{\beta\gamma_y}{\pi}\right)^{1/2}, \\ \frac{1}{2} \left(\frac{15\beta\gamma_y\gamma_z}{4\pi}\right)^{2/5}, \end{cases} \quad E_g^\beta \approx E_g^{\text{TF}} = \begin{cases} \frac{3}{10} \left(\frac{3\beta}{2}\right)^{2/3}, & d = 1, \\ \frac{2}{3} \left(\frac{\beta\gamma_y}{\pi}\right)^{1/2}, & d = 2, \\ \frac{5}{14} \left(\frac{15\beta\gamma_y\gamma_z}{4\pi}\right)^{2/5}, & d = 3, \end{cases}$$

with $E_g^{\text{TF}} := \mu_g^{\text{TF}} - E_{\text{int}}(\phi_g^{\text{TF}})$. For fixed $\gamma_y \geq 1$ and $\gamma_z \geq 1$ in (2.26) and when $\beta \gg 1$ (e.g. $N \gg 1$), from the above TF approximation, we can get the typical lengths (i.e. $R_x^{\text{TF}} = \sqrt{2\mu_g^{\text{TF}}}$, $R_y^{\text{TF}} = \sqrt{2\mu_g^{\text{TF}}/\gamma_y}$ and $R_z^{\text{TF}} = \sqrt{2\mu_g^{\text{TF}}/\gamma_z}$ of the support of the TF approximation ϕ_g^{TF} in x -, y - and z -directions, respectively) – TF radius– of the ground state ϕ_g^β for a BEC as: $R_x^{\text{TF}} = O(\beta^{1/(d+2)}) = O(N^{1/(d+2)})$ for $d = 1, 2, 3$, $R_y^{\text{TF}} = O(\beta^{1/(d+2)}) = O(N^{1/(d+2)})$ for $d = 2, 3$, and $R_z^{\text{TF}} = O(\beta^{1/5}) = O(N^{1/5})$ for $d = 3$. In addition, we also have $E_g^\beta \approx E_g^{\text{TF}} = \frac{d+2}{d+4} \mu_g^{\text{TF}} \approx \frac{d+2}{d+4} \mu_g^\beta = O(\beta^{2/(d+2)}) = O(N^{2/(d+2)})$, $\|\phi_g^\beta\|_{L^\infty} \approx \phi_g^{\text{TF}}(\mathbf{0}) = O(\beta^{-d/2(d+2)}) = O(N^{-d/2(d+2)})$ for $d = 1, 2, 3$. Thus it is easy to see that there is no limit of the ground state ϕ_g^β when $\beta \rightarrow \infty$ under the standard physics scaling (2.10) for a BEC. In addition, for computing the ground states and dynamics of a BEC, the bounded computational domain needs to be chosen depending on β such that the truncation error can be negligible!

3.3. Numerical methods. Various numerical methods for computing the ground state ϕ_g in (3.5) have been proposed and studied in the literature [7, 11, 12, 22, 34, 64]. Among them, one of the most efficient and simple methods is the following *gradient flow with discrete normalization* (GFDN) [7, 12]. Choose a time step $\tau := \Delta t > 0$ and denote time steps as $t_n = n\tau$ for $n = 0, 1, \dots$. At each time interval $[t_n, t_{n+1})$, by applying the steepest decent method to the energy functional $E(\phi)$ without constraint and then projecting the solution back to the unit sphere S at $t = t_{n+1}$ so as to satisfy the constraint (3.3), we have

$$\partial_t \phi = -\frac{1}{2} \frac{\delta E(\phi)}{\delta \phi} = \left[\frac{1}{2} \nabla^2 - V(\mathbf{x}) - \beta |\phi|^2 \right] \phi, \quad t_n < t < t_{n+1}, \quad (3.11)$$

$$\phi(\mathbf{x}, t_{n+1}) \triangleq \phi(\mathbf{x}, t_{n+1}^+) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{\|\phi(\cdot, t_{n+1}^-)\|}, \quad \mathbf{x} \in \mathbb{R}^d, \quad n \geq 0, \quad (3.12)$$

where $\phi := \phi(\mathbf{x}, t)$, $\phi(\mathbf{x}, t_n^\pm) = \lim_{t \rightarrow t_n^\pm} \phi(\mathbf{x}, t)$, and with the initial data

$$\phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d. \tag{3.13}$$

In fact, the gradient flow (3.11) can be obtained from the GPE (2.25) by $t \rightarrow -it$, thus the GFDN is known as *imaginary time method* in physics literatures [34, 64].

For the above GFDN, suppose $V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$ and $\|\phi_0\|^2 := \int_{\mathbb{R}^d} |\phi_0(\mathbf{x})|^2 dx = 1$, then we have [7, 12]

Theorem 3.5 (Energy diminishing [12]). *For $\beta = 0$, the GFDN (3.11)-(3.13) is energy diminishing for any time step $\tau > 0$ and initial data ϕ_0 , i.e.*

$$E(\phi(\cdot, t_{n+1})) \leq E(\phi(\cdot, t_n)) \leq \dots \leq E(\phi(\cdot, 0)) = E(\phi_0), \quad n = 0, 1, 2, \dots \tag{3.14}$$

Let $\tau \rightarrow 0$ in (3.11)-(3.13), we can obtain the following *normalized gradient flow* (NGF) [12]

$$\partial_t \phi(\mathbf{x}, t) = \left[\frac{1}{2} \nabla^2 - V(\mathbf{x}) - \beta |\phi|^2 + \mu_\phi(t) \right] \phi, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0, \tag{3.15}$$

where

$$\mu_\phi(t) = \frac{\mu(\phi(\cdot, t))}{\|\phi(\cdot, t)\|^2} = \frac{1}{\|\phi(\cdot, t)\|^2} \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla \phi|^2 + V(\mathbf{x}) |\phi|^2 + \beta |\phi|^4 \right] dx. \tag{3.16}$$

Theorem 3.6 (Energy diminishing [12]). *The NGF (3.15) with (3.13) is normalization conservative and energy diminishing, i.e.*

$$\|\phi(\cdot, t)\| \equiv \|\phi_0\| = 1, \quad \frac{d}{dt} E(\phi) = -2 \|\partial_t \phi(\cdot, t)\|^2 \leq 0, \quad t \geq 0, \tag{3.17}$$

which in turn implies

$$E(\phi(\cdot, t)) \geq E(\phi(\cdot, s)), \quad 0 \leq t \leq s < \infty. \tag{3.18}$$

With the above two theorems, the positive ground state can be obtained from the GFDN as $\phi_g(\mathbf{x}) = \lim_{t \rightarrow \infty} \phi(\mathbf{x}, t)$ provided that ϕ_0 is chosen as a positive function and time step τ is not too big when $\beta \geq 0$ [7, 12]. In addition, the GFDN (3.11)-(3.13) can be discretized by the *backward Euler finite difference* (BEFD) discretization [7, 12]. For simplicity of notation, here we only present the BEFD for the GFDN in 1D truncated on a bounded interval $U = (a, b)$ with homogeneous Dirichlet boundary conditions. Choose a mesh size $h := \Delta x = (b - a)/M > 0$ with M a positive integer, denote grid points as $x_j = a + jh$ for $j = 0, 1, \dots, M$, and let ϕ_j^n be the numerical approximation of $\phi(x_j, t_n)$. Then a BEFD discretization for the GFDN in 1D reads [7, 12]

$$\begin{aligned} \frac{\phi_j^{(1)} - \phi_j^n}{\tau} &= \frac{\phi_{j+1}^{(1)} - 2\phi_j^{(1)} + \phi_{j-1}^{(1)}}{2h^2} - \left[V(x_j) + \beta (\phi_j^n)^2 \right] \phi_j^{(1)}, \quad 1 \leq j \leq M - 1, \\ \phi_0^{(1)} = \phi_M^{(1)} &= 0, \quad \phi_j^0 = \phi_0(x_j), \quad \phi_j^{n+1} = \frac{\phi_j^{(1)}}{\|\phi^{(1)}\|_h}, \quad 0 \leq j \leq M, \quad n \geq 0, \end{aligned}$$

where $\|\phi^{(1)}\|_h^2 := h \sum_{j=1}^{M-1} |\phi_j^{(1)}|^2$. This BEFD method is implicit and unconditionally stable, the discretized system can be solved by the Thomas' algorithm, the memory cost is

$O(M)$ and computational cost is $O(M)$ per time step. The ground state can be obtained numerically from the above BEFD when $\max_{0 \leq j \leq M} \frac{|\phi_j^{n+1} - \phi_j^n|}{\tau} \leq \varepsilon$ with ε small enough, e.g. 10^{-6} . For extensions to 2D and 3D as well as other numerical methods, we refer [7, 11, 12, 22, 34, 64] and references therein.

4. Dynamics

For studying the dynamics of the GPE (2.25), the initial data is usually chosen as

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d. \tag{4.1}$$

The GPE (2.25) is a dispersive PDE and it is *time reversible* or *symmetric*, i.e. it is unchanged under the change of variable in time as $t \rightarrow -t$ and taken conjugate in the equation. Another important property is *time transverse* or *gauge invariant*, i.e. if $V \rightarrow V + \alpha$ with α a given real constant, then the solution $\psi \rightarrow \psi e^{-i\alpha t}$ which immediately implies that the density $\rho = |\psi|^2$ is unchanged. It conserves the normalization (or mass) and energy (or Hamiltonian), i.e. $N(\psi(\cdot, t)) \equiv N(\psi_0)$ and $E(\psi(\cdot, t)) \equiv E(\psi_0)$ for $t \geq 0$.

4.1. Well-posedness and dynamical properties. For studying well-posedness of the GPE (2.25), we introduce the functional spaces

$$L_V(\mathbb{R}^d) = \left\{ \phi \mid \int_{\mathbb{R}^d} V(\mathbf{x}) |\phi(\mathbf{x})|^2 d\mathbf{x} < \infty \right\}, \quad X := X(\mathbb{R}^d) = H^1(\mathbb{R}^d) \cap L_V(\mathbb{R}^d).$$

Theorem 4.1 (Well-posedness [7]). *Suppose the trapping potential is nonnegative and at most quadratic growth in far field, i.e., $V(\mathbf{x}) \in C^\infty(\mathbb{R}^d)$ and $D^{\mathbf{k}}V(\mathbf{x}) \in L^\infty(\mathbb{R}^d)$ for all $\mathbf{k} \in \mathbb{N}_0^d$ with $|\mathbf{k}| \geq 2$, then we have*

- (i) *For any initial data $\psi_0 \in X(\mathbb{R}^d)$, there exists a time $T_{\max} \in (0, +\infty]$ such that the Cauchy problem of the GPE (2.25) with (4.1) has a unique maximal solution $\psi \in C([0, T_{\max}), X)$. It is maximal in the sense that if $T_{\max} < \infty$, then $\|\psi(\cdot, t)\|_X \rightarrow \infty$ when $t \rightarrow T_{\max}^-$.*
- (ii) *As long as the solution $\psi(\mathbf{x}, t)$ remains in the energy space X , the L^2 -norm $\|\psi(\cdot, t)\|_2$ and energy $E(\psi(\cdot, t))$ are conserved for $t \in [0, T_{\max})$.*
- (iii) *The solution of the Cauchy problem is global in time, i.e., $T_{\max} = \infty$, if $d = 1$ or $d = 2$ with $\beta > C_b / \|\psi_0\|_2^2$ or $d = 3$ with $\beta \geq 0$.*

Theorem 4.2 (Finite time blow-up [7]). *In 2D and 3D, assume $V(\mathbf{x})$ is at most quadratic growth in far field and satisfies $V(\mathbf{x})d + \mathbf{x} \cdot \nabla V(\mathbf{x}) \geq 0$ for $\mathbf{x} \in \mathbb{R}^d$ ($d = 2, 3$). When $\beta < 0$, for any initial data $\psi_0(\mathbf{x}) \in X$ with finite variance $\int_{\mathbb{R}^d} |\mathbf{x}|^2 |\psi_0|^2 d\mathbf{x} < \infty$, the Cauchy problem of the GPE (2.25) with (4.1) will blow-up at finite time, i.e. $T_{\max} < \infty$, if one of the following holds:*

- (i) $E(\psi_0) < 0$;
- (ii) $E(\psi_0) = 0$ and $\text{Im} \left(\int_{\mathbb{R}^d} \overline{\psi_0}(\mathbf{x}) (\mathbf{x} \cdot \nabla \psi_0(\mathbf{x})) d\mathbf{x} \right) < 0$;
- (iii) $E(\psi_0) > 0$ and $\text{Im} \left(\int_{\mathbb{R}^d} \overline{\psi_0}(\mathbf{x}) (\mathbf{x} \cdot \nabla \psi_0(\mathbf{x})) d\mathbf{x} \right) < -\sqrt{E(\psi_0)d} \|\mathbf{x}\psi_0\|_{L^2}$.

If there is no external potential in the GPE (2.25), i.e. $V(\mathbf{x}) \equiv 0$, then the momentum and angular momentum are also conserved [4, 7, 70]. The GPE (2.25) admits the plane wave solution as $\psi(\mathbf{x}, t) = Ae^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$, where the time frequency ω , amplitude A and spatial wave number \mathbf{k} satisfy the following *dispersion relation* [4, 7, 70]: $\omega = \frac{|\mathbf{k}|^2}{2} + \beta|A|^2$. In 1D, i.e. $d = 1$, when $\beta < 0$, it admits the well-known bright soliton solution as [4, 70]

$$\psi_B(x, t) = \frac{A}{\sqrt{-\beta}} \operatorname{sech}(A(x - vt - x_0)) e^{i(vx - \frac{1}{2}(v^2 - A^2)t + \theta_0)}, \quad x \in \mathbb{R}, \quad t \geq 0, \quad (4.2)$$

where $\frac{A}{\sqrt{-\beta}}$ is the amplitude of the soliton with A a positive real constant, v is the velocity of the soliton, x_0 and θ_0 are the initial shifts in space and phase, respectively. Since the soliton solution is exponentially decaying for $|x| \rightarrow +\infty$, then the mass and energy are well defined and given by: $N(\psi_B) = -\frac{2A}{\beta}$ and $E(\psi_B) = \frac{Av^2}{-\beta} + \frac{A^3}{-3\beta}$. When $\beta > 0$, it admits dark solitons [67, 70].

Let $\psi := \psi(\mathbf{x}, t)$ be the solution of the GPE (2.25) with the harmonic potential (2.26) and initial data (4.1) satisfying $\|\psi_0\| = 1$, define the center-of-mass $\mathbf{x}_c(t) = \int_{\mathbb{R}^d} \mathbf{x} |\psi(\mathbf{x}, t)|^2 dx$, square of the condensate width $\delta_\alpha(t) = \int_{\mathbb{R}^d} \alpha^2 |\psi(\mathbf{x}, t)|^2 dx$ with $\alpha = x, y$ or z , and angular momentum expectation $\langle L_z \rangle(t) = \int_{\mathbb{R}^d} \psi(\mathbf{x}, t) L_z \psi(\mathbf{x}, t) dx$ with $L_z = -i(x\partial_y - y\partial_x)$ when $d = 2, 3$. Then we have [7, 13]

Lemma 4.3 (Angular momentum expectation [7, 13]). *For any initial data $\psi_0(\mathbf{x})$ in (4.1), when $\gamma_y = 1$ in (2.26), i.e. the trapping potential is radially/cylindrically symmetric in 2D/3D, then the angular momentum expectation is conserved, i.e.*

$$\langle L_z \rangle(t) \equiv \langle L_z \rangle(0) = \int_{\mathbb{R}^d} \overline{\psi_0(\mathbf{x})} L_z \psi_0(\mathbf{x}) dx, \quad t \geq 0. \quad (4.3)$$

Lemma 4.4 (Condensate width [7, 13]). *For any initial data $\psi_0(\mathbf{x})$ in (4.1), in 1D without interaction, i.e. $d = 1$ and $\beta = 0$ in (2.25), we have*

$$\delta_x(t) = E(\psi_0) + \left(\delta_x^{(0)} - E(\psi_0) \right) \cos(2t) + \delta_x^{(1)} \sin(2t), \quad t \geq 0; \quad (4.4)$$

and in 2D with a radially symmetric trap, i.e. $d = 2$ and $\gamma_y = 1$ in (2.26), we have

$$\delta_r(t) = E(\psi_0) + \left(\delta_r^{(0)} - E(\psi_0) \right) \cos(2t) + \delta_r^{(1)} \sin(2t), \quad t \geq 0, \quad (4.5)$$

where $\delta_r(t) = \delta_x(t) + \delta_y(t)$, $\delta_r^{(0)} := \delta_x^{(0)} + \delta_y^{(0)}$, and $\delta_r^{(1)} := \delta_x^{(1)} + \delta_y^{(1)}$ with $\delta_\alpha^{(0)} = \int_{\mathbb{R}^d} \alpha^2 |\psi_0(\mathbf{x})|^2 dx$ and $\delta_\alpha^{(1)} = 2 \int_{\mathbb{R}^d} \alpha \operatorname{Im}(\overline{\psi_0} \partial_\alpha \psi_0) dx$ for $\alpha = x$ or y . Thus δ_x in 1D and δ_r in 2D are periodic functions with frequency doubling the trapping frequency.

Lemma 4.5 (Center-of-mass [7, 13, 19]). *For any initial data $\psi_0(\mathbf{x})$ in (4.1), the dynamics of the center-of-mass satisfies the following second-order ODE*

$$\ddot{\mathbf{x}}_c(t) + \Lambda \mathbf{x}_c(t) = 0, \quad t \geq 0, \quad (4.6)$$

with the following initial data

$$\mathbf{x}_c(0) = \mathbf{x}_c^{(0)} = \int_{\mathbb{R}^d} \mathbf{x} |\psi_0(\mathbf{x})|^2 dx, \quad \dot{\mathbf{x}}_c(0) = \mathbf{x}_c^{(1)} = \int_{\mathbb{R}^d} \operatorname{Im}(\overline{\psi_0} \nabla \psi_0) dx,$$

where Λ is a $d \times d$ diagonal matrix as $\Lambda = 1$ when $d = 1$, $\Lambda = \operatorname{diag}(1, \gamma_y^2)$ when $d = 2$, and $\Lambda = \operatorname{diag}(1, \gamma_y^2, \gamma_z^2)$ when $d = 3$. This implies that each component of \mathbf{x}_c is a periodic function whose frequency is the same as the trapping frequency in that direction.

Lemma 4.6 (Exact solution [7, 13]). *If the initial data $\psi_0(\mathbf{x})$ in (4.1) is chosen as*

$$\psi_0(\mathbf{x}) = \phi_e(\mathbf{x} - \mathbf{x}_0) e^{i(\mathbf{w}_0 \cdot \mathbf{x} + g_0)}, \quad \mathbf{x} \in \mathbb{R}^d, \quad (4.7)$$

where $\mathbf{x}_0, \mathbf{w}_0 \in \mathbb{R}^d$ and $g_0 \in \mathbb{R}$ are given constants, and (μ_e, ϕ_e) is a solution of the nonlinear eigenvalue problem (3.2) with the constraint (3.3), then the GPE (2.25) with (2.26) and (4.7) admits the following unique exact solution

$$\psi(\mathbf{x}, t) = \phi_e(\mathbf{x} - \mathbf{x}_c(t)) e^{-i\mu_e t} e^{i(\mathbf{w}(t) \cdot \mathbf{x} + g(t))}, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0, \quad (4.8)$$

where $\mathbf{x}_c(t)$ satisfies the second-order ODE (4.6) with the initial condition $\mathbf{x}_c(0) = \mathbf{x}_0$ and $\dot{\mathbf{x}}_c(0) = \mathbf{w}_0$, and $\mathbf{w}(t)$ and $g(t)$ satisfy the following ODEs

$$\dot{\mathbf{w}}(t) = -\Lambda \mathbf{x}_c(t), \quad \dot{g}(t) = V(\mathbf{x}_c(t)) = \frac{1}{2} \mathbf{x}_c(t) \cdot (\Lambda \mathbf{x}_c(t)), \quad t > 0, \quad (4.9)$$

with initial data $\mathbf{w}(0) = \mathbf{w}_0$ and $g(0) = g_0$.

4.2. Numerical methods. Various numerical methods have been proposed and studied in the literature [4, 7, 14, 20, 34, 64] for computing the dynamics of the GPE (2.25) with (4.1). Among them, one of the most efficient and accurate as well as simple methods is the following *time-splitting sine pseudospectral* (TSSP) method [4, 7, 14]. For simplicity of notation, here we only present the TSSP method for the GPE (2.25) in 1D truncated on a bounded interval $U = (a, b)$ with homogeneous Dirichlet boundary conditions. Let ψ_j^n be the numerical approximation of $\psi(x_j, t_n)$ and ψ^n be the solution vector at time $t = t_n = n\tau$ with components $\{\psi_j^n\}_{j=0}^M$, then a second-order TSSP method for the GPE (2.25) in 1D reads [4, 7, 14]

$$\begin{aligned} \psi_j^{(1)} &= \frac{2}{M} \sum_{l=1}^{M-1} e^{-i\tau\mu_l^2/4} (\widetilde{\psi^n})_l \sin(\mu_l(x_j - a)), \quad \psi_j^{(2)} = e^{-i\tau(V(x_j) + \beta|\psi_j^{(1)}|^2)} \psi_j^{(1)}, \\ \psi_j^{n+1} &= \frac{2}{M} \sum_{l=1}^{M-1} e^{-i\tau\mu_l^2/4} (\widetilde{\psi^{(2)}})_l \sin(\mu_l(x_j - a)), \quad 0 \leq j \leq M, \end{aligned}$$

where $\mu_l = l\pi/(b - a)$ for $1 \leq l \leq M - 1$ and $(\widetilde{\psi^n})_l$ and $(\widetilde{\psi^{(2)}})_l$ are the discrete sine transform (DST) coefficients of ψ^n and $\psi^{(2)}$, respectively. This TSSP method for the GPE (2.25) is explicit, unconditionally stable, second-order accurate in time and spectral-order accurate in space [4, 7, 14]. It is time reversible or symmetric, time transverse invariant, conserves the mass at the discretized level and has the same dispersive relation as the GPE when $V(\mathbf{x}) \equiv 0$. The memory cost is $O(M)$ and computational cost is $O(M \ln M)$ per time step. For extensions to 2D/3D and other numerical methods, we refer to [4, 7, 14, 20, 34, 64] and references therein.

4.3. Bogoliubov excitation of ground state. An important class of time-dependent solutions of the GPE (2.25) is given by the small-amplitude oscillations, where the changes in space and time of the wave function (or order parameter) with respect to the stationary states, especially ground states, are small. In many cases these solutions emphasize the collective behavior exhibited by the interacting Bose gases and can be interpreted in terms of the elementary excitations of the system. For describing the dynamics of a BEC, it is natural

to consider the linearized behavior of small perturbations around its ground state ϕ_g with chemical potential μ_g and take the ansatz [38, 43, 45, 67]

$$\psi(\mathbf{x}, t) = e^{-i\mu_g t} \left[\phi_g(\mathbf{x}) + u(\mathbf{x})e^{-i\omega t} - \overline{v(\mathbf{x})}e^{i\omega t} \right], \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \quad (4.10)$$

where the Bogoliubov amplitudes $u(\mathbf{x})$ and $v(\mathbf{x})$ are treated as small and $\omega \in \mathbb{C}$ to be determined. Substituting (4.10) into (2.25) and collecting first-order terms proportional to $e^{\pm i\omega t}$, we obtain the Bogoliubov equations – linear eigenvalue problem for (ω, u, v) — as [38, 43, 45, 67]

$$\begin{aligned} \omega u(\mathbf{x}) &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + 2\beta|\phi_g(\mathbf{x})|^2 - \mu_g \right] u(\mathbf{x}) - \phi_g^2 v(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \\ -\omega v(\mathbf{x}) &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + 2\beta|\phi_g(\mathbf{x})|^2 - \mu_g \right] v(\mathbf{x}) - \overline{\phi_g^2} u(\mathbf{x}). \end{aligned} \quad (4.11)$$

In many ways, the above Bogoliubov equations are analogous to a nonrelativistic version of the Dirac equation, with u and v as the particle and hole amplitudes, including the $(+, -)$ metric seen in the minus sign on the left hand side of the second equation compared to the first equation in (4.11) [38, 43, 45, 67]. In addition, a detailed analysis shows that physically relevant Bogoliubov eigenfunctions must satisfy the following *positive* normalization condition [38, 43, 45, 67]:

$$\|u\|^2 - \|v\|^2 := \int_{\mathbb{R}^d} [|u(\mathbf{x})|^2 - |v(\mathbf{x})|^2] d\mathbf{x} = 1. \quad (4.12)$$

For solutions of the Bogoliubov equations, especially no external trapping potential in (2.25), we refer to [38, 43, 45, 67] and references therein.

4.4. Semiclassical scaling and limits. In the strongly repulsive interaction regime, i.e. $\beta \gg 1$ in the GPE (2.25) with (2.26), another scaling (under the normalization (2.27) with ψ being replaced by ψ^ε) – semiclassical scaling – is also very useful in practice, especially in numerical computation. By choosing $\mathbf{x} \rightarrow \mathbf{x}\varepsilon^{-1/2}$ and $\psi = \varepsilon^{d/4} \psi^\varepsilon$ with $0 < \varepsilon = 1/\beta^{2/(2+d)} < 1$ ($\Leftrightarrow t = \frac{1}{\omega\varepsilon}$, $x_s = \sqrt{\hbar/m\varepsilon\omega_x}$ and $E_s = \hbar\omega_x/\varepsilon$ in (2.10) for the GPE (2.8) when $d = 3$), we obtain [7, 14]

$$i\varepsilon \partial_t \psi^\varepsilon(\mathbf{x}, t) = \left[-\frac{\varepsilon^2}{2}\nabla^2 + V(\mathbf{x}) + |\psi^\varepsilon(\mathbf{x}, t)|^2 \right] \psi^\varepsilon(\mathbf{x}, t), \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0. \quad (4.13)$$

This GPE conserves the following energy

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

Similarly, the nonlinear eigenvalue problem (3.2) (under the normalization (3.3) with $\phi = \phi^\varepsilon$) reads

$$\mu^\varepsilon \phi^\varepsilon(\mathbf{x}) = \left[-\frac{\varepsilon^2}{2}\nabla^2 + V(\mathbf{x}) + |\phi^\varepsilon(\mathbf{x})|^2 \right] \phi^\varepsilon(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad (4.14)$$

where the eigenvalue (or chemical potential) μ^ε can be computed from its corresponding eigenfunction ϕ^ε by $\mu^\varepsilon = \mu^\varepsilon(\phi^\varepsilon) = E^\varepsilon(\phi^\varepsilon) + E_{\text{int}}^\varepsilon(\phi^\varepsilon)$ with $E_{\text{int}}^\varepsilon(\phi^\varepsilon) = \frac{1}{2} \int_{\mathbb{R}^d} |\phi^\varepsilon|^4 d\mathbf{x}$.

The constrained minimization problem for ground state collapses to: Find $\phi_g^\varepsilon \in S$ such that

$$E_g^\varepsilon := E^\varepsilon(\phi_g^\varepsilon) = \min_{\phi^\varepsilon \in S} E^\varepsilon(\phi^\varepsilon), \quad \text{with } \mu_g^\varepsilon := \mu^\varepsilon(\phi_g^\varepsilon) = E^\varepsilon(\phi_g^\varepsilon) + E_{\text{int}}^\varepsilon(\phi_g^\varepsilon). \quad (4.15)$$

Similarly to section 3.2, we can get the TF approximation to the ground state when $0 < \varepsilon \ll 1$:

$$\phi_g^\varepsilon(\mathbf{x}) \approx \phi_g^{\text{TF}}(\mathbf{x}) = \begin{cases} \sqrt{\mu_g^{\text{TF}} - V(\mathbf{x})}, & V(\mathbf{x}) < \mu_g^{\text{TF}}, \\ 0, & \text{otherwise,} \end{cases} \quad (4.16)$$

where

$$\mu_g^\varepsilon \approx \mu_g^{\text{TF}} = \begin{cases} \frac{1}{2} \left(\frac{3}{2}\right)^{2/3}, \\ \left(\frac{\gamma_y}{\pi}\right)^{1/2}, \\ \frac{1}{2} \left(\frac{15\gamma_y\gamma_z}{4\pi}\right)^{2/5}, \end{cases} \quad E_g^\varepsilon \approx E_g^{\text{TF}} = \begin{cases} \frac{3}{10} \left(\frac{3}{2}\right)^{2/3}, & d = 1, \\ \frac{2}{3} \left(\frac{\gamma_y}{\pi}\right)^{1/2}, & d = 2, \\ \frac{5}{14} \left(\frac{15\gamma_y\gamma_z}{4\pi}\right)^{2/5}, & d = 3. \end{cases}$$

From this TF approximation, for fixed $\gamma_y \geq 1$ and $\gamma_z \geq 1$ in (2.26) and when $0 < \varepsilon \ll 1$, we have $E_g^\varepsilon \approx E_g^{\text{TF}} = \frac{d+2}{d+4} \mu_g^{\text{TF}} \approx \frac{d+2}{d+4} \mu_g^\varepsilon = O(1)$, $\|\phi_g^\varepsilon\|_{L^\infty} \approx \phi_g^{\text{TF}}(\mathbf{0}) = O(1)$, and the TF radius $R_x^{\text{TF}} = \sqrt{2\mu_g^{\text{TF}}} = O(1)$, $R_y^{\text{TF}} = \sqrt{2\mu_g^{\text{TF}}}/\gamma_y = O(1)$ and $R_z^{\text{TF}} = \sqrt{2\mu_g^{\text{TF}}}/\gamma_z = O(1)$ for $d = 1, 2, 3$. In addition, the ground state $\phi_g^\varepsilon(\mathbf{x})$ converges to $\phi_g^{\text{TF}}(\mathbf{x})$ uniformly when $\varepsilon \rightarrow 0^+$. Furthermore, for computing numerically the ground states and dynamics of a BEC, the bounded computational domain can be chosen independent of ε [7, 14].

Taking the WKB ansatz $\psi^\varepsilon(\mathbf{x}, t) = \sqrt{\rho^\varepsilon(\mathbf{x}, t)} e^{iS^\varepsilon(\mathbf{x}, t)/\varepsilon}$ with $\rho^\varepsilon = |\psi^\varepsilon|^2$ and S^ε the density and phase of the wave function, respectively, inserting it into the GPE (4.13) and separating real and imaginary parts, we obtain the transport and Hamilton-Jacobi equations for density and phase, respectively [7, 32, 44]

$$\begin{aligned} \partial_t \rho^\varepsilon + \text{div}(\rho^\varepsilon \nabla S^\varepsilon) &= 0, & \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \\ \partial_t S^\varepsilon + \frac{1}{2} |\nabla S^\varepsilon|^2 + \rho^\varepsilon + V(\mathbf{x}) &= \frac{\varepsilon^2}{2} \frac{1}{\sqrt{\rho^\varepsilon}} \Delta \sqrt{\rho^\varepsilon}. \end{aligned} \quad (4.17)$$

Furthermore, defining the quantum velocity $\mathbf{u}^\varepsilon = \nabla S^\varepsilon$ and current $\mathbf{J}^\varepsilon = \rho^\varepsilon \mathbf{u}^\varepsilon$, we get from (4.17) the Euler system with a third-order dispersion correction term – quantum hydrodynamics (QHD) – as [7, 32, 44]

$$\begin{aligned} \partial_t \rho^\varepsilon + \text{div} \mathbf{J}^\varepsilon &= 0, & \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \\ \partial_t \mathbf{J}^\varepsilon + \text{div} \left(\frac{\mathbf{J}^\varepsilon \otimes \mathbf{J}^\varepsilon}{\rho^\varepsilon} \right) + \rho^\varepsilon \nabla V(\mathbf{x}) + \nabla P(\rho^\varepsilon) &= \frac{\varepsilon^2}{4} \nabla (\rho^\varepsilon \nabla^2 \ln \rho^\varepsilon), \end{aligned} \quad (4.18)$$

where the pressure is defined as $P(\rho^\varepsilon) = (\rho^\varepsilon)^2/2$. Letting $\varepsilon \rightarrow 0^+$ in (4.18), formally we get the Euler system [7, 32, 44]

$$\begin{aligned} \partial_t \rho^0 + \text{div} \mathbf{J}^0 &= 0, & \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \\ \partial_t \mathbf{J}^0 + \text{div} \left(\frac{\mathbf{J}^0 \otimes \mathbf{J}^0}{\rho^0} \right) + \rho^0 \nabla V(\mathbf{x}) + \nabla P(\rho^0) &= 0. \end{aligned} \quad (4.19)$$

For mathematical justification of the passage from the GPE (4.13) to the Euler system (4.19), we refer to [7, 32, 44] and references therein.

5. Extensions

In this section, we will present briefly mathematical models and theories as well as numerical methods for rotating BEC based on the GPE with an angular momentum rotation term, dipolar BEC based on the GPE with a long-range anisotropic dipole-dipole interaction (DDI) and spin-orbit-coupled BEC based on coupled GPEs with an internal atomic Josephson junction (JJ) and an spin-orbit coupling term.

5.1. For rotating BEC. At temperatures T much smaller than the critical temperature T_c , following the mean field theory [1, 2, 7, 31, 43, 57, 62, 69], a BEC in the rotational frame is well described by the macroscopic wave function $\psi := \psi(\mathbf{x}, t)$, whose evolution is governed by the GPE with an angular momentum rotation term

$$i\hbar\partial_t\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - \tilde{\Omega}L_z + Ng|\psi|^2 \right] \psi, \quad \mathbf{x} \in \mathbb{R}^3, \quad t > 0, \quad (5.1)$$

where $\tilde{\Omega}$ is the angular velocity, L_z is the z -component angular momentum operator defined as $L_z = -i\hbar(x\partial_y - y\partial_x)$ and ψ satisfies the normalization condition (2.5).

Under the harmonic potential (2.9), similarly to the nondimensionalization in section 2.2 and dimension reduction in 2.3 from 3D to 2D when $\omega_z \gg \max\{\omega_x, \omega_y\}$ for a disk-shaped condensate [2, 7, 13, 23], we can obtain the following dimensionless GPE with an angular momentum rotation term in d -dimensions ($d = 2, 3$):

$$i \partial_t\psi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) - \Omega L_z + \beta|\psi|^2 \right] \psi, \quad \mathbf{x} \in \mathbb{R}^d, \quad t > 0, \quad (5.2)$$

where $\Omega = \tilde{\Omega}/\omega_x$, $\beta = \kappa$ and $\kappa\sqrt{\gamma_z/2\pi}$ when $d = 3$ and 2 , respectively, the dimensionless harmonic potential is given in (2.26) for $d = 3, 2$, and the dimensionless angular momentum rotation term is given as $L_z = -i(x\partial_y - y\partial_x)$. The GPE (5.2) conserves the normalization (2.5) and energy per particle

$$E(\psi(\cdot, t)) = \int_{\mathbb{R}^d} \left[\frac{1}{2} |\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 - \Omega\bar{\psi}L_z\psi + \frac{\beta}{2} |\psi|^4 \right] d\mathbf{x} \equiv E(\psi(\cdot, 0)), \quad t \geq 0.$$

The ground state can be defined the same as (3.5) with the above energy functional. For the existence and uniqueness as well as nonexistence, we have [2, 7, 23, 69]

Theorem 5.1 (Existence and uniqueness [2, 7, 23, 69]). *Suppose that $V(\mathbf{x})$ is taken as the harmonic potential in (2.26), then we have*

- i) *There exists a ground state of the rotating BEC (5.2) when $|\Omega| < 1$ and $\beta \geq 0$ in 3D or $\beta > -C_b$ in 2D.*
- ii) *For any $\beta \geq 0$, there exists a critical rotation velocity $0 < \Omega_c^\beta \leq 1$ – first critical rotation speed – depending on β such that: when $\Omega_c^\beta < |\Omega| < 1$, quantized vortices will appear in the ground state ϕ_g .*
- iii) *In 2D with $\gamma_y = 1$ (radially symmetric $V(\mathbf{x})$), there exists $\beta_0 > 0$ such that when $\beta \geq \beta_0$, for $|\Omega| < \Omega_{c_1}^\beta$ ($\Omega_{c_1}^\beta$ depends on β), the ground state can be chosen as positive $|\phi_g|$, and $\phi_g(\mathbf{x}) = e^{i\theta_0}|\phi_g(\mathbf{x})|$ for some constant $\theta_0 \in \mathbb{R}$, and the positive ground state ϕ_g is unique.*

- iv) *There exists no ground state of the rotating BEC (5.2) if one of the following holds:*
 (a) $\beta < 0$ in 3D or $\beta < -C_b$ in 2D; (b) $|\Omega| > 1$.

Remark 5.2. From the various numerical results, for radially symmetric $V(\mathbf{x})$ in 2D (or cylindrically symmetric in 3D) and any fixed $\beta \geq 0$, the *first critical rotation speed* $0 < \Omega_c^\beta \leq 1$ depends on β and: when $|\Omega| < \Omega_c^\beta$, the ground state can be chosen as nonnegative $|\phi_g|$, and $\phi_g(\mathbf{x}) = e^{i\theta_0} |\phi_g(\mathbf{x})|$ for some constant $\theta_0 \in \mathbb{R}$, and the nonnegative ground state ϕ_g is unique; when $\Omega_c^\beta < |\Omega| < 1$, quantized vortices will appear in the ground state ϕ_g ; and when $\Omega_c^\beta = |\Omega|$, there exist at least two different ground states – one without quantized vortices and one with quantized vortices. We remark here that a rigorous mathematical justification is still missing.

For more results on the ground state of the rotating BEC (5.2) and efficient and accurate numerical methods for simulation, such as BEFD [7, 23] or BEFP [11], we refer to [2, 7, 9, 23, 43, 69] and references therein. Similarly, for the well-posedness of the Cauchy problem of (5.2) with the initial data (4.1) and its dynamical properties as well as efficient and accurate numerical methods, such as TSADI [21] or TSGLFHP [17], we refer to [4, 7, 43, 69] and references therein. Here we present a different formulation of the GPE (5.2) under the *rotating Lagrangian coordinates* so that the angular momentum rotation term will be removed [19].

For any time $t \geq 0$, let $A(t)$ be an orthogonal rotational matrix defined as

$$A(t) = \begin{pmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad d = 2, \quad A(t) = \begin{pmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad d = 3.$$

It is easy to verify that $A^{-1}(t) = A^T(t)$ for any $t \geq 0$ and $A(0) = I$ with I the identity matrix. For any $t \geq 0$, we introduce the *rotating Lagrangian coordinates* $\tilde{\mathbf{x}}$ as [19]

$$\tilde{\mathbf{x}} = A^{-1}(t)\mathbf{x} = A^T(t)\mathbf{x} \quad \Leftrightarrow \quad \mathbf{x} = A(t)\tilde{\mathbf{x}}, \quad \mathbf{x} \in \mathbb{R}^d, \quad (5.3)$$

and denote the wave function in the new coordinates as $\varphi := \varphi(\tilde{\mathbf{x}}, t)$

$$\varphi(\tilde{\mathbf{x}}, t) := \psi(\mathbf{x}, t) = \psi(A(t)\tilde{\mathbf{x}}, t), \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0. \quad (5.4)$$

Here, we refer the Cartesian coordinates \mathbf{x} as the *Eulerian coordinates*. Plugging (5.3) and (5.4) into (5.2), we obtain the GPE

$$i\partial_t \varphi(\tilde{\mathbf{x}}, t) = \left[-\frac{1}{2} \nabla^2 + W(\tilde{\mathbf{x}}, t) + \beta |\varphi(\tilde{\mathbf{x}}, t)|^2 \right] \varphi(\tilde{\mathbf{x}}, t), \quad \tilde{\mathbf{x}} \in \mathbb{R}^d, \quad t > 0, \quad (5.5)$$

where $W(\tilde{\mathbf{x}}, t) = V(A(t)\tilde{\mathbf{x}})$ for $\tilde{\mathbf{x}} \in \mathbb{R}^d$ and $t > 0$, which is time-independent, i.e. $W(\tilde{\mathbf{x}}, t) = V(\tilde{\mathbf{x}})$ if the harmonic potential (2.26) is radially/cylindrically symmetric in 2D/3D, i.e. $\gamma_y = 1$. In addition, the initial data for the GPE (5.5) from (4.1) is

$$\varphi(\tilde{\mathbf{x}}, 0) = \psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}) := \varphi_0(\mathbf{x}) = \varphi_0(\tilde{\mathbf{x}}), \quad \tilde{\mathbf{x}} = \mathbf{x} \in \mathbb{R}^d. \quad (5.6)$$

Based on the above new formulation, the results and numerical methods developed for non-rotating BEC, such as TSSP [4, 7, 14, 17, 20], can be directly applied for analyzing and simulating the dynamics of rotating BEC.

5.2. For dipolar BEC. 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 following 3D GPE [6, 7, 10, 24, 55, 71]

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

where $C_{dd} = \mu_0\mu_{\text{dip}}^2/3$ with μ_0 the vacuum magnetic permeability and μ_{dip} the permanent magnetic dipole moment, ψ satisfies the normalization condition (2.5), and the long-range and anisotropic DDI between two dipoles with the same dipole moment or orientation $\mathbf{n} = (n_1, n_2, n_3)^T \in \mathbb{R}^3$ (which is a given unit vector satisfying $|\mathbf{n}| = \sqrt{n_1^2 + n_2^2 + n_3^2} = 1$) is given by

$$V_{\text{dip}}(\mathbf{x}) = \frac{3}{4\pi} \frac{1 - 3(\mathbf{x} \cdot \mathbf{n})^2/|\mathbf{x}|^2}{|\mathbf{x}|^3} = \frac{3}{4\pi} \frac{1 - 3\cos^2(\theta)}{|\mathbf{x}|^3}, \quad \mathbf{x} \in \mathbb{R}^3, \quad (5.7)$$

where θ is the angle between the dipole axis \mathbf{n} and the vector \mathbf{x} . We remark here that it is still an open problem to derive the above GPE from the N -body linear Schrödinger equation (2.3) with V_{int} in (2.2) is taken as V_{dip} .

Again, under the harmonic potential (2.9), similarly to the nondimensionalization in section 2.2 and dimension reduction in 2.3 from 3D to 2D when $\omega_z \gg \max\{\omega_x, \omega_y\}$ for a disk-shaped condensate and to 1D when $\omega_z = \omega_y \gg \omega_x$ for a cigar-shaped condensate [6, 7, 30], by using the decomposition of contact and long-range (or repulsive and attractive) parts of the DDI (5.7) [10, 30]

$$U_{\text{dip}}(\mathbf{x}) = \frac{3}{4\pi|\mathbf{x}|^3} \left(1 - \frac{3(\mathbf{x} \cdot \mathbf{n})^2}{|\mathbf{x}|^2} \right) = -\delta(\mathbf{x}) - 3\partial_{\mathbf{nn}} \left(\frac{1}{4\pi|\mathbf{x}|} \right), \quad \mathbf{x} \in \mathbb{R}^3, \quad (5.8)$$

where the differential operators $\partial_{\mathbf{n}} = \mathbf{n} \cdot \nabla$ and $\partial_{\mathbf{nn}} = \partial_{\mathbf{n}}\partial_{\mathbf{n}}$, we can obtain the following dimensionless GPE with a DDI in d -dimensions ($d = 1, 2, 3$):

$$i\partial_t\psi(\mathbf{x}, t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\psi(\mathbf{x}, t)|^2 + \eta\varphi(\mathbf{x}, t) \right] \psi(\mathbf{x}, t), \quad (5.9)$$

$$\varphi(\mathbf{x}, t) = L_{\mathbf{n}}u(\mathbf{x}, t), \quad u(\mathbf{x}, t) = G * |\psi|^2, \quad \mathbf{x} \in \mathbb{R}^d, \quad t \geq 0,$$

where

$$\beta = \begin{cases} \frac{2\kappa + \lambda(1 - 3n_1^2)}{4\pi\varepsilon^2}, \\ \frac{\kappa + \lambda(3n_3^2 - 1)}{\varepsilon\sqrt{2\pi}}, \\ \kappa - \lambda, \end{cases} \quad \eta = -3\lambda \begin{cases} \frac{3n_1^2 - 1}{8\varepsilon\sqrt{2\pi}}, \\ 1/2, \\ 1, \end{cases} \quad L_{\mathbf{n}} = \begin{cases} \partial_{xx}, & d = 1, \\ \partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_3^2\nabla^2, & d = 2, \\ \partial_{\mathbf{nn}}, & d = 3, \end{cases}$$

with $\kappa = \frac{4\pi Na_s}{x_s}$, $\lambda = \frac{mN\mu_0\mu_{\text{dip}}^2}{3\hbar^2 x_s}$, $\varepsilon = \frac{1}{\sqrt{\gamma_z}}$, $\mathbf{n}_\perp = (n_1, n_2)^T$, and

$$G(\mathbf{x}) = \begin{cases} \frac{1}{\varepsilon\sqrt{2\pi}} \int_0^\infty \frac{e^{-s/2\varepsilon^2}}{\sqrt{s^2 + |\mathbf{x}|^2}} ds \\ 1/(2\pi|\mathbf{x}|), \\ \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}} \frac{e^{-s^2/2}}{\sqrt{|\mathbf{x}|^2 + \varepsilon^2 s^2}} ds, \\ 1/(4\pi|\mathbf{x}|), \end{cases} \quad \Leftrightarrow \widehat{G}(\xi) = \begin{cases} \frac{\varepsilon\sqrt{2}}{\sqrt{\pi}} \int_0^\infty \frac{e^{-\varepsilon^2 s^2/2}}{s + |\xi|^2} ds, & d = 1\&S\text{AM}, \\ 1/|\xi|, & d = 2\&S\text{DM}, \\ \frac{1}{2\pi^2} \int_{\mathbb{R}} \frac{e^{-\varepsilon^2 s^2/2}}{|\xi|^2 + s^2} ds, & d = 2\&S\text{AM}, \\ 1/|\xi|^2, & d = 3, \end{cases}$$

where $\widehat{f}(\xi)$ denotes the Fourier transform of a function $f(\mathbf{x})$ for $\mathbf{x}, \xi \in \mathbb{R}^d$. In addition, in 3D, u in (5.9) satisfies the Poisson equation [6, 7, 30]

$$-\nabla^2 u(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2, \quad \mathbf{x} \in \mathbb{R}^3, \quad \text{satisfying} \quad \lim_{|\mathbf{x}| \rightarrow \infty} u(\mathbf{x}, t) = 0, \quad t \geq 0; \quad (5.10)$$

and in 2D with SDM approximation, u in (5.9) satisfies the fractional Poisson equation [6, 7, 30]

$$(-\nabla^2)^{1/2} u(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2, \quad \mathbf{x} \in \mathbb{R}^2, \quad \text{satisfying} \quad \lim_{|\mathbf{x}| \rightarrow \infty} u(\mathbf{x}, t) = 0, \quad t \geq 0. \quad (5.11)$$

The GPE (5.9) conserves the normalization (2.5) and energy per particle

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

The ground state can be defined the same as (3.5) with the above energy functional. For the existence and uniqueness as well as nonexistence of the ground state of the dipolar BEC (5.9) and efficient and accurate numerical methods for simulation, such as BESP [10] or BEFP with nonuniform FFT [49], we refer to [6, 7, 10] and references therein. Similarly, for the well-posedness of the Cauchy problem of (5.9) with the initial data (4.1) and its dynamical properties as well as efficient and accurate numerical methods, such as TSSP [10] or TSFP with nonuniform FFT [49], we refer to [6, 7, 10] and references therein.

5.3. For spin-orbit-coupled BEC. At temperatures T much smaller than the critical temperature T_c , a spin-orbit-coupled BEC with two components can be well described by the macroscopic wave function $\Psi := \Psi(\mathbf{x}, t) = (\psi_1(\mathbf{x}, t), \psi_2(\mathbf{x}, t))^T$ whose evolution is governed by the following 3D coupled Gross-Pitaevskii equations (CGPEs) [5, 7, 8, 48, 60, 65, 67, 73] for $\mathbf{x} \in \mathbb{R}^3$ and $t > 0$ as

$$\begin{aligned} i\hbar \partial_t \psi_1 &= \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) + \frac{i\hbar \tilde{k}_0}{2m} \partial_x + \frac{\hbar \tilde{\delta}}{2} + N g_{11} |\psi_1|^2 + N g_{12} |\psi_2|^2 \right] \psi_1 + \frac{\hbar \tilde{\Omega}}{2} \psi_2, \\ i\hbar \partial_t \psi_2 &= \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) - \frac{i\hbar \tilde{k}_0}{2m} \partial_x - \frac{\hbar \tilde{\delta}}{2} + N g_{21} |\psi_1|^2 + N g_{22} |\psi_2|^2 \right] \psi_2 + \frac{\hbar \tilde{\Omega}}{2} \psi_1, \end{aligned}$$

where N is the total number of particles, \tilde{k}_0 describes the spin-orbit-coupling strength, $\tilde{\delta}$ is the detuning constant for Raman transition, $\tilde{\Omega}$ is the effective Rabi frequency describing the strength to realize the internal atomic Josephson junction (JJ) by a Raman transition, and the interactions of particles are described by $g_{jl} = \frac{4\pi \hbar^2 a_{jl}}{m}$ with $a_{jl} = a_{lj}$ ($j, l = 1, 2$) being the s -wave scattering lengths between the j th and l th components. The above CGPEs is normalized as

$$\|\Psi\|^2 := \int_{\mathbb{R}^3} [|\psi_1(\mathbf{x}, t)|^2 + |\psi_2(\mathbf{x}, t)|^2] d\mathbf{x} = 1. \quad (5.12)$$

Again, under the harmonic potential (2.9), similarly to the nondimensionalization in section 2.2 and dimension reduction in 2.3 from 3D to 2D and 1D, we can obtain the following dimensionless CGPEs under the normalization condition (5.12) for spin-orbit-coupled BEC

in d -dimensions ($d = 1, 2, 3$) for $\mathbf{x} \in \mathbb{R}^d$ and $t > 0$ as

$$\begin{aligned} i\partial_t\psi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + ik_0\partial_x + \frac{\delta}{2} + \beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2 \right] \psi_1 + \frac{\Omega}{2}\psi_2, \\ i\partial_t\psi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) - ik_0\partial_x - \frac{\delta}{2} + \beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2 \right] \psi_2 + \frac{\Omega}{2}\psi_1, \end{aligned} \quad (5.13)$$

where $k_0 = \frac{\bar{k}_0}{\omega_x}$, $\delta = \frac{\bar{\delta}}{\omega_x}$, $\Omega = \frac{\bar{\Omega}}{\omega_x}$, and $\beta_{11}, \beta_{12} = \beta_{21}, \beta_{22}$ are dimensionless interaction constants. This CGPEs conserves the normalization (or total mass)

$$N(\Psi(\cdot, t)) := \|\Psi(\cdot, t)\|^2 = \int_{\mathbb{R}^d} \sum_{j=1}^2 |\psi_j(\mathbf{x}, t)|^2 d\mathbf{x} \equiv N(\Psi(\cdot, 0)) = 1, \quad t \geq 0, \quad (5.14)$$

and the energy per particle

$$\begin{aligned} E(\Psi(\cdot, t)) &= \int_{\mathbb{R}^d} \left\{ \sum_{j=1}^2 \left[\frac{1}{2} |\nabla\psi_j|^2 + |\psi_j|^2 \left(V(\mathbf{x}) + \frac{1}{2} \sum_{l=1}^2 \beta_{jl} |\psi_l|^2 \right) \right] + \frac{\delta}{2} (|\psi_1|^2 - |\psi_2|^2) \right. \\ &\quad \left. + ik_0 (\bar{\psi}_1 \partial_x \psi_1 - \bar{\psi}_2 \partial_x \psi_2) + \Omega \operatorname{Re}(\psi_1 \bar{\psi}_2) \right\} d\mathbf{x} \equiv E(\Psi(\cdot, 0)), \quad t \geq 0. \end{aligned} \quad (5.15)$$

In addition, when $\Omega = 0$, then it also conserves the mass of each component

$$N(\psi_j(\cdot, t)) := \int_{\mathbb{R}^d} |\psi_j(\mathbf{x}, t)|^2 d\mathbf{x} \equiv N(\psi_j(\cdot, 0)), \quad t \geq 0, \quad j = 1, 2. \quad (5.16)$$

The ground state can be defined as: Find $\Phi_g \in S$ such that

$$E_g := E(\Phi_g) = \min_{\Phi \in S} E(\Phi), \quad (5.17)$$

where $S = \{\Phi = (\phi_1, \phi_2)^T \mid \|\Phi\| = 1, E(\Phi) < \infty\}$. Of course, when $\Omega = 0$, for any fixed $0 \leq \alpha \leq 1$, an α -dependent ground state can be defined as: Find $\Phi_g^\alpha \in S_\alpha$ such that

$$E_g^\alpha := E(\Phi_g^\alpha) = \min_{\Phi \in S_\alpha} E(\Phi), \quad (5.18)$$

where $S_\alpha = \{\Phi = (\phi_1, \phi_2)^T \mid \|\phi_1\|^2 = \alpha, \|\phi_2\|^2 = 1 - \alpha, E(\Phi) < \infty\}$. It is easy to see that

$$E_g = E(\Phi_g) = \min_{0 \leq \alpha \leq 1} E_g^\alpha = \min_{0 \leq \alpha \leq 1} \min_{\Phi \in S_\alpha} E(\Phi) = \min_{0 \leq \alpha \leq 1} \min_{\Phi \in S_\alpha} E(\Phi). \quad (5.19)$$

For the existence and uniqueness as well as nonexistence of the ground states of the spin-orbit-coupled BEC (5.3) based on the definition (5.17) for any $\Omega \in \mathbb{R}$ and the definition (5.18) for $\Omega = 0$, and efficient and accurate numerical methods for simulation, such as BEFD or BESP [5, 7, 8], we refer to [5, 7, 8, 65, 67, 73] and references therein. Similarly, for the well-posedness of the Cauchy problem of (5.3) with the initial data $\Psi(\mathbf{x}, 0) = \Psi_0(\mathbf{x})$ and its dynamical properties as well as efficient and accurate numerical methods, such as TSSP [5, 7], we refer to [5, 7, 8, 65, 67, 73] and references therein. Finally, by setting

$\psi_1(\mathbf{x}, t) = \varphi_1(\mathbf{x}, t)e^{i(\omega t + k_0 x)}$ and $\psi_2(\mathbf{x}, t) = \varphi_2(\mathbf{x}, t)e^{i(\omega t - k_0 x)}$ with $\omega = \frac{\delta - k_0^2}{2}$ in the CGPEs (5.13), we obtain for $\mathbf{x} \in \mathbb{R}^d$ and $t > 0$

$$\begin{aligned} i\partial_t \varphi_1 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \delta + \beta_{11}|\varphi_1|^2 + \beta_{12}|\varphi_2|^2 \right] \varphi_1 + \frac{\Omega}{2} e^{-i2k_0 x} \varphi_2, \\ i\partial_t \varphi_2 &= \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta_{21}|\varphi_1|^2 + \beta_{22}|\varphi_2|^2 \right] \varphi_2 + \frac{\Omega}{2} e^{i2k_0 x} \varphi_1. \end{aligned} \quad (5.20)$$

This CGPEs conserves the normalization (5.14) for any $\Omega \in \mathbb{R}$ and (5.16) when $\Omega = 0$ with ψ_j replaced by φ_j for $j = 1, 2$. It is very useful in designing the most efficient and accurate numerical methods for computing ground states and dynamics, such as BESP and TSSP [5, 7, 8]), especially for the box potential, comparing to the system (5.13).

6. Conclusions and future perspectives

Due to its massive relations and applications in many different areas, such as atomic, molecular and optical physics, quantum optics, condensed matter physics and low temperature physics, the research on theoretical, experimental and computational studies of BEC has been started almost century ago and has grown explosively (or exponentially) since 1995. Up to now, rich and extensive research results have been obtained in experimental and theoretical understanding of ground states and dynamics of BEC. The research in this area is still very active and highly demanded due to the latest experimental and/or technological advances in BEC, such as spinor BEC [18, 22, 47, 51], BEC with damping terms [15] or impurities [50] or random potentials [63], degenerate Fermi gas [45], Rydberg gas [53], spin-orbit-coupled BEC [60], BEC at finite temperature [72], etc. These achievements have brought great challenges to AMO community, condensed matter community, and computational and applied mathematics community for modeling, simulating and understanding various interesting phenomenons related to BEC. It becomes more and more interdisciplinary involving theoretical, computational and experimental physicists and computational and applied mathematicians as well as pure mathematicians.

Acknowledgements. The author is grateful to Beijing Computational Science Research Center for its hospitality during the writing of this paper.

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Department of Mathematics, National University of Singapore, Singapore, 119076, Singapore

E-mail: matbaowz@nus.edu.sg; URL: <http://www.math.nus.edu.sg/~bao/>