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Analysis and computation for the semiclassical limits of the ground and excited states of the Gross-Pitaevskii equation

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Abstract. In this paper we review our recent work on mathematical analysis and efficient numerical computation for the semiclassical limits of the ground and excited states of the Gross-Pitaevskii equation (GPE) with applications in Bose-Einstein condensation and nonlinear optics. We begin with the time-independent GPE and show how to reformulate it into a singularly perturbed nonlinear eigenvalue problem under a constraint. Matched asymptotic approximations for the ground and excited states are presented to locate the positions and characterize the widths of boundary layers and/or interior layers in the solution. Semiclassical limits of the ground and excited states of the GPE are obtained analytically based on the matched asymptotic approximations. We also review different efficient numerical methods for computing the ground and excited states of the GPE. Finally, numerical results are reported to confirm the semiclassical limits and to provide the convergence rates of the solutions to the semiclassical limits.

1. Introduction

In this paper, we consider the following time-independent Gross-Pitaevskii equation (GPE) [**PS, BT, BC, BJP, AD**]

$$\mu\,\phi(\mathbf{x}) = -\frac{1}{2}\nabla^2\phi(\mathbf{x}) + V(\mathbf{x})\phi(\mathbf{x}) + \beta|\phi(\mathbf{x})|^2\phi(\mathbf{x}), \qquad \mathbf{x}\in\Omega\subset\mathbb{R}^d, \tag{1.1}$$

where $\mathbf{x} = (x_1,\ldots,x_d)^T$ is the spatial coordinate, Ω is a subdomain of $\mathbb{R}^d$ ($d = 1,2,3$), $V(\mathbf{x})$ is a real-valued potential whose shape is determined by the type of system under investigation, and β is a constant. Equation (1.1) is also known as a nonlinear eigenvalue problem with applications in Bose-Einstein condensation (BEC) [**PS, AEMWC, BJP**], quantum physics and chemistry, nonlinear optics, etc., where ϕ is the macroscopic wave function of the condensate and positive/negative β corresponds to repulsive/attractive interaction between atoms. The

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wave function ϕ is required to satisfy the normalization condition

$$\|\phi\|^2 := \int_\Omega |\phi(\mathbf{x})|^2 \, d\mathbf{x} = 1. \tag{1.2}$$

For the nonlinear eigenvalue problem (1.1) under the constraint (1.2), any eigenvalue μ, which is also called as chemical potential in quantum physics, can be computed from its corresponding eigenfunction ϕ by

$$\begin{aligned} \mu &:= \mu_\beta(\phi) = \int_\Omega \left[\frac{1}{2}|\nabla\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + \beta|\phi(\mathbf{x})|^4\right] d\mathbf{x} \\ &= E_\beta(\phi) + \frac{\beta}{2}\int_\Omega |\phi(\mathbf{x})|^4 \, d\mathbf{x}, \end{aligned} \tag{1.3}$$

where $E_\beta(\phi)$ is the energy defined as

$$E_\beta(\phi) = \int_\Omega \left[\frac{1}{2}|\nabla\phi(\mathbf{x})|^2 + V(\mathbf{x})|\phi(\mathbf{x})|^2 + \frac{\beta}{2}|\phi(\mathbf{x})|^4\right] d\mathbf{x}. \tag{1.4}$$

In fact, the nonlinear eigenvalue problem (1.1) can be viewed as the Euler-Lagrange equation of the energy functional $E_\beta(\phi)$ in (1.4) under the constraint (1.2). In physics literature [**PS, AEMWC, BJP**], the ground state is defined as the minimizer of the energy functional in (1.4) over the unit sphere $S = \{\phi \mid \|\phi\| = 1, \ E_\beta(\phi) < \infty\}$. Any other eigenfunctions of the nonlinear eigenvalue problem (1.1) under the constraint (1.2), whose energy is greater than that of the ground state, are usually known as excited states.

The aim of this paper is to review and present recent works on asymptotic and numerical results for the ground and excited states of the time-independent GPE (1.1) under the constraint (1.2) in different limiting interaction regimes and then explicitly find the semiclassical limits of the ground and excited states. For analysis and efficient computation of the semiclassical limits of the time-dependent GPE, we refer to [**GMMP, GM, G, C, BJP1, BJP2**] and references therein.

The paper is organized as follows. In section 2, we reformulate the time-independent GPE (1.1) into a singularly perturbed nonlinear eigenvalue problem when $|\beta| \gg 1$. In section 3, we review numerical methods for computing the ground and excited states. In section 4, we present asymptotic approximations of the ground and excited states in different limiting interaction regime for the GPE with a box potential. Similar results are presented in sections 5 and 6 for the GPE with a harmonic potential and the GPE on a ring, respectively. Finally, some concluding remarks are drawn in section 7.

2. Time-independent Gross-Pitaevskii equation

In this section, we reformulate the time-independent GPE (1.1) with different potentials into a singularly perturbed nonlinear eigenvalue problem under a constraint when $|\beta| \gg 1$, i.e. in the strong interaction regime.

2.1. For the box potential with strongly repulsive interaction. When $\beta \gg 1$, i.e. with strongly repulsive interaction, Ω is bounded and $V(\mathbf{x})$ is chosen as a box potential, i.e. $V(\mathbf{x}) \equiv 0$ when $\mathbf{x} \in \Omega$ and $V(\mathbf{x}) = \infty$ otherwise, we choose the semiclassical re-scaling as

$$\varepsilon := \frac{1}{\sqrt{\beta}}, \qquad \mu^\varepsilon := \varepsilon^2\mu = \frac{\mu}{\beta}, \qquad \phi^\varepsilon(\mathbf{x}) = \phi(\mathbf{x}). \tag{2.1}$$

By dividing both sides of (1.1) by β, the time-independent GPE (1.1) under the constraint (1.2) is reformulated into the following singularly perturbed nonlinear eigenvalue problem

$$\mu^\varepsilon\ \phi^\varepsilon(\mathbf{x}) = -\frac{\varepsilon^2}{2}\nabla^2\phi^\varepsilon(\mathbf{x}) + |\phi^\varepsilon(\mathbf{x})|^2\phi^\varepsilon(\mathbf{x}), \qquad \mathbf{x}\in\Omega, \tag{2.2}$$

under the constraint (1.2) with $\phi = \phi^\varepsilon$.

The eigenvalue (or chemical potential) μ^ε can be computed from its corresponding eigenfunction ϕ^ε by

$$\mu^\varepsilon := \mu_\varepsilon(\phi^\varepsilon) = \int_\Omega \left[\frac{\varepsilon^2}{2}|\nabla\phi^\varepsilon(\mathbf{x})|^2 + |\phi^\varepsilon(\mathbf{x})|^4\right]\, d\mathbf{x} = E_\varepsilon(\phi^\varepsilon) + \frac{1}{2}\int_\Omega |\phi^\varepsilon(\mathbf{x})|^4\, d\mathbf{x}, \tag{2.3}$$

where the re-scaled energy $E_\varepsilon(\phi^\varepsilon)$ is defined as

$$E_\varepsilon(\phi^\varepsilon) = \int_\Omega \left[\frac{\varepsilon^2}{2}|\nabla\phi^\varepsilon(\mathbf{x})|^2 + \frac{1}{2}|\phi^\varepsilon(\mathbf{x})|^4\right]\, d\mathbf{x}. \tag{2.4}$$

By assuming that ϕ^ε is ε-oscillatory (i.e., $\phi^\varepsilon(\mathbf{x}) = \sqrt{\rho^\varepsilon(\mathbf{x})}\ e^{iS^\varepsilon(\mathbf{x})/\varepsilon}$ with $\rho^\varepsilon(\mathbf{x}) = |\phi^\varepsilon(\mathbf{x})|^2$ and $S^\varepsilon(\mathbf{x}) = \varepsilon\arg(\phi^\varepsilon(\mathbf{x}))$, the position density and phase of the wave function ϕ^ε, respectively) and sufficiently 'integrable' such that all terms have $O(1)$-integral in (2.3) and (2.4), and noting (1.2) with $\phi = \phi^\varepsilon$, we have [**BLZ, BC, BWM**]

$$\mu^\varepsilon = \mu_\varepsilon(\phi^\varepsilon) = O(1), \qquad E_\varepsilon(\phi^\varepsilon) = O(1), \qquad 0<\varepsilon\ll 1. \tag{2.5}$$

Then the leading asymptotic approximations of the eigenvalue in (1.3) and energy in (1.4) in this case can be given by

$$\mu = \mu_\beta(\phi) = \beta\ \mu_\varepsilon(\phi^\varepsilon) = O(\beta), \qquad E_\beta(\phi) = \beta\ E_\varepsilon(\phi^\varepsilon) = O(\beta), \quad \beta\gg 1. \tag{2.6}$$

2.2. For the harmonic potential with strongly repulsive interaction. When $\beta\gg 1$, i.e. with strongly repulsive interaction, $\Omega = \mathbb{R}^d$ is the whole space and $V(\mathbf{x})$ is chosen as a harmonic potential, i.e. $V(\mathbf{x}) = \frac{1}{2}\left(\gamma_1^2x_1^2 + \cdots + \gamma_d^2x_d^2\right)$ with γ_1, ..., γ_d being positive constants, under the normalization (1.2), we choose the semiclassical re-scaling as

$$\mathbf{x} = \varepsilon^{1/2}\,\tilde{\mathbf{x}}, \quad \phi^\varepsilon(\tilde{\mathbf{x}}) = \varepsilon^{-d/4}\,\phi(\mathbf{x}), \quad \mu^\varepsilon = \varepsilon^{-1}\,\mu, \quad \text{with} \quad \varepsilon = \beta^{-d/(d+2)}. \tag{2.7}$$

Substituting the above re-scaling parameters into (1.1), rearranging the parameters and dropping the $\tilde{}$, we again obtain a singularly perturbed nonlinear eigenvalue problem

$$\mu^\varepsilon\ \phi^\varepsilon(\mathbf{x}) = -\frac{\varepsilon^2}{2}\nabla^2\phi^\varepsilon(\mathbf{x}) + V(\mathbf{x})\phi^\varepsilon(\mathbf{x}) + |\phi^\varepsilon(\mathbf{x})|^2\phi^\varepsilon(\mathbf{x}), \qquad \mathbf{x}\in\mathbb{R}^d, \tag{2.8}$$

under the constraint (1.2) with $\phi = \phi^\varepsilon$.

Again, the eigenvalue (or chemical potential) μ^ε can be computed from its corresponding eigenfunction ϕ^ε by

$$\begin{aligned}\mu^\varepsilon &:= \mu_\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d}\left[\frac{\varepsilon^2}{2}|\nabla\phi^\varepsilon(\mathbf{x})|^2 + V(\mathbf{x})|\phi^\varepsilon(\mathbf{x})|^2 + |\phi^\varepsilon(\mathbf{x})|^4\right]\, d\mathbf{x}\\ &= E_\varepsilon(\phi^\varepsilon) + \frac{1}{2}\int_{\mathbb{R}^d}|\phi^\varepsilon(\mathbf{x})|^4\, d\mathbf{x},\end{aligned} \tag{2.9}$$

where the re-scaled energy $E_\varepsilon(\phi^\varepsilon)$ is defined as

$$E_\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d} \left[\frac{\varepsilon^2}{2} |\nabla \phi^\varepsilon(\mathbf{x})|^2 + V(\mathbf{x}) |\phi^\varepsilon(\mathbf{x})|^2 + \frac{1}{2} |\phi^\varepsilon(\mathbf{x})|^4 \right] d\mathbf{x}. \tag{2.10}$$

Again, by assuming that ϕ^ε is ε-oscillatory and sufficiently 'integrable' such that all terms have $O(1)$-integral in (2.9) and (2.10), and noting (1.2) with $\phi = \phi^\varepsilon$, we have

$$\mu^\varepsilon = \mu_\varepsilon(\phi^\varepsilon) = O(1), \qquad E_\varepsilon(\phi^\varepsilon) = O(1), \qquad 0 < \varepsilon \ll 1. \tag{2.11}$$

Then the leading asymptotic approximations of the eigenvalue in (1.3) and energy in (1.4) in this case can be given by

$$\mu_\beta(\phi) = \varepsilon^{-1}\, \mu_\varepsilon(\phi^\varepsilon) = O(\beta^{d/(d+2)}),\ E_\beta(\phi) = \varepsilon^{-1}\, E_\varepsilon(\phi^\varepsilon) = O(\beta^{d/(d+2)}), \quad \beta \gg 1. \tag{2.12}$$

2.3. With strongly attractive interaction. When $-\beta \gg 1$, i.e. with strongly attractive interaction, we choose the semiclassical re-scaling as

$$\varepsilon := \frac{1}{\sqrt{-\beta}}, \quad \mu^\varepsilon := \varepsilon^2 \mu = \frac{\mu}{-\beta}, \quad V_\varepsilon(\mathbf{x}) = \frac{V(\mathbf{x})}{-\beta}, \quad \phi^\varepsilon(\mathbf{x}) = \phi(\mathbf{x}). \tag{2.13}$$

By dividing both sides of (1.1) by $-\beta$, the time-independent GPE (1.1) under the constraint (1.2) is reformulated into the following singularly perturbed nonlinear eigenvalue problem

$$\mu^\varepsilon\ \phi^\varepsilon(\mathbf{x}) = -\frac{\varepsilon^2}{2} \nabla^2 \phi^\varepsilon(\mathbf{x}) + V_\varepsilon(\mathbf{x}) \phi^\varepsilon(\mathbf{x}) - |\phi^\varepsilon(\mathbf{x})|^2 \phi^\varepsilon(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \tag{2.14}$$

under the constraint (1.2) with $\phi = \phi^\varepsilon$.

Again, the eigenvalue (or chemical potential) μ^ε can be computed from its corresponding eigenfunction ϕ^ε by

$$\begin{aligned} \mu^\varepsilon &:= \mu_\varepsilon(\phi^\varepsilon) = \int_\Omega \left[\frac{\varepsilon^2}{2} |\nabla \phi^\varepsilon(\mathbf{x})|^2 + V_\varepsilon(\mathbf{x}) |\phi^\varepsilon(\mathbf{x})|^2 - |\phi^\varepsilon(\mathbf{x})|^4 \right] d\mathbf{x} \\ &= E_\varepsilon(\phi^\varepsilon) - \frac{1}{2} \int_{\mathbb{R}^d} |\phi^\varepsilon(\mathbf{x})|^4\, d\mathbf{x}, \end{aligned} \tag{2.15}$$

where the re-scaled energy $E_\varepsilon(\phi^\varepsilon)$ is defined as

$$E_\varepsilon(\phi^\varepsilon) = \int_\Omega \left[\frac{\varepsilon^2}{2} |\nabla \phi^\varepsilon(\mathbf{x})|^2 + V_\varepsilon(\mathbf{x}) |\phi^\varepsilon(\mathbf{x})|^2 - \frac{1}{2} |\phi^\varepsilon(\mathbf{x})|^4 \right] d\mathbf{x}. \tag{2.16}$$

Again, by assuming that ϕ^ε is ε-oscillatory and sufficiently 'integrable' such that all terms have $O(1)$-integral in (2.15) and (2.16) and noting (1.2) with $\phi = \phi^\varepsilon$, we have

$$\mu^\varepsilon = \mu_\varepsilon(\phi^\varepsilon) = O(1), \qquad E_\varepsilon(\phi^\varepsilon) = O(1), \qquad 0 < \varepsilon \ll 1. \tag{2.17}$$

Then the leading asymptotic approximations of the eigenvalue in (1.3) and energy in (1.4) in this case can be given by

$$\mu_\beta(\phi) = -\beta\, \mu_\varepsilon(\phi^\varepsilon) = O(-\beta),\ E_\beta(\phi) = -\beta\, E_\varepsilon(\phi^\varepsilon) = O(-\beta), \quad -\beta \gg 1. \tag{2.18}$$

2.4. General formulation. In this paper, we will consider the following time-independent GPE

$$\mu^\varepsilon\ \phi^\varepsilon(\mathbf{x}) = -\frac{\varepsilon^2}{2}\nabla^2\phi^\varepsilon(\mathbf{x}) + V_\varepsilon(\mathbf{x})\phi^\varepsilon(\mathbf{x}) + \gamma|\phi^\varepsilon(\mathbf{x})|^2\phi^\varepsilon(\mathbf{x}), \quad \mathbf{x}\in\Omega\subset\mathbb{R}^d, \tag{2.19}$$

under the normalization or constraint

$$\|\phi^\varepsilon\|^2 := \int_\Omega |\phi^\varepsilon(\mathbf{x})|^2\, d\mathbf{x} = 1; \tag{2.20}$$

where ε and γ are constants satisfying either $\varepsilon = 1$ and $|\gamma| \le 1$ or $0 < \varepsilon \le 1$ and $\gamma = \pm 1$, and $V_\varepsilon(\mathbf{x})$ is a given real-valued potential.

The eigenvalue (or chemical potential) μ^ε can be computed from its corresponding eigenfunction ϕ^ε by

$$\begin{aligned} \mu^\varepsilon &:= \mu_\varepsilon(\phi^\varepsilon) = \int_\Omega \left[\frac{\varepsilon^2}{2}|\nabla\phi^\varepsilon(\mathbf{x})|^2 + V_\varepsilon(\mathbf{x})|\phi^\varepsilon(\mathbf{x})|^2 + \gamma|\phi^\varepsilon(\mathbf{x})|^4\right] d\mathbf{x} \\ &= E_\varepsilon(\phi^\varepsilon) + \frac{\gamma}{2}\int_\Omega |\phi^\varepsilon(\mathbf{x})|^4\, d\mathbf{x}, \end{aligned} \tag{2.21}$$

and the energy functional is defined as

$$E_\varepsilon(\phi^\varepsilon) = \int_\Omega \left[\frac{\varepsilon^2}{2}|\nabla\phi^\varepsilon(\mathbf{x})|^2 + V_\varepsilon(\mathbf{x})|\phi^\varepsilon(\mathbf{x})|^2 + \frac{\gamma}{2}|\phi^\varepsilon(\mathbf{x})|^4\right] d\mathbf{x}. \tag{2.22}$$

Again, the ground state wave function $\phi_g^\varepsilon := \phi_g^\varepsilon(\mathbf{x})$ is found by minimizing the energy functional $E_\varepsilon(\phi^\varepsilon)$ over the unit sphere $S = \{\phi^\varepsilon(\mathbf{x}) \mid \|\phi^\varepsilon\| = 1,\ E_\varepsilon(\phi^\varepsilon) < \infty\}$, i.e. find $(\mu_g^\varepsilon, \phi_g^\varepsilon)$ such that

$$E_g^\varepsilon := E_\varepsilon(\phi_g^\varepsilon) = \min_{\phi^\varepsilon\in S} E_\varepsilon(\phi^\varepsilon), \qquad \mu_g^\varepsilon = \mu_\varepsilon(\phi_g^\varepsilon).$$

It can be easily shown that the ground state $\phi_g^\varepsilon(\mathbf{x})$ is an eigenfunction of the nonlinear eigenvalue problem (2.19) under the constraint (2.20). When $\gamma \ge 0$ and either Ω is bounded or $\Omega = \mathbb{R}^d$ with $V_\varepsilon(\mathbf{x})$ satisfying $\lim_{|\mathbf{x}|\to+\infty} V_\varepsilon(\mathbf{x}) = +\infty$, there exists a unique positive minimizer of the minimization problem (2.22) [**LSY, LS, LS1**].

Any other eigenfunction $\phi^\varepsilon(\mathbf{x})$ of (2.19) under the constraint (2.20) whose energy $E_\varepsilon(\phi^\varepsilon) > E_\varepsilon(\phi_g^\varepsilon)$ is usually known as an excited state in physics literature. In addition, suppose all different eigenfunctions of the nonlinear eigenvalue problem (2.19) under the constraint (2.20) are

$$\phi_g^\varepsilon(\mathbf{x}), \quad \phi_1^\varepsilon(\mathbf{x}), \quad \phi_2^\varepsilon(\mathbf{x}), \quad \ldots, \tag{2.23}$$

which are ranked according to their energies, i.e.

$$E_\varepsilon(\phi_g^\varepsilon) < E_\varepsilon(\phi_1^\varepsilon) < E_\varepsilon(\phi_2^\varepsilon) < \cdots, \tag{2.24}$$

then $\phi_l^\varepsilon(\mathbf{x})$ ($l = 1, 2, \ldots$) is usually known as the l-th excited state in quantum physics. We notice that the ground and excited states may differ up to a factor C with $|C| = 1$, i.e. if ϕ^ε is a solution, then $C\phi^\varepsilon$ is also a solution with any C satisfying $|C| = 1$.

3. Numerical methods for computing the ground and excited states

In this section, we present numerical methods for computing the ground and excited states of the time-independent GPE (2.19). For simplicity of notation, we introduce the methods for the case of one spatial dimension, i.e. $d = 1$ in (2.19) with $\Omega = (a, b)$. Generalizations to higher dimensions are straightforward for tensor product grids.

3.1. The normalized gradient flow and its discretization. Various algorithms for computing the ground and excited states, i.e. eigenfunctions of the nonlinear eigenvalue problem (2.19) under the constraint (2.20) have been studied in the literature (cf. [**CCPST, CST, D, AD, BD, A, BT, CCJ, CLS**] and references therein). Perhaps one of the more popular and efficient techniques for dealing the constraint (2.20) is through the following construction: Choose a time step $k = \Delta t > 0$ and denote a time sequence $0 = t_0 < t_1 < t_2 < \cdots < t_n < \cdots$ with $t_n = n\, k = n\, \Delta t$. To compute the ground and first excited states of the nonlinear eigenvalue problem (2.19) under the constraint (2.20), it is natural to consider the following normalized gradient flow (NGF) which was widely used in the literature for computing the ground and first excited states of the time-independent GPE [**AD, BD, BWM**]:

$$\partial_t \phi^\varepsilon(x,t) = \frac{\varepsilon^2}{2}\nabla^2\phi^\varepsilon - V_\varepsilon(x)\phi^\varepsilon - \gamma|\phi^\varepsilon|^2\phi^\varepsilon, \quad a < x < b,\ t_n \le t < t_{n+1}, \tag{3.1}$$

$$\phi^\varepsilon(x,t_{n+1}) := \phi^\varepsilon(x,t_{n+1}^+) = \frac{\phi^\varepsilon(x,t_{n+1}^-)}{\|\phi^\varepsilon(x,t_{n+1}^-)\|}, \qquad a < x < b, \quad n \ge 0, \tag{3.2}$$

$$\phi^\varepsilon(a,t) = \phi^\varepsilon(b,t) = 0, \qquad \phi^\varepsilon(x,0) = \phi_0^\varepsilon(x), \qquad a \le x \le b; \tag{3.3}$$

where $\phi^\varepsilon(x,t_n^\pm) = \lim_{t\to t_n^\pm}\phi^\varepsilon(x,t)$ and $\|\phi_0^\varepsilon\|^2 = \displaystyle\int_a^b |\phi_0^\varepsilon(x)|^2\, dx = 1$. When $\gamma = 0$ and $V_\varepsilon(x) \ge 0$, the above normalized gradient flow is energy diminishing for any time step Δt and initial data ϕ_0^ε, i.e. $E_\varepsilon(\phi^\varepsilon(\cdot,t_{n+1})) \le E_\varepsilon(\phi^\varepsilon(\cdot,t_n)) \le \cdots \le E_\varepsilon(\phi^\varepsilon(\cdot,t_0)) = E_\varepsilon(\phi_0^\varepsilon)$ [**BD, BWM**].

Various spatial/temporal discretization schemes were studied and compared in the literature for discretizing the normalized gradient flow (3.1)-(3.3) (cf. [**AD, BD, BWM, BCL, BC**] and references therein). Here we adapt the backward Euler finite difference (BEFD) discretization scheme for (3.1)-(3.3) with a uniform spatial mesh. We choose the spatial mesh size $h = \Delta x > 0$ with $h = (b-a)/M$ for M being a positive integer, and let the grid points be $x_j = a + jh$, $j = 0, 1, \ldots, M$. Let $\phi_j^{\varepsilon,n}$ be the approximation of $\phi^\varepsilon(x_j,t_n)$ and $\phi^{\varepsilon,n}$ be the solution vector with component $\phi_j^{\varepsilon,n}$. The gradient flow (3.1) is discretized in time by the backward Euler scheme and in space by the finite difference method, for $j = 1, 2, \ldots, M-1$ and $n \ge 0$, as

$$\frac{\phi_j^{\varepsilon,*} - \phi_j^{\varepsilon,n}}{\Delta t} = \frac{\varepsilon^2}{2}\frac{\phi_{j+1}^{\varepsilon,*} - 2\phi_j^{\varepsilon,*} + \phi_{j-1}^{\varepsilon,*}}{h^2} - V_\varepsilon(x_j)\phi_j^{\varepsilon,*} - \gamma|\phi_j^{\varepsilon,n}|^2\phi_j^{\varepsilon,*}\ . \tag{3.4}$$

The boundary and initial conditions (3.3) are discretized as

$$\phi_0^{\varepsilon,*} = \phi_M^{\varepsilon,*} = 0, \qquad \phi_j^{\varepsilon,0} = \phi_0^\varepsilon(x_j), \qquad j = 0, 1, 2, \ldots, N. \tag{3.5}$$

The normalized step (3.2) is discretized as

$$\phi_j^{\varepsilon,n+1} = \frac{\phi_j^{\varepsilon,*}}{\|\phi^{\varepsilon,*}\|}, \quad j = 0, 1, 2, \ldots, M, \quad \text{with } \|\phi^{\varepsilon,*}\| = \sqrt{\sum_{j=1}^{M-1} h \left|\phi_j^{\varepsilon,*}\right|^2}. \tag{3.6}$$

3.2. The continuous normalized gradient flow (CNGF) and its discretization. In fact, the normalized step (3.2) is equivalent to solving the following ODE *exactly*

$$\partial_t \phi^\varepsilon(x,t) = \mu_\phi(t,k)\phi^\varepsilon(x,t), \qquad a < x < b, \quad t_n < t < t_{n+1}, \quad n \geq 0, \tag{3.7}$$

$$\phi^\varepsilon(x,t_n^+) = \phi^\varepsilon(x,t_{n+1}^-), \qquad a \leq x \leq b; \tag{3.8}$$

where

$$\mu_\phi(t,k) \equiv \mu_\phi(t_{n+1},k) = -\frac{1}{2\,k} \ln \|\phi^\varepsilon(\cdot,t_{n+1}^-)\|^2, \qquad t_n \leq t \leq t_{n+1}. \tag{3.9}$$

Thus the NGF (3.1)-(3.3) can be viewed as a first-order splitting method for the following gradient flow with discontinuous coefficients:

$$\partial_t \phi^\varepsilon(x,t) = \frac{\varepsilon^2}{2}\Delta\phi^\varepsilon - V_\varepsilon(x)\phi^\varepsilon - \gamma\,|\phi^\varepsilon|^2\phi^\varepsilon + \mu_\phi(t,k)\phi^\varepsilon, \quad a < x < b, \tag{3.10}$$

$$\phi^\varepsilon(a,t) = \phi^\varepsilon(b,t) = 0, \qquad \phi^\varepsilon(x,0) = \phi_0^\varepsilon(x), \qquad a \leq x \leq b. \tag{3.11}$$

Letting $k \to 0$ and noticing that $\phi^\varepsilon(x,t_{n+1})$ on the right hand side of (3.8) is the solution of (3.1) at $t_{n+1} = t_n + k$, we obtain

$$\begin{aligned} \mu_\phi(t) &:= \lim_{k\to 0^+} \mu_\phi(t,k) = \lim_{k\to 0^+} \frac{\ln\|\phi^\varepsilon(\cdot,t_{n+1}^-)\|^2}{-2\,k} = \lim_{k\to 0^+} \frac{\ln\|\phi^\varepsilon(\cdot,t+k)\|^2}{-2\,k} \\ &= \lim_{k\to 0^+} \frac{\frac{d}{d\tau}\|\phi^\varepsilon(\cdot,t+\tau)\|^2\big|_{\tau=k}}{-2\|\phi^\varepsilon(\cdot,t+k)\|^2} = \lim_{k\to 0^+} \frac{\mu_\varepsilon(\phi^\varepsilon(\cdot,t+k)}{\|\phi^\varepsilon(\cdot,t+k)\|^2} = \frac{\mu_\varepsilon(\phi^\varepsilon(\cdot,t))}{\|\phi^\varepsilon(\cdot,t)\|^2}. \end{aligned} \tag{3.12}$$

This suggests us to consider the following CNGF:

$$\partial_t \phi^\varepsilon(x,t) = \frac{\varepsilon^2}{2}\Delta\phi^\varepsilon - V_\varepsilon(x)\phi - \gamma\,|\phi^\varepsilon|^2\phi^\varepsilon + \frac{\mu_\varepsilon(\phi^\varepsilon(\cdot,t))}{\|\phi^\varepsilon(\cdot,t)\|^2}\phi^\varepsilon, \quad a < x < b, \tag{3.13}$$

$$\phi^\varepsilon(a,t) = \phi^\varepsilon(b,t) = 0, \qquad \phi^\varepsilon(x,0) = \phi_0^\varepsilon(x), \qquad a \leq x \leq b. \tag{3.14}$$

In fact, the right hand side of (3.13) is the same as (2.19) if we view $\mu_\varepsilon(\phi^\varepsilon)/\|\phi^\varepsilon\|^2$ as a Lagrange multiplier for the constraint (2.20). Following the proof in [**BD, BWM**], for the above CNGF, we have the following theorem:

THEOREM 3.1. *Suppose that ϕ_0^ε satisfies $\|\phi_0^\varepsilon\| = 1$. Then the CNGF (3.13)-(3.14) is normalization conserving and energy diminishing, i.e.*

$$\|\phi^\varepsilon(\cdot,t)\|^2 = \int_a^b |\phi^\varepsilon(x,t)|^2\,dx = \|\phi_0^\varepsilon\|^2 = 1, \qquad t \geq 0, \tag{3.15}$$

$$\frac{d}{dt}E_\varepsilon(\phi^\varepsilon) = -2\,\|\partial_t\phi^\varepsilon(\cdot,t)\|^2 \leq 0\,, \qquad t \geq 0, \tag{3.16}$$

which in turn implies that

$$E_\varepsilon(\phi^\varepsilon(\cdot,t_2)) \leq E_\varepsilon(\phi^\varepsilon(\cdot,t_1)), \qquad 0 \leq t_1 \leq t_2 < \infty.$$

In addition, a second-order in space and time full discretization for the CNGF (3.13) can be given, for $j = 1, 2, \ldots, M-1$ and $n \geq 0$, as

$$\frac{\phi_j^{\varepsilon,n+1} - \phi_j^{\varepsilon,n}}{\Delta t} = \frac{\varepsilon^2}{2h^2}\left[\phi_{j+1}^{\varepsilon,n+1/2} - 2\phi_j^{\varepsilon,n+1/2} + \phi_{j-1}^{\varepsilon,n+1/2}\right] - V_\varepsilon(x_j)\phi_j^{\varepsilon,n+1/2}$$
$$-\frac{\gamma}{2}\left[|\phi_j^{\varepsilon,n+1}|^2 + |\phi_j^{\varepsilon,n}|^2\right]\phi_j^{\varepsilon,n+1/2} + \frac{\mu_\varepsilon^h(\phi^{\varepsilon,n}, \phi^{\varepsilon,n+1})}{\|\phi^{\varepsilon,n+1/2}\|^2}\phi_j^{\varepsilon,n+1/2}, \tag{3.17}$$

where

$$\phi_j^{\varepsilon,n+1/2} = \frac{1}{2}\left(\phi_j^{\varepsilon,n+1} + \phi_j^{\varepsilon,n}\right), \qquad j = 0, 1, \ldots, M,$$
$$\mu_\varepsilon^h(\phi^{\varepsilon,n}, \phi^{\varepsilon,n+1}) = h\sum_{j=0}^{M-1}\left[\frac{\varepsilon^2}{2}\left|\frac{\phi_{j+1}^{\varepsilon,n+1/2} - \phi_j^{\varepsilon,n+1/2}}{h}\right|^2 + V_\varepsilon(x_j)|\phi_j^{\varepsilon,n+1/2}|^2\right.$$
$$\left.+\frac{\gamma}{2}|\phi_j^{\varepsilon,n+1/2}|^2\left(|\phi_j^{\varepsilon,n+1}|^2 + |\phi_j^{\varepsilon,n}|^2\right)\right].$$

The initial and boundary conditions in (3.14) can be discretized as in (3.5) with $\phi^{\varepsilon,*} = \phi^{\varepsilon,n+1}$.

Following the proof in [**BW, BL**], for the full discretization of the CNGF, we have the following theorem:

THEOREM 3.2. *Under the conditions in Theorem 3.1, the above full discretization is normalization conserving and energy diminishing in the discretized level, i.e.*

$$\|\phi^{\varepsilon,n}\|^2 := h\sum_{j=1}^{M-1}|\phi_j^{\varepsilon,n}|^2 \equiv \|\phi^{\varepsilon,0}\|^2 = \|\phi_0^\varepsilon\|^2 := h\sum_{j=1}^{M-1}|\phi_0^\varepsilon(x_j)|^2, \tag{3.18}$$

$$E_\varepsilon(\phi^{\varepsilon,n}) \equiv E_\varepsilon(\phi^{\varepsilon,0}) = E_\varepsilon(\phi_0^\varepsilon), \qquad n \geq 0; \tag{3.19}$$

where

$$E_\varepsilon(\phi^{\varepsilon,n}) = h\sum_{j=0}^{M-1}\left[\frac{\varepsilon^2}{2}\left|\frac{\phi_{j+1}^{\varepsilon,n} - \phi_j^{\varepsilon,n}}{h}\right|^2 + V_\varepsilon(x_j)|\phi_j^{\varepsilon,n}|^2 + \frac{\gamma}{2}|\phi_j^{\varepsilon,n}|^4\right].$$

4. Semiclassical limits of the GPE with box potential

In this section, we will derive the approximations for the ground and excited states of the GPE with a box potential in different limiting interaction regimes and then obtain the semiclassical limits of the solutions. For simplicity, here we only present the results in 1D. Extensions to d-dimensions with $\Omega = (0,1)^d$ for linear and repulsive interaction cases are straightforward. When $d = 1$ and $\Omega = (0,1)$ with a box potential, i.e. $V_\varepsilon(x) = 0$ for $0 \leq x \leq 1$ and $V_\varepsilon(x) = \infty$ otherwise, the problem (2.19)-(2.20) collapses to

$$\mu^\varepsilon\ \phi^\varepsilon(x) = -\frac{\varepsilon^2}{2}\frac{d^2\phi^\varepsilon(x)}{dx^2} + \gamma|\phi^\varepsilon(x)|^2\phi^\varepsilon(x), \quad 0 < x < 1, \tag{4.1}$$

$$\phi^\varepsilon(0) = \phi^\varepsilon(1) = 0, \tag{4.2}$$

under the normalization or constraint (2.20) with $\Omega = (0,1)$.

4.1. In the weak interaction regime. In the case without interaction, i.e. $\varepsilon = 1$ and $\gamma = 0$, the problem (4.1) collapses into a linear eigenvalue problem and we can find a complete set of orthonormal eigenfunctions

$$\phi_l^b(x) = \sqrt{2}\sin((l+1)\pi x), \qquad l = 0, 1, 2, \dots. \tag{4.3}$$

The corresponding eigenvalues are

$$\mu_l = \frac{1}{2}(l+1)^2\pi^2, \qquad l = 0, 1, 2, \dots\ . \tag{4.4}$$

From these solutions, we can immediately get the ground and excited states as

$$\phi_g(x) = \phi_0^b(x), \qquad \phi_l(x) = \phi_l^b(x), \qquad l = 1, 2, \dots\ . \tag{4.5}$$

The corresponding energy and chemical potential of the ground and excited states are

$$E_g = \mu_g = \pi^2/2, \qquad E_l = \mu_l = (l+1)^2\pi^2/2, \qquad l = 1, 2, \dots\ . \tag{4.6}$$

In addition, based on these solutions, we can get the approximations of the ground and excited states in the weakly interaction regime, i.e. $\varepsilon = 1$ and $|\gamma| \ll 1$. In this case, the ground and excited states can be approximated as

$$\phi_g(x) \approx \phi_0^b(x), \qquad \phi_l(x) \approx \phi_l^b(x), \qquad l = 1, 2, \dots\ . \tag{4.7}$$

Furthermore, the energy and chemical potential of the ground and excited states can be approximated as

$$\begin{aligned} E_g &:= E_\varepsilon(\phi_g) \approx E_\varepsilon(\phi_0^b) = \frac{\pi^2}{2} + \frac{3\gamma}{2}, \quad E_l := E_\varepsilon(\phi_l) \approx E_\varepsilon(\phi_l^b) = \frac{(l+1)^2\pi^2}{2} + \frac{3\gamma}{2}, \\ \mu_g &:= \mu_\varepsilon(\phi_g) \approx \mu_\varepsilon(\phi_0^b) = \frac{\pi^2}{2} + 3\gamma, \quad \mu_l := \mu_\varepsilon(\phi_l) \approx \mu_\varepsilon(\phi_l^b) = \frac{(l+1)^2\pi^2}{2} + 3\gamma. \end{aligned}$$

4.2. In the strongly repulsive interaction regime. In this case, i.e. $\gamma = 1$ and $0 < \varepsilon \ll 1$, we formally drop the first term on the right hand side of (4.1) and obtain the Thomas-Fermi approximation of the ground state as

$$\mu_g^{\mathrm{TF}}\ \phi_g^{\mathrm{TF}}(x) = |\phi_g^{\mathrm{TF}}(x)|^2\phi_g^{\mathrm{TF}}(x), \qquad 0 < x < 1, \tag{4.8}$$

which implies

$$\phi_g^{\mathrm{TF}}(x) = \sqrt{\mu_g^{\mathrm{TF}}}, \qquad 0 < x < 1. \tag{4.9}$$

Plugging (4.9) into the constraint (2.20) with $\Omega = (0, 1)$, we get

$$1 = \int_0^1 |\phi_g^{\mathrm{TF}}(x)|^2\, dx = \int_0^1 \mu_g^{\mathrm{TF}}\, dx = \mu_g^{\mathrm{TF}}. \tag{4.10}$$

Here the leading order approximation for the ground state is given by

$$\phi_g^\varepsilon(x) \approx \phi_g^{\mathrm{TF}}(x) = 1, \qquad 0 < x < 1. \tag{4.11}$$

However, the approximation for the ground state (4.11) does *not* satisfy the zero boundary condition (4.2). This suggests the existence of two boundary layers in the region near $x = 0$ and $x = 1$ in the ground state of the GPE (4.1) with the box potential.

To get the matched asymptotic approximation, since the two boundary layers exist at the two boundaries $x = 0$ and $x = 1$ when $0 < \varepsilon \ll 1$, we solve (4.1) near

$x = 0$ and $x = 1$, respectively. Let us assume that the boundary layer is of width δ with $0 < \delta \ll 1$ and do a rescaling in the region near $x = 0$ with

$$x = \delta\, X, \qquad \phi^\varepsilon(x) = \phi_s\, \Phi(X), \qquad X \geq 0. \tag{4.12}$$

Substituting (4.12) into (4.1), we obtain

$$\mu^\varepsilon\, \Phi(X) = -\frac{\varepsilon^2}{2\delta^2}\, \Phi_{XX}(X) + \phi_s^2\, \Phi(X), \qquad X > 0, \tag{4.13}$$

$$\Phi(0) = 0, \qquad \lim_{X\to\infty} \Phi(X) = 1. \tag{4.14}$$

In order to balance all terms in (4.13), we need to choose

$$\delta = \varepsilon/\sqrt{\mu^\varepsilon}, \qquad \phi_s = \sqrt{\mu^\varepsilon}. \tag{4.15}$$

Solving the problem (4.13)-(4.14) with the choice of the parameters in (4.15), we get

$$\Phi(X) = \tanh(X), \qquad X \geq 0. \tag{4.16}$$

Since $\mu^\varepsilon \approx \mu_g^{\rm TF} = 1$ for the ground state, we can conclude that the width of the boundary layer near $x = 0$ is $\delta = O(\varepsilon)$ and the inner expansion for (4.1)-(4.2) near $x = 0$ is

$$\phi_g^\varepsilon(x) \approx \sqrt{\mu_g^\varepsilon}\, \tanh\left(\sqrt{\mu_g^\varepsilon} x/\varepsilon\right), \qquad \text{for} \quad x \geq 0 \quad \text{near} \quad x = 0. \tag{4.17}$$

Similarly, we can get the inner expansion for (4.1)-(4.2) near $x = 1$ as

$$\phi_g^\varepsilon(x) \approx \sqrt{\mu_g^\varepsilon}\, \tanh\left(\sqrt{\mu_g^\varepsilon}(1-x)/\varepsilon\right), \qquad \text{for} \quad x \leq 1 \quad \text{near} \quad x = 1. \tag{4.18}$$

Using the matched asymptotic technique, we get the asymptotic approximation for the ground state as

$$\begin{aligned} \phi_g^\varepsilon(x) \quad &\approx \quad \sqrt{\mu_g^{\rm MA}}\left[\tanh\left(\frac{x}{\varepsilon}\sqrt{\mu_g^{\rm MA}}\right) + \tanh\left(\frac{1-x}{\varepsilon}\sqrt{\mu_g^{\rm MA}}\right) - \tanh\left(\frac{1}{\varepsilon}\sqrt{\mu_g^{\rm MA}}\right)\right] \\ &:= \quad \phi_g^{\rm MA}(x), \qquad 0 \leq x \leq 1. \end{aligned} \tag{4.19}$$

Plugging (4.19) into the normalization constraint (2.20) with $\Omega = (0, 1)$, after some computations [**BLZ, BC**], we obtain

$$1 = \int_0^1 |\phi_g^{\rm MA}(x)|^2\, dx \approx \mu_g^{\rm MA} - 2\varepsilon\sqrt{\mu_g^{\rm MA}}. \tag{4.20}$$

Solving the above equation, we obtain the asymptotic approximation for the chemical potential of the ground state as

$$\mu_g^\varepsilon \approx \mu_g^{\rm MA} = 1 + 2\varepsilon\sqrt{1+\varepsilon^2} + 2\varepsilon^2, \qquad 0 < \varepsilon \ll 1. \tag{4.21}$$

Moreover, plugging (4.19) into (2.21) with $\Omega = (0, 1)$ $V_\varepsilon(\mathbf{x}) = 0$, after some computations [**BLZ, BC**], we obtain the asymptotic approximation for the energy of the ground state as

$$E_g^\varepsilon \approx E_g^{\rm MA} \approx \frac{1}{2}\mu_g^{\rm MA} + \frac{1}{3}\mu_g^{\rm MA}\varepsilon\sqrt{\mu_g^{\rm MA}} \approx \frac{1}{2} + \frac{4}{3}\varepsilon\sqrt{1+\varepsilon^2} + 2\varepsilon^2, \qquad 0 < \varepsilon \ll 1. \tag{4.22}$$

Based on the above matched asymptotic approximation for the ground state, we can obtain the semiclassical limits of the ground state wave function ϕ_g^ε, density

function $\rho_g^\varepsilon := |\phi_g^\varepsilon|^2$, energy E_g^ε and chemical potential μ_g^ε as

$$\phi_g^0(x) := \lim_{\varepsilon\to 0^+} \phi_g^\varepsilon(x) = \begin{cases} 1 & 0 < x < 1, \\ 0 & x = 0, 1, \end{cases} \tag{4.23}$$

$$\rho_g^0(x) := \lim_{\varepsilon\to 0^+} \rho_g^\varepsilon(x) = \begin{cases} 1 & 0 < x < 1, \\ 0 & x = 0, 1; \end{cases} \tag{4.24}$$

$$E_g^0 := \lim_{\varepsilon\to 0^+} E_g^\varepsilon = \frac{1}{2}, \qquad \mu_g^0 := \lim_{\varepsilon\to 0^+} \mu_g^\varepsilon = 1. \tag{4.25}$$

Similarly, for the lth ($l \in \mathbb{N}$) excited state of (4.1)-(4.2), there are two boundary layers near $x = 0$ and $x = 1$ and l interior layers located at $x_j = \frac{j}{l+1}$ ($j = 1, 2, \ldots, l$). By using the matched asymptotic technique, we get the asymptotic approximation for the lth excited state as [**BLZ, BC**]

$$\begin{aligned} \phi_l^\varepsilon(x) \quad &\approx \quad \phi_l^{\rm MA}(x) = \sqrt{\mu_l^{\rm MA}} \left[\sum_{j=0}^{[(l+1)/2]} \tanh\left(\frac{1}{\varepsilon}\sqrt{\mu_l^{\rm MA}} \left(x - \frac{2j}{l+1} \right) \right) \right. \\ &\left. + \sum_{j=0}^{[l/2]} \tanh\left(\frac{1}{\varepsilon}\sqrt{\mu_l^{\rm MA}} \left(\frac{2j+1}{l+1} - x \right) \right) - C_l \tanh\left(\frac{1}{\varepsilon}\sqrt{\mu_l^{\rm MA}} \right) \right], \end{aligned} \tag{4.26}$$

where $[\tau]$ takes the integer part of the real number τ, the constant $C_l = 1$ when l is odd and $C_l = 0$ when l is even, and $\mu_l^{\rm MA}$ is the asymptotic approximation of eigenvalue (or chemical potential) of the lth ($l \in \mathbb{N}$) excited state given as [**BLZ, BC**]

$$\mu_l := \mu_\varepsilon(\phi_l^\varepsilon) \approx \mu_l^{\rm MA} = 1 + 2(l+1)\varepsilon\sqrt{1 + (l+1)^2\varepsilon^2} + 2(l+1)^2\varepsilon^2. \tag{4.27}$$

In addition, the asymptotic approximation of the energy of the lth ($l \in \mathbb{N}$) excited state can be given as [**BLZ, BC**]

$$E_l := E_\varepsilon(\phi_l^\varepsilon) \approx E_l^{\rm MA} = \frac{1}{2} + \frac{4}{3}(l+1)\varepsilon\sqrt{1 + (l+1)^2\varepsilon^2} + 2(l+1)^2\varepsilon^2. \tag{4.28}$$

Again, based on the above matched asymptotic approximation for the excited states, we can obtain the semiclassical limits of the excited state wave function ϕ_l^ε, density function $\rho_l^\varepsilon := |\phi_l^\varepsilon|^2$, energy E_l^ε and chemical potential μ_l^ε as

$$\phi_l^0(x) := \lim_{\varepsilon\to 0^+} \phi_l^\varepsilon(x) = \begin{cases} 1, & \frac{j}{l+1} < x < \frac{j+1}{l+1} \text{ with } 0 \le j \le l \ \&j \text{ is even}, \\ -1, & \frac{j}{l+1} < x < \frac{j+1}{l+1} \text{ with } 0 \le j \le l \ \&j \text{ is odd}, \\ 0, & x = \frac{j}{l+1},\ j = 0, 1, \ldots, l+1, \end{cases} \tag{4.29}$$

$$\rho_l^0(x) := \lim_{\varepsilon\to 0^+} \rho_l^\varepsilon(x) = \begin{cases} 1, & \frac{j}{l+1} < x < \frac{j+1}{l+1},\ j = 0, 1, \ldots, l, \\ 0, & x = \frac{j}{l+1},\ j = 0, 1, \ldots, l+1; \end{cases} \tag{4.30}$$

$$E_l^0 := \lim_{\varepsilon\to 0^+} E_l^\varepsilon = \frac{1}{2}, \qquad \mu_l^0 := \lim_{\varepsilon\to 0^+} \mu_l^\varepsilon = 1. \tag{4.31}$$

Based on the above asymptotic results, we make the following observations for the ground and excited states of the time-independent GPE (4.1)-(4.2) under the constraint (2.20) with $\Omega = (0, 1)$ in the semiclassical regime, i.e. $0 < \varepsilon \ll 1$ and $\gamma = 1$:

- Boundary layers are observed at $x = 0$ and $x = 1$ for ground and all excited states. The width of these layers is of $O(\varepsilon)$.

ε	$\varepsilon=\frac{1}{5}$	$\varepsilon=\frac{1}{10}$	$\varepsilon=\frac{1}{20}$	$\varepsilon=\frac{1}{40}$	$\varepsilon=\frac{1}{80}$	$\varepsilon=\frac{1}{160}$
$\|\phi_g^0-\phi_g^\varepsilon\|$	0.3387	0.2589	0.1894	0.1358	0.096	0.0674
$\|E_g^0-E_g^\varepsilon\|$	0.3649	0.1555	0.0719	0.0341	0.0169	0.0084
$\|\mu_g^0-\mu_g^\varepsilon\|$	0.4881	0.2211	0.1051	0.0512	0.0253	0.0126

TABLE 1. Errors between the ground state and its semiclassical limit for the time-independent GPE with box potential.

ε	$\varepsilon=\frac{1}{10}$	$\varepsilon=\frac{1}{20}$	$\varepsilon=\frac{1}{40}$	$\varepsilon=\frac{1}{80}$	$\varepsilon=\frac{1}{160}$	$\varepsilon=\frac{1}{320}$
$\|\phi_1^0-\phi_1^\varepsilon\|$	0.3387	0.2589	0.1894	0.1358	0.0962	0.0675
$\|E_1^0-E_1^\varepsilon\|$	0.3649	0.1554	0.0719	0.0346	0.0169	0.0084
$\|\mu_1^0-\mu_1^\varepsilon\|$	0.4880	0.2211	0.1051	0.0512	0.0253	0.0126

TABLE 2. Errors between the first excited state and its semiclassical limit for the time-independent GPE with box potential.

ε	$\varepsilon=\frac{1}{20}$	$\varepsilon=\frac{1}{40}$	$\varepsilon=\frac{1}{80}$	$\varepsilon=\frac{1}{160}$	$\varepsilon=\frac{1}{320}$	$\varepsilon=\frac{1}{640}$
$\|\phi_5^0-\phi_5^\varepsilon\|$	0.3807	0.3054	0.2282	0.1653	0.1178	0.0832
$\|E_5^0-E_5^\varepsilon\|$	0.6445	0.2525	0.1121	0.0529	0.0257	0.0126
$\|\mu_5^0-\mu_5^\varepsilon\|$	0.8096	0.3483	0.1616	0.0778	0.0382	0.0189

TABLE 3. Errors between the fifth excited state and its semiclassical limit for the time-independent GPE with box potential.

- For the lth ($l\in\mathbb{N}$) excited state, interior layers are observed at $x_j=\frac{j}{l+1}$ ($j=1,2,\ldots,l$). The widths of these layers are of $O(\varepsilon)$ and they are twice the size of the widths of the boundary layers.
- If we rank all different eigenfunctions monotonously according to their energies, then the corresponding eigenvalues (or chemical potentials) are in the same order (see (4.21), (4.22), (4.27) and (4.28)).
- The semiclassical limits of the ground and excited states exist and they can be found explicitly.

To verify the above asymptotic results, we compute the ground and excited states numerically for each fixed ε. Table 1 lists the errors between the ground state and its semiclassical limit for different ε. Tables 2 and 3 show similar results for the first and fifth excited states, respectively.

From Tabs. 1, 2 and 3, the numerical results confirm our asymptotic results for the ground and excited states. In addition, they also suggest the following convergence rate:

$$\|\phi_g^\varepsilon-\phi_g^0\|=O(\varepsilon^{1/2}),\quad E_g^\varepsilon=E_g^0+O(\varepsilon),\quad \mu_g^\varepsilon=\mu_g^0+O(\varepsilon),\quad 0<\varepsilon\ll 1,$$
$$\|\phi_l^\varepsilon-\phi_l^0\|=O(\varepsilon^{1/2}),\quad E_l^\varepsilon=E_l^0+O(\varepsilon),\quad \mu_l^\varepsilon=\mu_l^0+O(\varepsilon),\quad l=1,2,\ldots\ .$$

4.3. In the strongly attractive interaction regime in 1D. In this case, i.e. $\gamma=-1$ and $0<\varepsilon\ll 1$, by using the soliton solution of the 1D nonlinear

Schrödinger equation (NLSE) with attractive cubic nonlinearity [**AC**], we can obtain the approximate ground state in this regime as

$$\phi_g^\varepsilon(x) \approx \phi^\varepsilon(x) = \frac{1}{2\varepsilon}\mathrm{sech}\left(\frac{(x-0.5)}{2\varepsilon^2}\right), \qquad 0 \le x \le 1. \tag{4.32}$$

Plugging (4.32) into (4.1), we get the approximate ground state chemical potential and energy as

$$\mu_g^\varepsilon \approx -\frac{1}{8\varepsilon^2}, \quad E_g^\varepsilon = \mu_g^\varepsilon + \frac{1}{2}\int_0^1 |\phi_g^\varepsilon(x)|^4 dx \approx -\frac{1}{8\varepsilon^2} + \frac{1}{2}\int_0^1 |\phi^\varepsilon(x)|^4 dx = -\frac{1}{24\varepsilon^2}. \tag{4.33}$$

Based on the above asymptotic approximation for the ground state, we can obtain the semiclassical limits of the ground state wave function ϕ_g^ε, density function $\rho_g^\varepsilon := |\phi_g^\varepsilon|^2$, energy E_g^ε and chemical potential μ_g^ε as

$$\phi_g^0(x) := \lim_{\varepsilon\to 0^+} \phi_g^\varepsilon(x) = \delta^{1/2}(x-0.5), \quad \rho_g^0(x) := \lim_{\varepsilon\to 0^+} \rho_g^\varepsilon(x) = \delta(x-0.5), \tag{4.34}$$

$$E_g^0 := \lim_{\varepsilon\to 0^+} E_g^\varepsilon = -\infty, \qquad \mu_g^0 := \lim_{\varepsilon\to 0^+} \mu_g^\varepsilon = -\infty; \tag{4.35}$$

where $\delta(x)$ is the Dirac delta function.

5. Semiclassical limits of the GPE with harmonic potential

In this section, we will derive the approximations for the ground and first excited states of the GPE with a harmonic potential in different limiting interaction regimes and then obtain the semiclassical limits of the solutions. For simplicity, here we only present results in 1D. Extensions to d-dimensions for linear and repulsive interaction cases are straightforward. When $d = 1$ and $\Omega = \mathbb{R}$ with harmonic potential, i.e. $V_\varepsilon(x) = x^2/2$ for the cases of: (i) $\varepsilon = 1$ and $|\gamma| \le 1$; or (ii) $0 < \varepsilon \le 1$ and $\gamma = 1$; and $V_\varepsilon(x) = \varepsilon^2 x^2/2$ for the case of $0 < \varepsilon \le 1$ and $\gamma = -1$, the problem (2.19)-(2.20) collapses into

$$\mu^\varepsilon\ \phi^\varepsilon(x) = -\frac{\varepsilon^2}{2}\frac{d^2\phi^\varepsilon(x)}{dx^2} + V_\varepsilon(x)\phi^\varepsilon(x) + \gamma|\phi^\varepsilon(x)|^2\phi^\varepsilon(x), \quad -\infty < x < \infty, \tag{5.1}$$

under the normalization or constraint (2.20) with $\Omega = \mathbb{R}$.

5.1. In the weak interaction regime. In the case without interaction, i.e. $\varepsilon = 1$ and $\gamma = 0$, the problem (5.1) collapses into a linear eigenvalue problem and we can find a complete set of orthonormal eigenfunctions [**L, BD, BCL**]

$$\phi_l^h(x) = (2^l\, l!)^{-1/2}\frac{1}{\pi^{1/4}}e^{-x^2/2}H_l(x), \qquad l = 0, 1, 2, \ldots, \tag{5.2}$$

where $H_l(x)$ ($l = 0, 1, 2, \ldots$) are the standard Hermite polynomials. The corresponding eigenvalues are

$$\mu_l = \frac{l+1}{2}, \qquad l = 0, 1, 2, \ldots\ . \tag{5.3}$$

From these solutions, we can immediately get the ground and excited states as

$$\phi_g(x) = \phi_0^h(x), \qquad \phi_l(x) = \phi_l^h(x), \qquad l = 1, 2, \ldots\ . \tag{5.4}$$

The corresponding energy and chemical potential of the ground and excited states are

$$E_g = \mu_g = \frac{1}{2}, \qquad E_l = \mu_l = \frac{l+1}{2}, \qquad l = 1, 2, \ldots\ . \tag{5.5}$$

In addition, based on these solutions, we can get the approximations of the ground and excited states in the weak interaction regime, i.e. $\varepsilon = 1$ and $|\gamma| \ll 1$. In this case, the ground and excited states can be approximated as

$$\phi_g(x) \approx \phi_0^h(x), \qquad \phi_l(x) \approx \phi_l^h(x), \qquad l = 1, 2, \dots . \tag{5.6}$$

Furthermore, the energy and chemical potential of the ground and excited states can be approximated as

$$\begin{aligned} E_g &:= E_\varepsilon(\phi_g) \approx E_\varepsilon(\phi_0^h) = \frac{1}{2} + \frac{\gamma C_0}{2}, \quad E_l := E_\varepsilon(\phi_l) \approx E_\varepsilon(\phi_l^h) = \frac{l+1}{2} + \frac{\gamma C_l}{2}, \\ \mu_g &:= \mu_\varepsilon(\phi_g) \approx \mu_\varepsilon(\phi_0^h) = \frac{1}{2} + \gamma C_0, \quad \mu_l := \mu_\varepsilon(\phi_l) \approx \mu_\varepsilon(\phi_l^h) = \frac{l+1}{2} + \gamma C_l; \end{aligned}$$

where

$$C_l = \int_{-\infty}^{\infty} |\phi_l^h(x)|^4 \, dx, \qquad l = 0, 1, 2, \dots .$$

5.2. In the strongly repulsive interaction regime. In this case, i.e. $\gamma = 1$ and $0 < \varepsilon \ll 1$, we formally drop the first term on the right hand side of (5.1) and obtain the Thomas-Fermi approximation of the ground state as

$$\mu^{\rm TF} \, \phi^{\rm TF}(x) = \frac{x^2}{2} \phi^{\rm TF}(x) + |\phi^{\rm TF}(x)|^2 \phi^{\rm TF}(x), \qquad x \in \mathbb{R}, \tag{5.7}$$

which immediately implies that the Thomas-Fermi approximation for the ground state is

$$\phi_g^{\rm TF}(x) = \begin{cases} \sqrt{\mu_g^{\rm TF} - \frac{x^2}{2}}, & x^2 < 2\mu_g^{\rm TF}, \\ 0, & \text{otherwise.} \end{cases} \tag{5.8}$$

Thus there is no boundary or interior layer in the ground state of the time-independent GPE (5.1) with harmonic potential. Plugging (5.8) into the constraint (2.20) with $\Omega = \mathbb{R}$, we get

$$1 = \int_{-\infty}^{\infty} |\phi_g^{\rm TF}(x)|^2 \, dx = \int_{-\sqrt{2\mu_g^{\rm TF}}}^{\sqrt{2\mu_g^{\rm TF}}} \left(\mu_g^{\rm TF} - \frac{x^2}{2} \right) \, dx = \frac{2}{3} \left(2\mu_g^{\rm TF} \right)^{3/2}. \tag{5.9}$$

Solving the above equation, we can obtain the asymptotic approximation for the eigenvalue (or chemical potential) of the ground state as

$$\mu_g^\varepsilon = \mu_\varepsilon(\phi_g^\varepsilon) \approx \mu_g^{\rm TF} = \frac{1}{2} \left(\frac{3}{2} \right)^{2/3}. \tag{5.10}$$

Furthermore, we can also obtain the asymptotic approximation for the energy of the ground state as

$$\begin{aligned} E_g^\varepsilon &= E_\varepsilon(\phi_g^\varepsilon) = \mu_\varepsilon(\phi_g^\varepsilon) - \frac{1}{2} \int_{-\infty}^{\infty} |\phi_g^\varepsilon(x)|^4 \, dx \\ &\approx \mu_g^{\rm TF} - \frac{1}{2} \int_{-\infty}^{\infty} |\phi_g^{\rm TF}(x)|^4 \, dx = \mu_g^{\rm TF} - \frac{2}{5} \mu_g^{\rm TF} = \frac{3}{10} \left(\frac{3}{2} \right)^{2/3}. \end{aligned} \tag{5.11}$$

Based on the above Thomas-Fermi approximation for the ground state, we can obtain the semiclassical limits of the ground state wave function ϕ_g^ε, density function

$\rho_g^\varepsilon := |\phi_g^\varepsilon|^2$, energy E_g^ε and chemical potential μ_g^ε as

$$\phi_g^0(x) := \lim_{\varepsilon\to 0^+} \phi_g^\varepsilon(x) = \begin{cases} \sqrt{\mu_g^{\rm TF} - \frac{x^2}{2}}, & x^2 \le 2\mu_g^{\rm TF}, \\ 0 & \text{otherwise}, \end{cases} \tag{5.12}$$

$$\rho_g^0(x) := \lim_{\varepsilon\to 0^+} \rho_g^\varepsilon(x) = \begin{cases} \mu_g^{\rm TF} - \frac{x^2}{2}, & x^2 \le 2\mu_g^{\rm TF}, \\ 0 & \text{otherwise}; \end{cases} \tag{5.13}$$

$$E_g^0 := \lim_{\varepsilon\to 0^+} E_g^\varepsilon = \frac{3}{10}\left(\frac{3}{2}\right)^{2/3}, \qquad \mu_g^0 := \lim_{\varepsilon\to 0^+} \mu_g^\varepsilon = \frac{1}{2}\left(\frac{3}{2}\right)^{2/3}. \tag{5.14}$$

In addition, the Thomas-Fermi approximation for the first excited state is

$$\phi_1^{\rm TF}(x) = \begin{cases} \sqrt{\mu_1^{\rm TF} - \frac{x^2}{2}}, & 0 < x \le \sqrt{2\mu_1^{\rm TF}}, \\ -\sqrt{\mu_1^{\rm TF} - \frac{x^2}{2}}, & -\sqrt{2\mu_1^{\rm TF}} \le x < 0, \\ 0, & \text{otherwise}. \end{cases} \tag{5.15}$$

Similarly, we can get the Thomas-Fermi approximation for the eigenvalue (or chemical potential) and energy of the first excited state as

$$\mu_1^\varepsilon = \mu_\varepsilon(\phi_1^\varepsilon) \approx \mu_1^{\rm TF} = \frac{1}{2}\left(\frac{3}{2}\right)^{2/3}, \qquad E_1^\varepsilon = E_\varepsilon(\phi_1^\varepsilon) = E_1^{\rm TF} \approx \frac{3}{10}\left(\frac{3}{2}\right)^{2/3}. \tag{5.16}$$

Since $\mu_1^{\rm TF} > 0$ is independent of ε, when $0 < \varepsilon \ll 1$, there is an interior layer located at $x = 0$ in the first excited state of the time-independent GPE (5.1) with harmonic potential.

To get the matched asymptotic approximation for the first excited state, let us assume that the interior layer is of width δ with $0 < \delta \ll 1$ and do a rescaling in the region near $x = 0$ with

$$x = \delta\, X, \qquad \phi^\varepsilon(x) = \phi_s\, \Phi(X), \qquad X \ge 0. \tag{5.17}$$

Substituting (5.17) into (5.1), we obtain

$$\mu^\varepsilon\, \Phi(X) = -\frac{\varepsilon^2}{2\delta^2}\, \Phi_{XX}(X) + \frac{\delta^2 X^2}{2}\Phi(\delta X) + \phi_s^2\, \Phi^3(X), \qquad X > 0, \tag{5.18}$$

$$\Phi(0) = 0, \qquad \lim_{X\to\infty} \Phi(X) = 1. \tag{5.19}$$

Since δ is small and we want to find the approximate solution of (5.18) for $|X|$ that is not too large, we drop the second term in the right hand side of (5.18) and choose δ and ϕ_s as those in (4.15), we can obtain that (4.16) is an approximate solution of (5.18) for $|X|$ that is not too large. Since $\mu^\varepsilon \approx \mu_1^{\rm TF} = O(1)$ for the first excited state, we can conclude that the width of the interior layer at $x = 0$ is $\delta = O(\varepsilon)$ and the inner expansion of (5.1) near $x = 0$ is

$$\phi_1^\varepsilon(x) = \sqrt{\mu_1^\varepsilon}\tanh\left(\frac{x}{\varepsilon}\sqrt{\mu_1^\varepsilon}\right), \qquad \text{for} \quad x \text{ near } 0. \tag{5.20}$$

Again, by using the matched asymptotic technique, we get the asymptotic approximation for the first excited state as [**BCL, BC**]

$$\begin{aligned} \phi_1^\varepsilon(x) &\approx \phi_1^{\rm MA}(x) \\ &= \begin{cases} \sqrt{\mu_1^{\rm MA}}\tanh\left(\frac{x}{\varepsilon}\sqrt{\mu_1^{\rm MA}}\right) - \frac{|x|x}{2\left[\sqrt{\mu_1^{\rm MA} - x^2/2} + \sqrt{\mu_1^{\rm MA}}\right]}, & x^2 \le 2\mu_1^{\rm MA}, \\ 0, & \text{otherwise}; \end{cases} \end{aligned} \tag{5.21}$$

ε	$\varepsilon = 0.4$	$\varepsilon = 0.2$	$\varepsilon = 0.1$	$\varepsilon = 0.05$	$\varepsilon = 0.025$	$\varepsilon = 0.0125$
$\|\phi_g^0 - \phi_g^\varepsilon\|$	0.2296	0.1471	0.0943	0.0605	0.0388	0.0251
$\|E_g^0 - E_g^\varepsilon\|$	7.35E-2	2.32E-2	7.05E-3	2.08E-3	5.99E-4	1.70E-4
$\|\mu_g^0 - \mu_g^\varepsilon\|$	4.33E-2	1.24E-2	3.47E-3	9.25E-4	2.15E-4	2.43E-5

TABLE 4. Errors between the ground state and its semiclassical limit for the time-independent GPE with harmonic potential.

ε	$\varepsilon = 0.4$	$\varepsilon = 0.2$	$\varepsilon = 0.1$	$\varepsilon = 0.05$	$\varepsilon = 0.025$	$\varepsilon = 0.0125$
$\|\phi_g^0 - \phi_g^\varepsilon\|$	0.6096	0.4144	0.2818	0.1927	0.1341	0.0934
$\|E_g^0 - E_g^\varepsilon\|$	4.26E-1	1.85E-1	8.33E-2	3.88E-2	1.86E-2	9.10E-3
$\|\mu_g^0 - \mu_g^\varepsilon\|$	3.68E-1	1.63E-1	7.62E-2	3.68E-2	1.80E-2	8.89E-3

TABLE 5. Errors between the first excited state and its semiclassical limit the time-independent GPE with harmonic potential.

where $\mu_1^{\rm MA} = \mu_1^{\rm TF} + O(\varepsilon)$ can be determined from the normalization constraint (2.20) with $\Omega = \mathbb{R}$ and $\phi = \phi_1^{\rm MA}$. Again, based on the above matched asymptotic approximation for the first excited state, we can obtain the semiclassical limits of the first excited state wave function ϕ_1^ε, density function $\rho_1^\varepsilon := |\phi_1^\varepsilon|^2$, energy E_1^ε and chemical potential μ_1^ε as

$$\phi_1^0(x) := \lim_{\varepsilon\to 0^+} \phi_1^\varepsilon(x) = \begin{cases} \sqrt{\mu_1^{\rm TF} - \frac{x^2}{2}}, & 0 < x^2 \le 2\mu_1^{\rm TF}, \\ -\sqrt{\mu_1^{\rm TF} - \frac{x^2}{2}}, & -2\mu_1^{\rm TF} \le x^2 < 0, \\ 0 & \text{otherwise}, \end{cases} \tag{5.22}$$

$$\rho_1^0(x) := \lim_{\varepsilon\to 0^+} \rho_1^\varepsilon(x) = \begin{cases} \mu_1^{\rm TF} - \frac{x^2}{2}, & 0 < x^2 \le 2\mu_1^{\rm TF}, \\ 0 & \text{otherwise}; \end{cases} \tag{5.23}$$

$$E_1^0 := \lim_{\varepsilon\to 0^+} E_1^\varepsilon = \frac{3}{10}\left(\frac{3}{2}\right)^{2/3}, \qquad \mu_1^0 := \lim_{\varepsilon\to 0^+} \mu_1^\varepsilon = \frac{1}{2}\left(\frac{3}{2}\right)^{2/3}. \tag{5.24}$$

Based on the above asymptotic results, we make the following observations for the ground and first excited states of the time-independent GPE (5.1) under the constraint (2.20) with $\Omega = \mathbb{R}$:

- For the ground state, there is no boundary and interior layer.
- For the first excited state, an interior layer is located at $x = 0$ and its width is of $O(\varepsilon)$.
- The semiclassical limits of the ground and first excited states exist and they can be found explicitly.

Again, to verify the above asymptotic results, we compute the ground and first excited state numerically for each fixed ε. Table 4 lists the errors between the ground state and its semiclassical limit for different ε. Table 5 shows similar results for the first excited state.

From Tabs. 4 and 5, the numerical results confirm our asymptotic results for the ground and first excited states. In addition, they also suggest the following

convergence rate:

$$\|\phi_g^\varepsilon - \phi_g^0\| = O(\varepsilon^{1/2}), \quad E_g^\varepsilon = E_g^0 + O(\varepsilon^2), \quad \mu_g^\varepsilon = \mu_g^0 + O(\varepsilon^2),$$
$$\|\phi_1^\varepsilon - \phi_1^0\| = O(\varepsilon^{1/2}), \quad E_1^\varepsilon = E_1^0 + O(\varepsilon), \quad \mu_1^\varepsilon = \mu_1^0 + O(\varepsilon), \quad 0 < \varepsilon \ll 1.$$

5.3. In the strongly attractive interaction regime in 1D. In this case, i.e. $\gamma = -1$ and $0 < \varepsilon \ll 1$, dropping the second term on the right hand of (5.1) and using the soliton solution of the 1D nonlinear Schrödinger equation (NLSE) with attractive cubic nonlinearity [**AC**], we can obtain the approximate ground state in this regime as

$$\phi_g^\varepsilon(x) \approx \phi^\varepsilon(x) = \frac{1}{2\varepsilon}\operatorname{sech}\left(\frac{x}{2\varepsilon^2}\right), \qquad -\infty < x < \infty. \tag{5.25}$$

Plugging (5.25) into (5.1), we get the approximate ground state chemical potential and energy as

(5.26)
$$\mu_g^\varepsilon \approx -\frac{1}{8\varepsilon^2}, \quad E_g^\varepsilon = \mu_g^\varepsilon + \frac{1}{2}\int_{-\infty}^{\infty} |\phi_g^\varepsilon(x)|^4 dx \approx -\frac{1}{8\varepsilon^2} + \frac{1}{2}\int_{-\infty}^{\infty} |\phi^\varepsilon(x)|^4 dx = -\frac{1}{24\varepsilon^2}.$$

Based on the above asymptotic approximation for the ground state, we can obtain the semiclassical limits of the ground state wave function ϕ_g^ε, density function $\rho_g^\varepsilon := |\phi_g^\varepsilon|^2$, energy E_g^ε and chemical potential μ_g^ε as

$$\phi_g^0(x) := \lim_{\varepsilon\to 0^+} \phi_g^\varepsilon(x) = \delta^{1/2}(x), \quad \rho_g^0(x) := \lim_{\varepsilon\to 0^+} \rho_g^\varepsilon(x) = \delta(x), \quad x \in \mathbb{R}, \tag{5.27}$$

$$E_g^0 := \lim_{\varepsilon\to 0^+} E_g^\varepsilon = -\infty, \qquad \mu_g^0 := \lim_{\varepsilon\to 0^+} \mu_g^\varepsilon = -\infty. \tag{5.28}$$

6. Semiclassical limits of the GPE on a ring

In this section, we will derive the approximations for the ground and excited states of the GPE on a ring with $\Omega = (0, 1)$ and periodic boundary conditions in different limiting interaction regimes and then obtain the semiclassical limits. Extensions to the case of GPE on a torus for linear and repulsive interaction cases are straightforward. On the ring, the problem (2.19)-(2.20) collapses into

$$\mu^\varepsilon\ \phi^\varepsilon(x) = -\frac{\varepsilon^2}{2}\frac{d^2\phi^\varepsilon(x)}{dx^2} + \gamma|\phi^\varepsilon(x)|^2\phi^\varepsilon(x), \quad 0 < x < 1, \tag{6.1}$$

$$\phi^\varepsilon(x+1) = \phi^\varepsilon(x), \qquad 0 \le x \le 1, \tag{6.2}$$

under the normalization or constraint (2.20) with $\Omega = (0, 1)$. We notice that the ground and excited states may differ up to a shift, i.e. if $\phi^\varepsilon(x)$ is a solution, then $\phi^\varepsilon(x + x_0)$ is also a solution with any fixed x_0.

6.1. In the weak interaction regime. In the case without interaction, i.e. $\varepsilon = 1$ and $\gamma = 0$, the problem (6.1) collapses into a linear eigenvalue problem and we can find a complete set of orthonormal eigenfunctions

$$\phi_0^r(x) = 1, \qquad \phi_l^r(x) = \sqrt{2}\sin(2l\pi x), \qquad l = 1, 2, \dots\ . \tag{6.3}$$

The corresponding eigenvalues are

$$\mu_l^r = 2l^2\pi^2, \qquad l = 0, 1, 2, \dots\ . \tag{6.4}$$

From these solutions, we can immediately get the ground and excited states as

$$\phi_g(x) = \phi_0^r(x), \qquad \phi_l(x) = \phi_l^r(x), \qquad l = 1, 2, \dots\ . \tag{6.5}$$

The corresponding energy and chemical potential of the ground and excited states are

$$E_g = \mu_g = 0, \qquad E_l = \mu_j = 2l^2\pi^2, \qquad l = 1, 2, \dots . \tag{6.6}$$

In addition, based on these solutions, we can get the approximations of the ground and excited states in the weak interaction regime, i.e. $\varepsilon = 1$ and $|\gamma| \ll 1$. In this case, the ground and excited states can be approximated as

$$\phi_g(x) \approx \phi_0^r(x), \qquad \phi_l(x) \approx \phi_l^r(x), \qquad l = 1, 2, \dots . \tag{6.7}$$

Furthermore, the energy and chemical potential of the ground and excited states can be approximated as

$$\begin{aligned} E_g &:= E_\varepsilon(\phi_g) \approx E_\varepsilon(\phi_0^r) = \frac{3\gamma}{2}, \qquad E_l := E_\varepsilon(\phi_l) \approx E_\varepsilon(\phi_l^r) = 2l^2\pi^2 + \frac{3\gamma}{2}, \\ \mu_g &:= \mu_\varepsilon(\phi_g) \approx \mu_\varepsilon(\phi_0^b) = 3\gamma, \qquad \mu_l := \mu_\varepsilon(\phi_l) \approx \mu_\varepsilon(\phi_l^r) = 2l^2\pi^2 + 3\gamma. \end{aligned}$$

6.2. In the strongly repulsive interaction regime. In this case, i.e. $\gamma = 1$ and $0 < \varepsilon \ll 1$, due to the repulsive interaction and periodic boundary condition, we can conclude that the ground state is

$$\phi_g^\varepsilon(x) = 1, \qquad 0 \le x \le 1. \tag{6.8}$$

The corresponding energy and chemical potential are

$$E_g^\varepsilon = \frac{1}{2}, \qquad \mu_g^\varepsilon = 1.$$

Based on the above results, we can obtain the semiclassical limits of the ground state wave function ϕ_g^ε, density function $\rho_g^\varepsilon := |\phi_g^\varepsilon|^2$, energy E_g^ε and chemical potential μ_g^ε as

$$\phi_g^0(x) := \lim_{\varepsilon\to 0^+} \phi_g^\varepsilon(x) = 1, \qquad \rho_g^0(x) := \lim_{\varepsilon\to 0^+} \rho_g^\varepsilon(x) = 1, \tag{6.9}$$

$$E_g^0 := \lim_{\varepsilon\to 0^+} E_g^\varepsilon = \frac{1}{2}, \qquad \mu_g^0 := \lim_{\varepsilon\to 0^+} \mu_g^\varepsilon = 1. \tag{6.10}$$

For the excited states, similar to the case of box potential, we can get the matched asymptotic approximation for the lth excited state as [**BLZ, BC**]

$$\begin{aligned} \phi_l^\varepsilon(x) \approx & \left[\sum_{j=1}^{l} \left(\tanh\left(\frac{1}{\varepsilon}\sqrt{\mu_l^{\rm MA}}\left(\frac{2j-1}{2l} - x\right)\right) + \tanh\left(\frac{1}{\varepsilon}\sqrt{\mu_l^{\rm MA}}\left(x - \frac{j}{l}\right)\right)\right)\right. \\ & \left. + \tanh\left(\frac{x}{\varepsilon}\sqrt{\mu_l^{\rm MA}}\right)\right]\sqrt{\mu_l^{\rm MA}} := \phi_l^{\rm MA}(x), \qquad 0 \le x \le 1, \end{aligned} \tag{6.11}$$

and $\mu_l^{\rm MA}$ is the asymptotic approximation of the eigenvalue (or chemical potential) of the lth ($l \in \mathbb{N}$) excited state given as [**BLZ, BC**]

$$\mu_l := \mu_\varepsilon(\phi_l^\varepsilon) \approx \mu_l^{\rm MA} = 1 + O(\varepsilon). \tag{6.12}$$

In addition, the asymptotic approximation of the energy of the lth ($l \in \mathbb{N}$) excited state can be given as [**BLZ, BC**]

$$E_l := E_\varepsilon(\phi_l^\varepsilon) \approx E_l^{\rm MA} = \frac{1}{2} + O(\varepsilon). \tag{6.13}$$

Again, based on the above matched asymptotic approximation for the excited states, we can obtain the semiclassical limits of the excited state wave function ϕ_l^ε, density function $\rho_l^\varepsilon := |\phi_l^\varepsilon|^2$, energy E_l^ε and chemical potential μ_l^ε as

$$\phi_l^0(x) := \lim_{\varepsilon\to 0^+} \phi_l^\varepsilon(x) = \begin{cases} 1, & \frac{(j-1)}{l} < x < \frac{(2j-1)}{2l} \text{ with } 1 \le j \le l, \\ -1, & \frac{(2j-1)}{2l} < x < \frac{j}{l} \text{ with } 1 \le j \le l, \\ 0, & x = \frac{j}{2l},\ j = 0, 1, \ldots, 2l, \end{cases} \tag{6.14}$$

$$\rho_l^0(x) := \lim_{\varepsilon\to 0^+} \rho_l^\varepsilon(x) = \begin{cases} 1, & \frac{(j-1)}{2l} < x < \frac{j}{2l},\ j = 1, 2, \ldots, 2l, \\ 0, & x = \frac{j}{2l},\ j = 0, 1, \ldots, 2l; \end{cases} \tag{6.15}$$

$$E_l^0 := \lim_{\varepsilon\to 0^+} E_l^\varepsilon = \frac{1}{2}, \qquad \mu_l^0 := \lim_{\varepsilon\to 0^+} \mu_l^\varepsilon = 1. \tag{6.16}$$

Based on the above asymptotic results, we make the following observations for the ground and excited states of the time-independent GPE (6.1)-(6.2) on a ring in the semiclassical regime, i.e. $0 < \varepsilon \ll 1$ and $\gamma = 1$:

- The ground state is independent of the interaction strength.
- For the lth ($l \in \mathbb{N}$) excited state, interior layers are observed at $x_j = \frac{j}{2l}$ ($j = 0, 1, \ldots, 2l$). The widths of these layers are of $O(\varepsilon)$.
- The semiclassical limits of the ground and excited states exist and they can be found explicitly.

Finally, in the strongly attractive interaction regime, i.e. $\gamma = -1$ and $0 < \varepsilon \ll 1$, the same results are still valid as in the case of the GPE with box potential in the subsection 4.3. We omitted the details here for brevity.

7. Concluding remarks

We have reviewed and presented asymptotic approximations of the ground and excited states of the time-independent Gross-Pitaevskii equation (GPE) with applications in Bose-Einstein condensation, quantum physics and chemistry, nonlinear optics, etc. Matched asymptotic approximations were obtained for different external potentials in the regimes of weak interaction regime, strongly repulsive interaction regime and strongly attractive interaction regime in 1D. Boundary and/or interior layers were observed in the ground and/or excited states in the strongly repulsive interaction regime. Based on the matched asymptotic approximations, we also obtained explicitly the semiclassical limits of the ground and excited states of the time-independent GPE. In addition, efficient and accurate numerical methods for computing the ground and excited states were discussed and numerical results were reported to verify our asymptotic results.

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