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Ground states of Bose–Einstein condensates with higher order interaction

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HIGHLIGHTS

- Ground state exists for positive higher order interactions.
- Ground state is unique with certain negative contact interaction.
- Higher order interaction competes with contact interaction.
- Thomas-Fermi limits are different in whole space and bounded domain.
- Asymptotic profiles of ground states satisfy free boundary problems.

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ABSTRACT

We analyze the ground state of a Bose–Einstein condensate in the presence of higher-order interaction (HOI), modeled by a modified Gross–Pitaevskii equation (MGPE). In fact, due to the appearance of HOI, the ground state structures become very rich and complicated. We establish the existence and non-existence results under different parameter regimes, and obtain their limiting behaviors and/or structures with different combinations of HOI and contact interactions. Both the whole space case and the bounded domain case are considered, where different structures of ground states are identified.

1. Introduction

Bose–Einstein condensates (BECs) have been thoroughly studied since its first experimental realization in 1995 [1,2] and many of its properties have been investigated theoretically based on the mean-field Gross–Pitaevskii equation (GPE). In the derivation of GPE, one key assumption is that the binary interaction between the particles can be well described by the shape-independent approximation (or pseudopotential approximation), i.e. a Dirac function, where the interaction strength is characterized by the s-wave scattering length [3]. It is well-known that such approximation is valid in low energies (or low densities) and becomes less valid in high energies (or high densities). Therefore, numerous efforts have been devoted to the improvements of the pseudopotential approximation for the two-body interaction, which lead to better mean field theory towards the understanding of BEC experiments.

In [3,4], a higher order interaction (HOI) correction to the pseudopotential approximation has been analyzed. As a consequence, at temperature T much lower than the critical temperature T_c, a BEC with HOI can be described by the wave function $\psi := \psi(\mathbf{x}, t)$ whose evolution is governed by the dimensionless modified Gross–Pitaevskii equation (MGPE) in three dimensions (3D) [3–5]

$$i\partial_t \psi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + g_0|\psi|^2 - g_1\nabla^2|\psi|^2 \right] \psi, \qquad (1.1)$$

where t is time, $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ is the Cartesian coordinate, g_0 is the contact interaction constant (positive for repulsive interaction and negative for attractive interaction), g_1 is the constant describing the higher order correction of the contact interaction due to the finite size effects, and $V(\mathbf{x})$ is a given real-valued external trapping potential and is commonly chosen to be the harmonic potential in typical experiments as

$$V(\mathbf{x}) = \frac{1}{2}\left(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2\right), \quad \mathbf{x} \in \mathbb{R}^3. \qquad (1.2)$$

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When the trapping potential in (1.2) is strongly anisotropic, i.e. $\gamma_x, \gamma_y \ll \gamma_z$ for a quasi-2D BEC or $\gamma_x \ll \gamma_y, \gamma_x \ll \gamma_z$ for a quasi-1D BEC, similar to the dimension reduction of the conventional GPE for a BEC [6–9], the MGPE (1.1) in 3D can be formally reduced to two dimensions (2D) or one dimension (1D) for the disk-shaped or cigar-shaped BEC [5,10], respectively. In fact, the resulting MGPE can be written in a unified form in d dimensions ($d = 1, 2, 3$) with $\mathbf{x} \in \mathbb{R}^d$ and $\mathbf{x} = x \in \mathbb{R}$ for $d = 1$, $\mathbf{x} = (x, y)^T \in \mathbb{R}^2$ for $d = 2$ and $\mathbf{x} = (x, y, z)^T \in \mathbb{R}^3$ for $d = 3$ as

$$i\partial_t \psi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\psi|^2 - \delta\nabla^2|\psi|^2\right]\psi, \tag{1.3}$$

where

$$V(\mathbf{x}) = \begin{cases} \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), & d = 3, \\ \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2), & d = 2, \\ \frac{1}{2}\gamma_x^2 x^2, & d = 1. \end{cases} \tag{1.4}$$

For other potentials such as box potential, optical lattice potential and double-well potential, we refer to [6,9] and references therein. Thus, in the subsequent discussion, we will treat the external potential $V(\mathbf{x})$ in (1.3) as a general real-valued function and the parameters β and δ as arbitrary real constants. In addition, without loss of generality, we assume $V(\mathbf{x}) \ge 0$ in the rest of this paper. The dimensionless MGPE (1.3) conserves the total mass

$$N(t) := \|\psi(\cdot, t)\|^2 = \int_{\mathbb{R}^d} |\psi(\mathbf{x}, t)|^2 d\mathbf{x} \equiv \|\psi(\cdot, 0)\|^2 = 1, \quad t \ge 0, \tag{1.5}$$

and the energy per particle

$$E(\psi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{\delta}{2}\left|\nabla|\psi|^2\right|^2\right] d\mathbf{x}. \tag{1.6}$$

Theoretically, other higher order terms can be included in the MGPE (1.3) as the higher order corrections of the two-body interaction [4]. Here, we focus on the current MGPE (1.3) to understand the idea behind the theory. In fact, MGPE (1.3) has been found in other applications (in a generalized form), such as the modeling of ultrashort laser pulses in plasmas [11,12], description of the thin-film superfluid condensates [13], study of the Heisenberg ferromagnets [14]. MGPE (1.3) with $\delta = 0$ has been thoroughly studied in the literature and we refer the readers to [6,7,9,15–20] and reference therein. However, there have been only a few mathematical results for MGPE (1.3), including the local well-posedness of the Cauchy problem [21,22], existence of solutions to the time independent version of (1.3) [23,24], the stability of standing waves [25], spectral method for (1.3) [26], etc. To the best of our knowledge, all the known mathematical results for MGPE (1.3) are not based on the BEC applications, and only some physical studies are available for MGPE (1.3) originating from BEC, like the ground state properties [27,28] and the dynamical instabilities [29,30]. In [5], we have studied the dimension reduction of MGPE in lower dimensions. Here, we will present our mathematical results on ground states of BEC based on the MGPE (1.3). In particular, much effort will be devoted to the study of the existence and qualitative properties as well as the asymptotic profiles of the ground state under different parameter regimes.

The paper is organized as follows. In Section 2, we establish existence, uniqueness and non-existence results of ground states under different parameter regimes as well as qualitative properties including regularity and decay of the ground state in the far field. We study the asymptotic profiles of ground states in different parameter regimes under a harmonic potential in Section 3 and under a box potential in Section 4. In particular, we are interested in the regimes with vanishing δ ($\delta \to 0^+$) and large interactions $\delta \to +\infty$, $|\beta| \to \infty$. Some conclusions are drawn in Section 5.

2. Mathematical analysis of the ground state

In this section, we focus on the existence and uniqueness of the ground states as well as the qualitative properties such as regularity and far field decay.

2.1. Existence and uniqueness

Introduce the function space

$$X = \left\{\phi \in H^1(\mathbb{R}^d) \middle| \|\phi\|_X^2 = \|\phi\|^2 + \|\nabla\phi\|^2 + \int_{\mathbb{R}^d} V(\mathbf{x})|\phi(\mathbf{x})|^2 \, d\mathbf{x} < \infty\right\}.$$

The ground state $\phi_g := \phi_g(\mathbf{x})$ of a BEC modeled by the MGPE (1.3) is defined as the minimizer of the energy functional (1.6) under the constraint (1.5), i.e. Find $\phi_g \in S$ such that

$$E_g := E(\phi_g) = \min_{\phi \in S} E(\phi), \tag{2.1}$$

where S is defined as

$$S := \{\phi \in X \mid \|\phi\| = 1, \quad E(\phi) < \infty\}. \tag{2.2}$$

In addition, the ground state ϕ_g is a solution to the following nonlinear eigenvalue problem, i.e. the Euler–Lagrange equation of the problem (2.1)

$$\mu\phi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + \beta|\phi|^2 - \delta\nabla^2|\phi|^2\right]\phi, \tag{2.3}$$

under the normalization constraint $\phi \in S$, where the corresponding eigenvalue (or chemical potential) $\mu := \mu(\phi)$ can be computed as (multiply (2.3) by ϕ and integrate over $\mathbf{x}$)

$$\mu = E(\phi) + \int_{\mathbb{R}^d} \left(\frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}\left|\nabla|\phi|^2\right|^2\right) d\mathbf{x}. \tag{2.4}$$

The following embedding results hold [6].

Lemma 2.1. *Under the assumption that $V(\mathbf{x}) \ge 0$ for $\mathbf{x} \in \mathbb{R}^d$ is a confining potential, i.e. $\lim_{R\to\infty} \mathrm{ess\,inf}_{|\mathbf{x}|<R} V(\mathbf{x}) = \infty$, we have that the embedding $X \hookrightarrow L^p(\mathbb{R}^d)$ is compact provided that exponent p satisfies*

$$\begin{cases} p \in [2, 6), & d = 3, \\ p \in [2, \infty), & d = 2, \\ p \in [2, \infty], & d = 1. \end{cases} \tag{2.5}$$

The existence and uniqueness of the ground state when $\delta = 0$ has been thoroughly studied in [6,31–33]. When $\delta \ne 0$, we have the existence and uniqueness results below.

Theorem 2.1 (*Existence and Uniqueness*). *Suppose $\delta \ne 0$ and $V(\mathbf{x}) \ge 0$ satisfies the confining condition, i.e. $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty$, then there exists a minimizer $\phi_g \in S$ of (2.1) if and only if $\delta > 0$. Furthermore, $e^{i\theta}\phi_g$ is also a ground state of (2.1) for any $\theta \in [0, 2\pi)$. The ground state ϕ_g can be chosen as non-negative $|\phi_g|$ and the non-negative ground state is unique if $\delta \ge 0$ and $\beta \ge 0$.*

The uniqueness result can be generalized to the case with negative β when the problem is defined on a bounded connected open domain Ω, i.e. the potential $V(\mathbf{x}) = +\infty$ for $\mathbf{x} \notin \Omega$. In such case, the zero Dirichlet boundary conditions on $\partial\Omega$ are imposed for the wave functions, and for any $\delta > 0$, there exists $C_\Omega > 0$ (depending on Ω) such that when $\beta > -\delta/C_\Omega$, the non-negative ground state $\phi_g \in H_0^1(\Omega)$ of (2.1) is unique.

Proof. (i) We start with the existence. Assume $\delta > 0$, by the inequality [34]

$$|\nabla|\phi(\mathbf{x})|| \le |\nabla\phi(\mathbf{x})|, \quad \text{a.e.} \quad \mathbf{x} \in \mathbb{R}^d, \tag{2.6}$$

we deduce

$$E(\phi) \ge E(|\phi|), \tag{2.7}$$

where equality holds iff $\phi = e^{i\theta}|\phi|$ for some constant $\theta \in [0, 2\pi)$. Therefore, it suffices to consider the real non-negative minimizers of (2.1). On the other hand, Nash inequality $\|f\|_{L^2}^{1+2/d} \le C\|f\|_{L^1}^{2/d}\|\nabla f\|_{L^2}$ and Young's inequality imply that for $\rho = |\phi|^2$ ($\phi \in S$),

$$\int_{\mathbb{R}^d} |\phi|^4 \, d\mathbf{x} \le (C\int_{\mathbb{R}^d} \rho(\mathbf{x})\, d\mathbf{x})^{4/d+2}\|\nabla|\phi|^2\|^{2d/d+2}$$
$$\le \frac{C}{\varepsilon} + \varepsilon\|\nabla\rho\|^2, \quad \forall\varepsilon > 0,$$

and we can conclude that $E(\phi)$ ($\phi \in S$) is bounded from below

$$E(\phi) \ge \int_{\mathbb{R}^d} \left(\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\delta}{4}\left|\nabla|\phi|^2\right|^2\right) d\mathbf{x} - C.$$

Taking a nonnegative minimizing sequence $\{\phi_n\}_{n=1}^{\infty} \subset S$, we find the ϕ_n is uniformly bounded in X and there exist $\phi_\infty \in X$ and a subsequence (denote as the original sequence for simplicity) such that

$$\phi_n \rightharpoonup \phi_\infty \quad \text{in} \quad X, \tag{2.8}$$

Lemma 2.1 ensures that $\phi_n \to \phi_\infty$ in L^p with p given in the lemma and so $\nabla|\phi_n|^2$ converges to $\nabla|\phi_\infty|^2$ in the sense of distribution. Noticing that $\|\nabla|\phi_n|^2\|$ is uniformly bounded and hence $\nabla|\phi_n|^2$ converges weakly in L^2 and we then get $\nabla|\phi_n|^2 \rightharpoonup \nabla|\phi_\infty|^2$ in L^2. Thus we know $\phi_\infty \in S$ with ϕ_∞ being nonnegative, and under the condition $\delta > 0$,

$$E(\phi_\infty) \le \liminf_{n\to\infty} E(\phi_n) = \min_{\phi\in S} E(\phi), \tag{2.9}$$

which shows that ϕ_∞ is a ground state.

Secondly, for the case $\beta > 0$ and $\delta > 0$, we prove the uniqueness of the nonnegative ground state. Denote $\rho = |\phi|^2$, then for $\phi = \sqrt{\rho} \in S$, the energy is

$$E(\sqrt{\rho}) = \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\sqrt{\rho}|^2 + V(\mathbf{x})\rho + \frac{\beta}{2}|\rho|^2 + \frac{\delta}{2}|\nabla\rho|^2\right] d\mathbf{x}. \tag{2.10}$$

The sum of first three terms of the energy is strictly convex in ρ [6,31], and the last term is also convex because it is quadratic in ρ and $\delta > 0$. Hence, we know $E(\sqrt{\rho})$ is strictly convex in ρ and the uniqueness of the nonnegative ground state follows [6,31].

When $\delta < 0$, we show the nonexistence of the ground state. Choosing a non-negative smooth function $\varphi(\mathbf{x}) \in S$ with compact support and denoting $\varphi_\varepsilon(\mathbf{x}) = \varepsilon^{-d/2}\varphi(\mathbf{x}/\varepsilon) \in S$, we have

$$\begin{aligned} E(\varphi_\varepsilon) = \int_{\mathbb{R}^d}\Bigg[&\frac{1}{2\varepsilon^2}|\nabla\varphi|^2 + V(\varepsilon\mathbf{x})|\varphi|^2 + \frac{\beta}{2\varepsilon^d}|\varphi|^4 \\ &+ \frac{\delta}{2\varepsilon^{2+d}}\left|\nabla|\varphi|^2\right|^2\Bigg] d\mathbf{x}. \end{aligned} \tag{2.11}$$

From the above equation, we see that $\lim_{\varepsilon\to 0^+} E(\varphi_\varepsilon) \to -\infty$ if $\delta < 0$ and there exists no ground state.

(ii) For problems defined on a bounded connected open domain, we have $\phi_g \in H_0^1(\Omega)$. Using Poincaré inequality, there exists $C_\Omega > 0$ such that

$$\|f\|_{L^2(\Omega)} \le C_\Omega\|\nabla f\|_{L^2(\Omega)}. \tag{2.12}$$

Denote $\rho = |\phi|^2$, then for $\phi = \sqrt{\rho} \in S$, and we claim the energy $E(\sqrt{\rho})$ is convex in ρ for $\beta \ge -\delta/C_\Omega$. To see this, we only need examine the case $\beta \in (-\delta/C_\Omega, 0)$. For any $\sqrt{\rho_j} \in S$ with $\rho_j \in H_0^1(\Omega)$ and $\theta \in [0, 1]$, we have

$$\begin{aligned} &\theta E(\sqrt{\rho_1}) + (1-\theta)E(\sqrt{\rho_2}) - E(\sqrt{\theta\rho_1 + (1-\theta)\rho_2}) \\ \ge &\frac{1}{2}\theta(1-\theta)\left(\beta\|\rho_1 - \rho_2\|^2 + \delta\|\nabla(\rho_1 - \rho_2)\|^2\right) \\ \ge &\frac{1}{2}\theta(1-\theta)\left(-\delta\|\nabla(\rho_1 - \rho_2)\|^2 + \delta\|\nabla(\rho_1 - \rho_2)\|^2\right) = 0, \end{aligned}$$

where we used the fact $\|\nabla\sqrt{\rho}\|^2$ is convex in ρ. This shows $E(\sqrt{\rho})$ is convex when $\beta > -\frac{\delta}{C_\Omega}$. The uniqueness follows. □

Remark 2.1. In the general whole space case, the energy functional $E(\sqrt{\rho})$ is no longer convex and the uniqueness when $\beta < 0$ is not clear (see recent results obtained by Guo et al. in [32] about the uniqueness when $\delta = 0$ with small $|\beta|$).

2.2. Regularity and decay

Concerning the ground state of (2.1), we have the following properties.

Theorem 2.2. *Let $\delta > 0$ and $\phi_g \in S$ be the nonnegative ground state of (2.1), we have the following properties:*

(i) There exist $\alpha > 0$ and $C > 0$ such that $|\phi_g(\mathbf{x})| \le Ce^{-\alpha|\mathbf{x}|}$, $\mathbf{x} \in \mathbb{R}^d$.

(ii) If $V(\mathbf{x}) \in L^\infty_{\text{loc}}(\mathbb{R}^d)$, we have ϕ_g is once continuously differentiable and $\nabla\phi_g$ is Hölder continuous with order 1. In particular, if $V(\mathbf{x}) \in C^\infty$, ϕ_g is smooth.

Proof. (i) We show the L^∞ bound of ϕ_g by a Moser's iteration and De Giorgi's iteration following [24]. From the fact that $\phi_g \in S$ minimizes energy (1.6), it is easy to check that ϕ_g satisfies the Euler–Lagrange equation (2.3), which shows that for any test function $\varphi \in C_0^\infty(\mathbb{R}^d)$, the following holds for $\phi = \phi_g$

$$\begin{aligned} &\int_{\mathbb{R}^d}\left[\frac{1}{2}\nabla\phi\cdot\nabla\varphi + V(\mathbf{x})\phi\varphi + \delta\phi\nabla\phi\cdot\nabla(\phi\varphi)\right] d\mathbf{x} \\ = &\int_{\mathbb{R}^d}\left[-\beta|\phi|^2\phi\varphi + \mu\phi\varphi\right] d\mathbf{x}. \end{aligned} \tag{2.13}$$

Using the Moser and De Giorgi iterations [35], we will prove that any weak solution $\phi \in X \cap \{E(\phi) < \infty\}$ of (2.13) is bounded and decays exponentially as $|\mathbf{x}| \to \infty$. In detail, we first observe that by an approximation argument, the test function φ can be any functions in X such that $\int_{\mathbb{R}^d}|\varphi|^2|\nabla\phi|^2\, d\mathbf{x} < \infty$ and $\int_{\mathbb{R}^d}|\phi|^2|\nabla\varphi|^2\, d\mathbf{x} < \infty$.

Firstly, we show that for all $q \ge 1$, $\int_{\mathbb{R}^d}(1 + \phi^{2q})|\nabla\phi|^2\, d\mathbf{x} < \infty$. Choose $q_0 = 12$, since $\nabla\phi^2 \in L^2$ and $\phi \in H^1$, $\phi \in L^p(\mathbb{R}^d)$ ($\forall p \in [2, q_0]$, $d = 1, 2, 3$). Let $\varphi = |\phi_M|^{q_0-4}\phi_M$ ($M > 0$) be the test function, where $\phi_M(\mathbf{x}) = \phi(\mathbf{x})$ if $\mathbf{x} \in \{|\phi(\mathbf{x})| \le M\}$, and $\phi_M(\mathbf{x}) = \pm M$ if $\mathbf{x} \in \{\phi(\mathbf{x}) \gtrless \pm M\}$. Plugging $\varphi = |\phi_M|^{q_0-4}\phi_M$ into (2.13), we obtain

$$\begin{aligned} &(q_0 - 3)\int_{\mathbb{R}^d}(\frac{1}{2} + \delta\phi^2)|\phi_M|^{q_0-4}\nabla\phi\cdot\nabla\phi_M\, d\mathbf{x} \\ &+ \delta\int_{\mathbb{R}^d}\phi\phi_M|\phi_M|^{q_0-4}|\nabla\phi|^2\, d\mathbf{x} + \int_{\mathbb{R}^d}V(\mathbf{x})\phi\phi_M|\phi_M|^{q_0-4}\, d\mathbf{x} \\ = &\int_{\mathbb{R}^d}\left(-\beta|\phi|^2\phi + \mu\phi\right)|\phi_M|^{q_0-4}\phi_M\, d\mathbf{x}. \end{aligned}$$

Letting $M \to \infty$, we get

$$\begin{aligned} &(q_0 - 2)\delta\int_{\mathbb{R}^d}|\phi|^{2\tilde{q}}|\nabla\phi|^2\, d\mathbf{x} + \int_{\mathbb{R}^d}V(\mathbf{x})|\phi|^{2\tilde{q}}\, d\mathbf{x} \\ \le &\int_{\mathbb{R}^d}\left(|\beta||\phi|^{q_0} + |\mu||\phi|^{q_0-2}\right) d\mathbf{x}, \end{aligned} \tag{2.14}$$

which shows $\int_{\mathbb{R}^d} |\phi|^{2\tilde{q}} |\nabla\phi|^2 \, d\mathbf{x} < \infty$ ($\tilde{q} = \frac{q_0}{2} - 1$). So $\nabla\phi^{\tilde{q}+1} \in L^2$ and for $q_1 = 6(\tilde{q}+1) = 3q_0 = 36$, $\phi \in L^p(\mathbb{R}^d)$ ($\forall p \in [2, q_1]$, $d = 1, 2, 3$). Then, the Moser iteration can continue with $q_j = 3^j q_0$, and $\phi \in L^{q_j}(\mathbb{R}^d)$ (it is obvious when $d = 1, 2$) which verifies our claim. In particular $\phi \in L^p$ for any $p \in [2, \infty)$.

Secondly, we show that $\phi \in L^\infty(\mathbb{R}^d)$ and $\lim_{|\mathbf{x}|\to\infty} \phi(\mathbf{x}) = 0$ by De Giorgi's iteration. Denoting $f = -\beta|\phi|^2\phi + \mu\phi$ and choosing test function $\varphi(\mathbf{x}) = (\xi(\mathbf{x}))^2(\phi(\mathbf{x}) - k)_+$ with $k \geq 0$ in (2.13), where $(\phi(\mathbf{x}))_+ = \max\{\phi, 0\}$ and $\xi(\mathbf{x})$ is a smooth cutoff function, we have

$$\int_{\mathbb{R}^d} \left[(\frac{1}{2} + \delta\phi^2 + \delta\phi(\phi - k)_+)|\xi|^2 |\nabla(\phi - k)_+|^2 + V(\mathbf{x})|\xi|^2 \phi(\phi - k)_+ \right] d\mathbf{x}$$
$$= \int_{\mathbb{R}^d} \left[-(1 + 2\delta\phi^2)(\phi - k)_+ \xi \nabla(\phi - k)_+ \cdot \nabla\xi + f\xi^2(\phi - k)_+ \right] d\mathbf{x}.$$

Cauchy inequality gives that

$$\int_{\mathbb{R}^d} -(1 + 2\delta\phi^2)(\phi - k)_+ \xi \nabla(\phi - k)_+ \cdot \nabla\xi \, d\mathbf{x}$$
$$\leq \varepsilon \int_{\mathbb{R}^d} (1 + \phi^2)|\nabla(\phi - k)_+|^2 \, d\mathbf{x} + C_\varepsilon \int_{\mathbb{R}^d} (1 + \phi^2)|\nabla\xi|^2 (\phi - k)_+^2 \, d\mathbf{x}.$$

Now choosing sufficiently small ε and defining function $\Phi_k(\mathbf{x}) = (1 + \phi)(\phi - k)_+$, we can get

$$\int_{\mathbb{R}^d} |\nabla\Phi_k|^2 |\xi|^2 \, d\mathbf{x} \leq C \int_{\mathbb{R}^d} |\nabla\xi|^2 \Phi_k^2 \, d\mathbf{x} + C \int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 \, d\mathbf{x}, \quad (2.15)$$

and

$$\int_{\mathbb{R}^d} |\nabla(\xi\Phi_k)|^2 \, d\mathbf{x} \leq C \int_{\mathbb{R}^d} |\nabla\xi|^2 \Phi_k^2 \, d\mathbf{x} + C \int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 \, d\mathbf{x}, \quad (2.16)$$

Since $f = -\beta|\phi|^2\phi + \mu\phi \in L^q(\mathbb{R}^d)$ for any $2 \leq q < \infty$, we can proceed to obtain L^∞ bound of ϕ by De Giorgi's iteration. Let $B_r(\mathbf{x})$ be the ball centered at $\mathbf{x}$ with radius r, and we use B_r for short to denote the ball centered at origin. For $0 < r < R \leq 1$, we choose C_0^∞ nonnegative cutoff function $\xi(\mathbf{x}) = 1$ for $\mathbf{x} \in B_r(\mathbf{x}_0)$ and $\xi(\mathbf{x}) = 0$ for $\mathbf{x} \notin B_R(\mathbf{x}_0)$ such that $|\nabla\xi(\mathbf{x})| \leq \frac{2}{R-r}$. Since for large q,

$$\int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 \, d\mathbf{x} \leq \|\xi f\|_{L^q} \|(\phi - k)_+ \xi\|_{L^6} |\{\Phi_k \xi > 0\}|^{\frac{5}{6} - \frac{1}{q}}, \quad (2.17)$$

where $|A|$ denotes the Lebesgue measure of set A, we have by Höder inequality and Sobolev inequality in 2D and 3D, for any $\varepsilon > 0$,

$$\int_{\mathbb{R}^d} |f|(\phi - k)_+ \xi^2 \, d\mathbf{x}$$
$$\leq C\|\xi f\|_{L^q} \|\nabla((\phi - k)_+ \xi)\| |\{\Phi_k \xi > 0\}|^{\frac{5}{6} - \frac{1}{q}}$$
$$\leq \varepsilon \|\nabla((\phi - k)_+ \xi)\|^2 + C_\varepsilon \|\xi f\|_{L^q}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3} - \frac{2}{q}}$$
$$\leq 2\varepsilon(\|\nabla(\Phi_k \xi)\|^2 + \|\Phi_k \nabla\xi\|^2) + C_\varepsilon \|\xi f\|_{L^q}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3} - \frac{2}{q}}.$$

Thus, from above inequality and (2.16), we arrive at

$$\|\nabla(\xi\Phi_k)\|^2 \leq C \left(\|\Phi_k \nabla\xi\|^2 + \|\xi f\|_{L^q}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3} - \frac{2}{q}} \right). \quad (2.18)$$

Since $\xi\Phi_k \in H_0^1(B_1(\mathbf{x}_0))$, we conclude by Sobolev inequality that $\forall p \in [2, 6]$,

$$\|\xi\Phi_k\|^2 \leq \|\xi\Phi_k\|_{L^6}^2 |\{\Phi_k \xi > 0\}|^{1 - \frac{2}{6}}$$
$$\leq C(d) \|\nabla(\xi\Phi_k)\|^2 |\{\Phi_k \xi > 0\}|^{\frac{2}{3}}. \quad (2.19)$$

By choosing $q = 3$, (2.18) and (2.19) imply that

$$\|\xi\Phi_k\|^2 \leq \left(\|\Phi_k \nabla\xi\|^2 |\{\Phi_k \xi > 0\}|^{\frac{2}{3}} + \|f\|_{L^3(B_1(\mathbf{x}_0))}^2 |\{\Phi_k \xi > 0\}|^{\frac{5}{3}} \right) \quad (2.20)$$

Denote

$$A(k, r) = \{\mathbf{x} | \mathbf{x} \in B_r(\mathbf{x}_0), \quad \phi > k\}. \quad (2.21)$$

and for $k > 0$, $0 < r < R \leq 1$, we have

$$\int_{A(k,r)} \Phi_k^2 \, d\mathbf{x} \leq C(\frac{1}{(R - r)^2} |A(k, R)|^{\frac{2}{3}} \int_{A(k,R)} \Phi_k^2 \, d\mathbf{x} + \|f\|_{L^3(B_1(\mathbf{x}_0))}^2 |A(k, R)|^{\frac{5}{3}}). \quad (2.22)$$

We claim that there exists $\tilde{C}$, such that for $k = \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|(1 + \phi)\phi\|_{L^2(B_1(\mathbf{x}_0))})$,

$$\int_{A(k, \frac{1}{2})} \Phi_k^2 \, d\mathbf{x} = 0. \quad (2.23)$$

Taking $h > k > k_0$ and $0 < r < 1$, we find $A(h, r) \subset A(k, r)$ with

$$\int_{A(h,r)} \Phi_h^2 \, d\mathbf{x} \leq \int_{A(k,r)} \Phi_k^2 \, d\mathbf{x}. \quad (2.24)$$

In addition, since $\Phi_k = (1 + \phi)(\phi - k)_+$, we have

$$|A(h, r)| = |B_r(\mathbf{x}_0) \cap \{\phi - k \geq h - k\}|$$
$$\leq \frac{1}{(h - k)^2} \int_{A(k,r)} \Phi_k^2 \, d\mathbf{x}. \quad (2.25)$$

Now, let us choose $\frac{1}{2} \leq r < R \leq 1$. We obtain from (2.22) that

$$\int_{A(h,r)} \Phi_h^2 \, d\mathbf{x}$$
$$\leq C \left(\frac{1}{(R - r)^2} \int_{A(h,R)} \Phi_h^2 \, d\mathbf{x} + \|f\|_{L^3(B_1(\mathbf{x}_0))}^2 |A(h, R)| \right) |A(h, R)|^{\frac{2}{3}}$$
$$\leq C \left(\frac{1}{(R - r)^2} + \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}^2}{(h - k)^2} \right) \frac{1}{(h - k)^{\frac{4}{3}}} \left(\int_{A(k,R)} \Phi_k^2 \, d\mathbf{x} \right)^{\frac{5}{3}},$$

and

$$\|\Phi_h\|_{L^2(B_r(\mathbf{x}_0))} \leq C \left(\frac{1}{R - r} + \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}}{h - k} \right) \times \frac{1}{(h - k)^{\frac{2}{3}}} \|\Phi_k\|_{L^2(B_R(\mathbf{x}_0))}^{\frac{5}{3}}. \quad (2.26)$$

Denote function

$$\chi(k, r) = \|\Phi_k\|_{L^2(B_r(\mathbf{x}_0))}. \quad (2.27)$$

For some value of $k > 0$ to be determined later, we define for $l = 0, 1, 2, \ldots,$

$$k_l = (1 - \frac{1}{2^l})k, \quad r_l = \frac{1}{2} + \frac{1}{2^{l+1}}, \quad (2.28)$$

then $k_l - k_{l-1} = \frac{k}{2^l}$ and $r_{l-1} - r_l = \frac{1}{2^{l+1}}$. From (2.26), we find

$$\chi(k_l, r_l) \leq C \left(2^{l+1} + \frac{2^l \|f\|_{L^3(B_1(\mathbf{x}_0))}}{k} \right) \frac{2^{\frac{2}{3}l}}{k^{\frac{2}{3}}} (\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}}$$
$$\leq 2C \frac{\|f\|_{L^3(B_1(\mathbf{x}_0))} + k}{k^{\frac{5}{3}}} 2^{\frac{5}{3}l} (\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}}.$$

Then, we prove that there exists $\gamma > 0$ such that

$$\chi(k_l, r_l) \leq \frac{\chi(k_0, r_0)}{\gamma^l}, \quad \gamma > 1. \quad (2.29)$$

We argue by induction. When $l = 0$, it is obvious true. Suppose (2.29) is true for $l - 1$, i.e.

$$(\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}} \leq \frac{\gamma^{\frac{5}{3}} (\chi(k_0, r_0))^{\frac{2}{3}}}{\gamma^{\frac{2}{3}l}} \cdot \frac{\chi(k_0, r_0)}{\gamma^l}.$$

Then, we have

$$\begin{aligned}\chi(k_l, r_l) \leq & 2C\frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}+k}{k^{\frac{5}{3}}}2^{\frac{5}{3}l}(\chi(k_{l-1}, r_{l-1}))^{\frac{5}{3}} \\ \leq & 2C\gamma^{\frac{5}{3}}(\chi(k_0, r_0))^{\frac{2}{3}}\frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}+k}{k^{\frac{5}{3}}}\cdot\frac{2^{\frac{5}{3}l}}{\gamma^{\frac{2}{3}l}}\cdot\frac{\chi(k_0, r_0)}{\gamma^l}.\end{aligned}$$

Let us choose $\gamma > 1$ such that $\gamma^{\frac{2}{3}} = 2^{\frac{5}{3}}$. Now we want to pick k sufficiently large such that

$$2C\gamma^{\frac{5}{3}}\frac{\|f\|_{L^3(B_1(\mathbf{x}_0))}+k}{k}\left(\frac{\chi(k_0, r_0)}{k}\right)^{\frac{2}{3}} \leq 1. \tag{2.30}$$

Choosing $k = \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \chi(k_0, r_0))$ for sufficiently large $\tilde{C}$, we get desired inequality (2.30). This gives that (2.29) is true for l and hence induction is done. Letting $l \to \infty$ in (2.29), we find $\chi(k, \frac{1}{2}) = 0$, which implies that

$$\Phi_k(\mathbf{x}) = 0, \quad \forall \mathbf{x} \in B_{\frac{1}{2}}(\mathbf{x}_0), \tag{2.31}$$

i.e.,

$$\begin{aligned}\sup_{B_{\frac{1}{2}}(\mathbf{x}_0)} \phi_+ \leq & \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \chi(k_0, r_0)) \\ \leq & \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|\Phi_0\|_{L^2(B_1(\mathbf{x}_0))}) \\ \leq & \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|\phi\|_{L^2(B_1(\mathbf{x}_0))} + \|\phi\|_{L^4(B_1(\mathbf{x}_0))}).\end{aligned}$$

The same estimates apply for $-\phi$ and we can conclude that

$$\|\phi\|_{L^\infty(B_{\frac{1}{2}}(\mathbf{x}_0))} \leq \tilde{C}(\|f\|_{L^3(B_1(\mathbf{x}_0))} + \|\phi\|_{L^2(B_1(\mathbf{x}_0))} + \|\phi\|_{L^4(B_1(\mathbf{x}_0))}).$$

This shows ϕ is bounded and $\lim_{|\mathbf{x}|\to 0}\phi(\mathbf{x}) = 0$.

Thirdly, we prove that $\int_{\mathbb{R}^d\setminus B_R}(|\nabla\phi|^2 + |\phi|^2)\,d\mathbf{x}$ decays exponentially as $R \to \infty$. Choose test function $\varphi = \eta^2(\mathbf{x})\phi$ in (2.13) with $\eta(\mathbf{x})$ being a smooth nonnegative cutoff function such that $\eta(\mathbf{x}) = 0$ for $\mathbf{x} \in B_R$ and $\eta(\mathbf{x}) = 1$ for $\mathbf{x} \in \mathbb{R}^d \setminus B_{R+1}$, then the following holds

$$\begin{aligned}&\int_{\mathbb{R}^d\setminus B_R}\left((\frac{1}{2} + 2\delta\phi^2)|\nabla\phi|^2\eta^2 + V(\mathbf{x})|\phi|^2\eta^2 + \beta\phi^4\eta^2 - \mu\phi^2\eta^2\right)d\mathbf{x} \\ &= -\int_{B_{R+1}\setminus B_R}\left(1 + 2\delta\phi^2\right)\eta\phi\nabla\phi\cdot\nabla\eta\,d\mathbf{x}.\end{aligned}$$

Since $\lim_{|\mathbf{x}|\to\infty}V(\mathbf{x}) = \infty$ and ϕ is bounded, we find that for large R,

$$\int_{\mathbb{R}^d\setminus B_R}(|\phi|^2 + |\nabla\phi|^2)\,d\mathbf{x} \leq C\int_{B_{R+1}\setminus B_R}(|\phi|^2 + |\nabla\phi|^2)\,d\mathbf{x}. \tag{2.32}$$

Let $a_n = \int_{\mathbb{R}^d\setminus B_{R_n}}(|\phi|^2 + |\nabla\phi|^2)\,d\mathbf{x}$ with $R_n = R + n$ $(n = 0, 1, 2, \ldots)$, then $a_n \leq C(a_{n+1} - a_n)$ and $a_{n+1} \leq \alpha a_n$ with $\alpha = \frac{C}{1+C}$. Hence $a_{n+1} \leq \alpha^n a_0$ which would imply the exponential decay of a_n as well as $\int_{\mathbb{R}^d\setminus B_R}(|\nabla\phi|^2 + |\phi|^2)\,d\mathbf{x}$.

Lastly, combining the exponential decay of $\int_{\mathbb{R}^d\setminus B_R}(|\nabla\phi|^2 + |\phi|^2)\,d\mathbf{x}$ and De Giorgi's iteration shown above, we can derive the exponential fall-off of $\|\phi\|_{L^\infty}$.

(ii) The regularity of the ground state ϕ_g can be proved by a variable of change method [23,25]. Let $v = F(t)$ be the solution of the ODE $F'(t) = \sqrt{\frac{1}{2} + 2\delta t^2}$ with $F(0) = 0$, then $F(t)$ is strictly increasing function, its inverse exists $t = G(v)$. Let $u = F(\phi)$, then $\phi = G(u)$ and the energy functional $E(\cdot)$ (1.6) becomes

$$E(\phi) = \int_{\mathbb{R}^d}\left(|\nabla u|^2 + V(\mathbf{x})G^2(u) + \frac{\beta}{2}G^4(u)\right)d\mathbf{x} := \tilde{E}(u). \tag{2.33}$$

$u_g = F(\phi_g)$ is the minimizer of $\tilde{E}(u)$ under constraint $\int_{\mathbb{R}^d} G(u)^2\,d\mathbf{x} = 1$. It follows that u_g satisfies the following Euler–Lagrange equation (for C_0^∞ test function)

$$-\nabla^2 u + V(\mathbf{x})G(u)G'(u) + \beta|G(u)|^2G(u)G'(u) = \lambda G(u)G'(u). \tag{2.34}$$

Since ϕ_g is bounded, we know u_g is bounded, hence $G(u_g)$ and $G'(u_g)$ are bounded with $\nabla^2 u_g \in L^\infty_{\mathrm{loc}}$. We conclude that u_g is once continuously differentiable and ∇u_g is Hölder continuous with order 1. Noticing that $\nabla^2\phi_g = G'(u_g)\nabla^2 u_g + G''(u_g)|\nabla u_g|^2$, we find that ϕ_g is once continuously differentiable and $\nabla\phi_g$ is Hölder continuous with order 1. In addition, if $V \in C^\infty$, we can obtain $\phi_g \in C^\infty$ by a bootstrap argument using the L^∞ bound of ϕ_g. $\square$

3. Limiting behavior of ground states in the whole space

In this section, we consider the behavior of the ground state (2.1) in different β and δ parameter regimes for typical potentials in the whole space, e.g. harmonic potential. In the next section, we will discuss about the box potential case (typical potential in bounded domains).

For the whole space, the harmonic trapping potential (1.4) is the most relevant experimental case and we will focus on such potentials. Our results are valid for more general confining potentials in d $(d = 1, 2, 3)$ dimensions, e.g. confining potentials satisfying the homogeneous conditions $V(\lambda\mathbf{x}) = |\lambda|^s V(\mathbf{x})$, for some $s > 0$ and any $\lambda \in \mathbb{R}$.

There are two interesting parameter regimes including the large β, δ limit and the vanishing δ limit. Below, we start with the strong interaction regime, i.e. $\delta \gg 1$ and $|\beta| \gg 1$ $(\delta \geq 0$ is necessary for the existence of the ground state).

3.1. Thomas–Fermi (TF) limit

When the number of particles in BEC is relatively large, the interaction between particles is dominant while the kinetic energy term can be neglected, leading to the Thomas–Fermi (TF) limit/approximation. The TF limit for the GPE has been thoroughly studied in [6,31,34] while the generalization to the MGPE is missing. As shown in [5], the TF limit for the MGPE is more complicated and more interesting where new phenomena can be observed due to the competition between the cubic nonlinear term and the new one. In this section, we aim to give a rigorous mathematical characterization of the TF approximations in different parameter regimes under a specific external potential, i.e. the harmonic potential.

When $V(\mathbf{x})$ is the harmonic potential (1.4), we consider the limiting profile of ground states (2.1) under different sets of parameters $\delta \gg 1$ and $|\beta| \gg 1$. For any $\phi(\mathbf{x}) \in S$, choose proper scaling $\phi^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2}\phi(\mathbf{x}/\varepsilon) \in S$ where ε^{-1} is the length scale for the condensate width, i.e.

$$\phi(\mathbf{x}) = \varepsilon^{d/2}\phi^\varepsilon(\mathbf{x}\varepsilon), \tag{3.35}$$

we find the energy $E(\cdot)$ (1.6) can be written as

$$\begin{aligned}E(\phi) &= \int_{\mathbb{R}^d}\left[\frac{\varepsilon^2}{2}|\nabla\phi^\varepsilon|^2 + \frac{1}{\varepsilon^2}V(\mathbf{x})|\phi^\varepsilon|^2 + \frac{\beta\varepsilon^d}{2}|\phi^\varepsilon|^4\right. \\ &\qquad \left.+\frac{\delta\varepsilon^{2+d}}{2}\left|\nabla|\phi^\varepsilon|^2\right|^2\right]d\mathbf{x} \\ &= \frac{1}{\varepsilon^2}\int_{\mathbb{R}^d}\left[\frac{\varepsilon^4}{2}|\nabla\phi^\varepsilon|^2 + V(\mathbf{x})|\phi^\varepsilon|^2 + \frac{\beta\varepsilon^{d+2}}{2}|\phi^\varepsilon|^4\right. \\ &\qquad \left.+\frac{\delta\varepsilon^{4+d}}{2}\left|\nabla|\phi^\varepsilon|^2\right|^2\right]d\mathbf{x},\end{aligned} \tag{3.36}$$

which indicates that the ground state of (2.1) is equivalent to the ground state of the following energy functional $E^\varepsilon(\cdot)$ under the constraint $\phi^\varepsilon \in S$ through relation (3.35),

$$\begin{aligned}E^\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d}&\left[\frac{\varepsilon^4}{2}|\nabla\phi^\varepsilon|^2 + V(\mathbf{x})|\phi^\varepsilon|^2 + \frac{\beta\varepsilon^{d+2}}{2}|\phi^\varepsilon|^4\right. \\ &\left.+\frac{\delta\varepsilon^{4+d}}{2}\left|\nabla|\phi^\varepsilon|^2\right|^2\right]d\mathbf{x}.\end{aligned} \tag{3.37}$$

Now, we give the characterization of the ground state ϕ_g for (2.1) when the two interaction strengths $|\beta|$ and $\delta > 0$ are very large. By comparing the contributions from each term in the energy (3.37) [5], we can identify the following different regimes:

Case 1: $\beta \to +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \ll 1$, i.e. $\delta = o(\beta^{\frac{4+d}{2+d}})$;

Case 2: $\beta \to +\infty$ and $\lim_{\beta\to+\infty}\delta/\beta^{\frac{4+d}{2+d}} = \delta_\infty > 0$;

Case 3: $\beta \to +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \gg 1$, i.e. $\beta = o(\delta^{\frac{2+d}{4+d}})$ as $\delta \to +\infty$;

and for $\beta \to -\infty$

Case 1′: $\beta \to -\infty$ and $\delta/|\beta|^{\frac{4+d}{2+d}} \ll 1$, i.e. $\delta = o(|\beta|^{\frac{4+d}{2+d}})$;

Case 2′: $\beta \to -\infty$ and $\lim_{\beta\to-\infty}\delta/|\beta|^{\frac{4+d}{2+d}} = \delta_\infty > 0$;

Case 3′: $\beta \to -\infty$ and $\delta/|\beta|^{\frac{4+d}{2+d}} \gg 1$, i.e. $|\beta| = o(\delta^{\frac{2+d}{4+d}})$ as $\delta \to +\infty$.

Intuitively, for cases 1 and 1′, the β cubic term in (3.37) is dominant and determines the length scale ε^{-1} of the ground state, which increases ($\varepsilon \to 0^+$) for growing repulsive interactions $\beta \to +\infty$. For growing attractive interactions $\beta \to -\infty$ in case 1′, it is readily to check that only the cubic β term (attractive) and the δ term (repulsive) are important, where the length scale ε could go to 0 or $+\infty$ (see Theorem 3.3). For cases 3 and 3′, the δ higher order interaction term in (3.37) is dominant and the length scale $\varepsilon \to 0^+$ as $\delta \to +\infty$. For cases 2 and 2′, the δ higher order interaction term and the β cubic term are comparable and the length scale $\varepsilon \to 0^+$. As shown later, the energy E^ε (3.37) with proper choice of ε ($\varepsilon \to 0^+$ for cases 1, 2, 3, 2′ and 3′; $\varepsilon \to +\infty$ for case 1′ and consider $E^\varepsilon/(\beta\varepsilon^{d+2})$) converges to the following functionals,

$$E_1(\phi) = \int_{\mathbb{R}^d}\left(V(\mathbf{x})|\phi|^2 + \frac{1}{2}|\phi|^4\right)d\mathbf{x}, \quad \text{for case 1,} \tag{3.38}$$

$$E_2(\phi) = \int_{\mathbb{R}^d}\left(V(\mathbf{x})|\phi|^2 + \frac{|\phi|^4}{2} + \frac{\delta_\infty}{2}|\nabla|\phi|^2|^2\right)d\mathbf{x}, \quad \text{for case 2,} \tag{3.39}$$

$$E_3(\phi) = \int_{\mathbb{R}^d}\left(V(\mathbf{x})|\phi|^2 + \frac{1}{2}|\nabla|\phi|^2|^2\right)d\mathbf{x}, \quad \text{for case 3 and 3′,} \tag{3.40}$$

$$E_{2'}(\phi) = \int_{\mathbb{R}^d}\left(V(\mathbf{x})|\phi|^2 - \frac{1}{2}|\phi|^4 + \frac{\delta_\infty}{2}\left|\nabla|\phi|^2\right|^2\right)d\mathbf{x}, \quad \text{for case 2′,} \tag{3.41}$$

$$E_{1'}(\phi) = \int_{\mathbb{R}^d}\left(\frac{1}{2}\left|\nabla|\phi|^2\right|^2 - \frac{1}{2}|\phi|^4\right)d\mathbf{x}, \quad \text{for case 1′,} \tag{3.42}$$

under the constraint

$$\|\phi\| = 1. \tag{3.43}$$

The limiting profiles of the ground state (2.1) can be proved to be the minimizers of the above energy functionals (3.38)–(3.42) with constraint $\|\phi\| = 1$ in different cases under proper scaling factor ε.

First of all, we investigate some basic properties of the limiting profiles, i.e. the minimizer of the energy functionals (3.38)–(3.42) under (3.43).

Theorem 3.1 (*Properties of the Limiting Profiles*). *Assume $0 \le V(\mathbf{x}) \in L^\infty_{\text{loc}}(\mathbb{R}^d)$ ($d = 1, 2, 3$) satisfies $\lim_{|\mathbf{x}|\to\infty}V(\mathbf{x}) = +\infty$, for each energy functional (3.38)–(3.42) with constraint (3.43), there exists a nonnegative minimizer $\sqrt{\rho_g} = \phi_g$ with $\|\phi_g\| = 1$ and such nonnegative minimizer is unique for (3.38)–(3.40). We denote the density $\rho_g = |\phi_g|^2$ and $\rho_g \ge 0$ with $\|\rho_g\|_{L^1} = 1$. The following properties for the minimizer ϕ_g (or density ρ_g) hold.*

(1) For (3.38), the density ρ_g is given by $\rho_g = \max\{\mu - V(\mathbf{x}), 0\}$ with $\mu = E_1(\sqrt{\rho_g}) + \frac{1}{2}\|\rho_g\|^2_{L^2}$ and $\|\rho_g\|_{L^1} = 1$.

(2) For (3.39), $\rho_g \in C^{1,\alpha}_{\text{loc}} \subset W^{2,p}_{\text{loc}}$ ($1 < p < \infty$ and $\alpha < 1$) solves the free boundary value problems

$$-\delta_\infty\Delta\rho_g + \rho_g = (\mu - V(\mathbf{x}))\,\chi_{\{\rho_g>0\}}, \tag{3.44}$$

where $\mu = 2E_2(\sqrt{\rho_g}) - \int_{\mathbb{R}^d}V(\mathbf{x})\rho_g d\mathbf{x}$. The conditions at the free boundaries are

$$\rho_g|_{\partial\{\rho_g>0\}} = 0, \quad |\nabla\rho_g||_{\partial\{\rho_g>0\}} = 0. \tag{3.45}$$

If $V(\mathbf{x})$ is radially increasing, we have that $\rho_g(\mathbf{x})$ is radially decreasing and compactly supported.

(3) For (3.40), $\rho_g \in C^{1,\alpha}_{\text{loc}} \subset W^{2,p}_{\text{loc}}$ ($1 < p < \infty$ and $\alpha < 1$) solves the free boundary value problems

$$-\delta_\infty\Delta\rho_g = (\mu - V(\mathbf{x}))\,\chi_{\{\rho_g>0\}}, \tag{3.46}$$

where $\mu = 2E_3(\sqrt{\rho_g}) - \int_{\mathbb{R}^d}V(\mathbf{x})\rho_g\, d\mathbf{x}$. The conditions at the free boundaries are given as (3.45). If $V(\mathbf{x})$ is radially increasing, $\rho_g(\mathbf{x})$ is radially decreasing and compactly supported.

(4) For (3.42), there exists a non-increasing radially symmetric minimizer ϕ_g which is unique and compactly supported. The density $\rho_g = |\phi_g|^2 \in C^{1,\alpha}_{\text{loc}} \subset W^{2,p}_{\text{loc}}$ ($1 < p < \infty$ and $\alpha < 1$). In fact, ρ_∞ solves the equation

$$-\Delta\rho_g - \rho_g = \mu\chi_{\{\rho_g>0\}}, \quad \mu = 2E_{1'}(\sqrt{\rho_g}). \tag{3.47}$$

Proof. The existence and uniqueness results (except for (3.42)) are straightforward following Theorem 2.1 and the conventional GPE case [6,31]. We omit the details here and the proof for (3.42) will be shown below.

(1) It is the classical TF density [31].

(2) We first show (3.44) is valid. We adapt an approach for the classical obstacle problem in [36]. Since $\rho_g \ge 0$ minimizes $E_2(\sqrt{\rho})$ under the constraints $\|\rho\|_{L^1} = 1$ and $\rho \ge 0$, in addition $V(\mathbf{x}) \ge 0$, we can conclude that ρ_g minimizes the following energy

$$\tilde{E}(\rho) = \int_{\mathbb{R}^d}\left(V(\mathbf{x})|\rho| + \frac{\rho^2}{2} + \frac{\delta_\infty}{2}|\nabla\rho|^2\right)d\mathbf{x}, \quad \int_{\mathbb{R}^d}\rho(\mathbf{x})\,d\mathbf{x} = 1, \tag{3.48}$$

i.e. ρ_g is still a minimizer if we remove the nonnegative constraint with the price to have a non-smooth $V(\mathbf{x})|\rho|$ term. The reason is that if $\int_{\mathbb{R}^d}\rho(\mathbf{x})\,d\mathbf{x} = 1$, we can write $\rho_+(\mathbf{x}) = \max\{\rho(\mathbf{x}), 0\}$ and $\rho_-(\mathbf{x}) = \max\{-\rho(\mathbf{x}), 0\}$, and $\int_{\mathbb{R}^d}\rho_+(\mathbf{x}) \ge 1$. Since all the terms in energy $\tilde{E}(\rho)$ are positive, we have $\tilde{E}(\rho_+/\|\rho_+\|_{L^1}) \le \tilde{E}(\rho_+) \le \tilde{E}(\rho)$. Thus, the minimizer must be nonnegative and the unique minimizer of (3.48) (by convexity) is ρ_g.

Now, we would like to derive the equation for ρ_g. In order to do this, we introduce the following regularization of (3.48). Mollify the step function $\chi_{[0,\infty)}(s)$ ($s \in \mathbb{R}$) to get smooth function $g_\varepsilon(s) \in C^\infty(\mathbb{R})$ ($\varepsilon > 0$) such that $g_\varepsilon(s) = 1$ if $s > 0$, $g_\varepsilon(s) = 0$ if $s \le -\varepsilon$ and $g'_\varepsilon(s) \ge 0$ for all $s \in \mathbb{R}$. Moreover, $g_\varepsilon(s) \to \chi_{(0,\infty)}$ as $\varepsilon \to 0^+$. Denote $G_\varepsilon(s) = \int_{-\infty}^s g_\varepsilon(s)\,ds$ and $G'' \ge 0$ indicating that G_ε is a convex function. Now, let us consider

$$\tilde{E}^\varepsilon(\rho) = \int_{\mathbb{R}^d}\left(V(\mathbf{x})G_\varepsilon(\rho(\mathbf{x})) + \frac{\rho^2}{2} + \frac{\delta_\infty}{2}|\nabla\rho|^2\right)d\mathbf{x}, \qquad \int_{\mathbb{R}^d}\rho(\mathbf{x})\,d\mathbf{x} = 1, \tag{3.49}$$

which is still a convex minimization problem and we have a unique minimizer $\rho_g^\varepsilon(\mathbf{x}) \ge 0$. Moreover, we can find the equations for $\rho_g^\varepsilon(\mathbf{x})$.

For any compactly supported smooth function $\varphi \in C_c^\infty(\mathbb{R}^d)$, consider $h(s) = \tilde{E}^\varepsilon(\rho_s(\mathbf{x}))$ where $\rho_s(\mathbf{x}) = (\rho_g^\varepsilon + s\varphi)/\int_{\mathbb{R}^d}(\rho_g^\varepsilon + s\varphi)\,d\mathbf{x}$ and $s \in (-s_0, s_0)$ with sufficiently small $s_0 > 0$ such that $\int_{\mathbb{R}^d}(\rho_g^\varepsilon + s\varphi)\,d\mathbf{x} \ge 1/2$, we then have $h(s)$ attains its minimum at $s = 0$. By standard computations and arguments [34,37], we can get that there exists a Lagrangian multiplier μ_ε, such that ρ_g^ε solves (in the weak sense)

$$-\delta_\infty\Delta\rho_g^\varepsilon + \rho_g^\varepsilon = \mu^\varepsilon - V(\mathbf{x})g_\varepsilon(\rho_g^\varepsilon). \tag{3.50}$$

It is easy to see that μ^ε is uniformly bounded and $\mu^\varepsilon - V(\mathbf{x})g_\varepsilon(\rho_g^\varepsilon) \in L^\infty_{\mathrm{loc}}$, which implies that for any bounded smooth domain $\Omega \subset \mathbb{R}^d$, ρ_g^ε is uniformly bounded in $W^{2,p}(\Omega)$ $(p \in (1,p))$ by classical elliptic regularity results [34,37]. Using Sobolev embedding, ρ_g^ε is uniformly bounded in $C^{1,\alpha}(\Omega)$ (for some $0 < \alpha < 1$) locally and hence there exist $\tilde{\rho} \in W^{2,p}(\Omega)$ such that as $\varepsilon \to 0^+$ (take a subsequence $\varepsilon_k \to 0^+$ if necessary), ρ_g^ε converges to $\tilde{\rho}$ strongly in $C^{1,\alpha}_{\mathrm{loc}}$ and weakly in $W^{2,p}_{\mathrm{loc}}$. Consequently, $\tilde{\rho} \ge 0$ and $\|\tilde{\rho}\|_{L^1} = 1$ ($V(\mathbf{x})$ is a confining potential). In fact, we can show $\tilde{\rho} = \rho_g$. Passing to the limit as $\varepsilon \to 0^+$ in $\tilde{E}(\rho_g^\varepsilon) \le \tilde{E}^\varepsilon(\rho_g^\varepsilon) \le \tilde{E}^\varepsilon(\rho_g)$ $(G_\varepsilon(|s|) \ge |s|)$, we observe that $\tilde{E}(\tilde{\rho}) \le \limsup_{\varepsilon\to 0^+} \tilde{E}^\varepsilon(\rho_g^\varepsilon) \le \tilde{E}(\rho_g)$ and it is obvious $\tilde{\rho} = \rho_g$.

Now, we have $\rho_g \in W^{2,p}_{\mathrm{loc}} \cap C^{1,\alpha}_{\mathrm{loc}}$ and we want to show that

$$-\delta_\infty \Delta\rho_g + \rho_g = (\mu - V(\mathbf{x}))\chi_{\{\rho_g>0\}}, \quad \text{a.e.} \quad \mathbf{x} \in \mathbb{R}^d. \tag{3.51}$$

Since $\rho_g^\varepsilon \in W^{2,p}_{\mathrm{loc}}$ is a strong solution of (3.50), (3.50) is valid almost everywhere. In addition, $\rho_g^\varepsilon \to \rho_g$ in $C^{1,\alpha}_{\mathrm{loc}}$, so we can pass to the limit as $\varepsilon \to 0^+$ in (3.50) to get

$$-\delta_\infty \Delta\rho_g + \rho_g = \mu - V(\mathbf{x}), \quad \text{a.e.} \quad \mathbf{x} \in \{\rho_g > 0\}, \tag{3.52}$$

where μ is a limiting point of μ_ε as $\varepsilon \to 0^+$ (take a subsequence if necessary here). On the other hand, $\rho_g \in W^{2,p}_{\mathrm{loc}}$ implies $\Delta\rho_g = 0$ a.e. $\mathbf{x} \in \{\rho_g = 0\}$. Together, we have shown ρ_g is the solution of the free boundary value problem (3.44) and μ can be computed via multiplying both sides of (3.44) by ρ_g and integrating over $\mathbb{R}^d$.

When $V(\mathbf{x}) = V(r)$ $(r = |\mathbf{x}|)$ is radially increasing, it is easy to find $\rho_g(\mathbf{x})$ is radially decreasing by Schwarz rearrangement [34,38,39]. Here we would like to show such ground state is compactly supported. For simplicity, we write $\rho_g(\mathbf{x}) = \rho_g(|\mathbf{x}|) = \rho_g(r)$ $(r = |\mathbf{x}|)$ and $\rho_g'(r) \le 0$. Integrating (3.44) over ball $B_R = \{|\mathbf{x}| < R\}$, we get

$$\int_{B_R} \left(V(\mathbf{x})\chi_{\{\rho_g>0\}} + \rho_g(\mathbf{x})\right) d\mathbf{x} - \delta_\infty \int_{\partial B_R} \partial_n\rho_g(\mathbf{x}) dS = \mu \int_{B_R} \chi_{\{\rho_g>0\}}\, d\mathbf{x},$$

where $\partial_n\rho_g(\mathbf{x})|_{\partial B_R} \le 0$ ($\rho_g(r)$ is non-increasing). On the other hand, $\lim_{r\to\infty} V(r) = \infty$, choosing R_0 large enough such that $V(r) \ge 2\mu$ $(r \ge R_0)$, we have

$$\int_{B_R\setminus B_{R_0}} \left[(V(\mathbf{x}) - \mu)\chi_{\{\rho_g>0\}} + \rho_g(\mathbf{x})\right] d\mathbf{x} \le \mu|B_{R_0}|,$$

which is true for all $R > 0$. Thus, we arrive at

$$|B^c_{R_0} \cap \chi_{\{\rho_g>0\}}| \le |B_{R_0}|, \tag{3.53}$$

and it implies that $|\{\rho_g > 0\}| < \infty$. Therefore ρ_g is compactly supported.

(3) The proof is quite similar to the proof of item (2) and is omitted for brevity.

(4) We show the fact that the decreasing radially symmetric minimizer ρ_∞ of (3.42) exists and is unique. In view of Nash inequality, $E_{1'}(\sqrt{\rho})$ is bounded from below under constraint $\|\rho\|_{L^1} = 1$ with $\rho \ge 0$. By Schwarz rearrangement, we can take a minimizing sequence of non-increasing radially symmetric functions $\{\rho_n\}_{n=1}^\infty$ where $\|\rho_n\|_{L^1} = 1$ and $\|\rho_n\|_{H^1} \le C$. Therefore, there exists $\rho_\infty \in H^1$ such that a subsequence (denoted as the original sequence) $\rho_n \to \rho_\infty$ weakly in H^1. In addition, for the non-increasing radially symmetric function ρ_n,

$$|\rho_n(\mathbf{x})| \le \frac{C}{R^d}\|\rho_n\|_{L^1} \le \frac{C}{R^d}, \quad |\mathbf{x}| \ge R > 0, \tag{3.54}$$

which would imply $\rho_n \to \rho_\infty$ strongly in L^2 and so $\rho_\infty \ge 0$ with $\|\rho_\infty\|_{L^1} \le 1$. In fact, we can show $\|\rho_\infty\|_{L^1} = 1$. Denote $I_\alpha = \inf_{\rho\ge 0, \|\rho\|_{L^1}=\alpha} E_{1'}(\rho)$ $(\alpha > 0)$, then it is obvious $I_\alpha = \alpha^2 I_1$. For any $\rho \ge 0$ with $\|\rho\|_{L^1} = 1$, denote $\rho_\eta = \eta^{-d}\rho(\mathbf{x}/\eta)$ $(\eta > 0)$ and we have $\|\rho_\eta\|_{L^1} = 1$ and $E_{1'}(\rho_\eta) = \frac{1}{2\eta^{d+2}}\|\nabla\rho\|^2 - \frac{1}{2\eta^d}\|\rho\|^2 < 0$ for $\eta > \|\nabla\rho\|/\|\rho\|$, which immediately suggests that $I_1 < 0$. If $\|\rho_\infty\|_{L^1} = \alpha < 1$, by the convergence of ρ_n, we get

$$\alpha^2 I_1 = I_\alpha \le E_{1'}(\sqrt{\rho_\infty}) \le \liminf_{n\to+\infty} E_{1'}(\sqrt{\rho_n}) = I_1, \tag{3.55}$$

which leads to $I_1 \ge 0$ contradicting to the fact $I_1 < 0$. Thus $\|\rho_\infty\|_{L^1} = 1$ and ρ_∞ is a non-increasing radially symmetric minimizer of (3.42). Next, we show such minimizer is unique. Following Theorem 3.1, we can get the equations for the minimizers of (3.42) as

$$-\Delta\rho - \rho = \mu\chi_{\{\rho>0\}}, \tag{3.56}$$

and a non-increasing radially symmetric minimizer ρ is compactly supported with the regularity stated in Theorem 3.1. If there are two non-increasing radially symmetric minimizers ρ_1 and ρ_2 to the energy (3.42), we have

$$-\Delta\rho_1 - \rho_1 = \mu_1\chi_{\{\rho_1>0\}}, \quad -\Delta\rho_2 - \rho_2 = \mu_2\chi_{\{\rho_2>0\}},$$

and $\mu_1 = \mu_2 = 2I_1$ (multiplying both sides of the equation by ρ_j, j=1,2, and integrate). Thus, by integrating the equations, we know ρ_1 and ρ_2 have the same supports (denote as the ball B_R). $\rho_1 = \rho_2$ is then a consequence of classical ODE theory by noticing that $\rho_j(R) = \partial_r\rho_j(R) = 0$. The existence and uniqueness of non-increasing radially symmetric minimizers are proved. □

Below, we specify the convergence towards the limiting profiles in Theorem 3.1 in different cases.

Theorem 3.2 (*positive β limit*)**.** *Let $V(\mathbf{x})$ $(\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3)$ be given in (1.4), $\delta > 0$, $\phi_g \in S$ be the positive ground state of (2.1), and $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2}\phi_g(\mathbf{x}/\varepsilon) \in S$ for some $\varepsilon > 0$ depending on β and δ.*

(1) For Case 1, i.e. $\beta \to +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \ll 1$, set $\varepsilon = \beta^{-\frac{1}{2+d}}$. For $\beta \to +\infty$ $(\varepsilon \to 0^+)$, we have

$$\rho_g^\varepsilon = |\phi_g^\varepsilon(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) = |\phi_\infty(\mathbf{x})|^2 \text{ in } L^2, \tag{3.57}$$

where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy (3.38).

(2) For Case 2, i.e. $\beta \to +\infty$ and $\lim_{\beta\to+\infty}\delta/\beta^{\frac{4+d}{2+d}} = \delta_\infty > 0$, set $\varepsilon = \beta^{-\frac{1}{2+d}}$. For $\delta \to +\infty$ $(\varepsilon \to 0^+)$, we have

$$\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) = |\phi_\infty(\mathbf{x})|^2 \text{ in } H^1, \tag{3.58}$$

where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy (3.39).

(3) For Case 3, i.e. $\beta \to +\infty$ and $\delta/\beta^{\frac{4+d}{2+d}} \gg 1$, set $\varepsilon = \delta^{-\frac{1}{4+d}}$. For $\delta \to +\infty$ $(\varepsilon \to 0^+)$, we have

$$\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) = |\phi_\infty(\mathbf{x})|^2 \text{ in } H^1, \tag{3.59}$$

where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy (3.40).

Proof. We separate the three cases.

(1) Using (3.37) and choosing $\varepsilon = \beta^{-1/(d+2)}$, we find $\phi_g^\varepsilon \in S$ minimizes

$$E^\varepsilon(\phi^\varepsilon) = \int_{\mathbb{R}^d}\left[\frac{\varepsilon^4}{2}|\nabla\phi^\varepsilon|^2 + V(\mathbf{x})|\phi^\varepsilon|^2 + \frac{|\phi^\varepsilon|^4}{2} + \frac{\delta\varepsilon^{4+d}}{2}\left|\nabla|\phi^\varepsilon|^2\right|^2 d\mathbf{x}\right]. \tag{3.60}$$

On the other hand, $E_1(\phi)$ has a unique nonnegative minimizer ϕ_∞ and by an approximation argument, we can take any smooth approximation of $\phi_\infty(\mathbf{x})$ in S and find that for any $\eta > 0$ with $\delta = o(\beta^{\frac{d+4}{d+2}})$

$$E_1(\phi_\infty) \le E^\varepsilon(\phi_g^\varepsilon) \le E_1(\phi_\infty) + \eta + C(\eta)(\varepsilon^4 + o(1)),$$

which implies

$$\lim_{\varepsilon\to 0^+} E_1(\phi_g^\varepsilon) = E_1(\phi_\infty). \tag{3.61}$$

Hence we know ϕ_g^ε ($\varepsilon \to 0^+$) is a minimizing sequence for $E_1(\cdot)$. On the other hand,

$$\begin{aligned}
&E_1(\phi_g^\varepsilon) - E_1(\phi_\infty)\\
&= \int_{\mathbb{R}^d} \left[(V(\mathbf{x}) + |\phi_\infty|^2)(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2) + \frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2\right] d\mathbf{x}\\
&= \int_{\mathbb{R}^d} \left[\max\{V(\mathbf{x}), \mu\}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2) + \frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2\right] d\mathbf{x}\\
&\geq \int_{\mathbb{R}^d} \left[\mu|\phi_g^\varepsilon|^2 - \mu|\phi_\infty|^2 + \frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2\right] d\mathbf{x}\\
&= \frac{1}{2}\int_{\mathbb{R}^d} (|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 d\mathbf{x},
\end{aligned}$$

and the conclusion follows.

(2) Similar to the part (1), it is easy to show $\lim_{\varepsilon\to 0^+} E_2(\phi_g^\varepsilon) = E_2(\phi_\infty)$. Noticing that for any function $0 \leq \sqrt{\rho(\mathbf{x})} \in H^1$ with $\int_{\mathbb{R}^d} \rho(\mathbf{x}) = 1$, we have $E_2(\sqrt{(\rho_\infty + s\rho)/(1+s)})$ ($s \geq 0$) attains minimum at $s = 0$. By direct computation, we find

$$\begin{aligned}
&\frac{d}{ds}E_2\left(\sqrt{\frac{\rho_\infty + s\rho}{1+s}}\right)\Bigg|_{s=0}\\
&= \int_{\mathbb{R}^d} (V(\mathbf{x})\rho(\mathbf{x}) + \rho_\infty(\mathbf{x})\rho(\mathbf{x}) + \delta_\infty \nabla\rho_\infty(\mathbf{x}) \cdot \nabla\rho(\mathbf{x}))\, d\mathbf{x}\\
&\quad - \int_{\mathbb{R}^d} (V(\mathbf{x})\rho_\infty(\mathbf{x}) + \rho_\infty^2(\mathbf{x}) + \delta_\infty|\nabla\rho_\infty(\mathbf{x})|^2)\, d\mathbf{x}\\
&\geq 0.
\end{aligned}$$

A simple calculation shows

$$\begin{aligned}
&E_2(\phi_g^\varepsilon) - E_2(\phi_\infty)\\
&= \frac{d}{ds}E_2\left(\sqrt{\frac{\rho_\infty + s\rho^\varepsilon}{1+s}}\right)\Bigg|_{s=0}\\
&\quad + \int_{\mathbb{R}^d} \left[\frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 + \frac{\delta_\infty}{2}(\nabla|\phi_g^\varepsilon|^2 - \nabla|\phi_\infty|^2)^2\right] d\mathbf{x}\\
&\geq \int_{\mathbb{R}^d} \left[\frac{1}{2}(|\phi_g^\varepsilon|^2 - |\phi_\infty|^2)^2 + \frac{\delta_\infty}{2}(\nabla|\phi_g^\varepsilon|^2 - \nabla|\phi_\infty|^2)^2\right] d\mathbf{x},
\end{aligned}$$

which implies $\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2$ converges to $\rho_\infty(\mathbf{x})$ in H^1.

(3) Using (3.37) and choosing $\varepsilon = \delta^{-\frac{1}{4+d}}$, we find $\phi_g^\varepsilon \in S$ minimizes

$$\begin{aligned}
&E^\varepsilon(\phi^\varepsilon)\\
&= \int_{\mathbb{R}^d} \left[\frac{\varepsilon^4}{2}|\nabla\phi^\varepsilon|^2 + V(\mathbf{x})|\phi^\varepsilon|^2 + \frac{\beta\varepsilon^{d+2}|\phi^\varepsilon|^4}{2} + \frac{1}{2}\left|\nabla|\phi^\varepsilon|^2\right|^2\right] d\mathbf{x}.
\end{aligned} \tag{3.62}$$

Nash inequality and Young inequality imply that for $\rho^\varepsilon = |\phi^\varepsilon|^2$ ($\phi^\varepsilon \in S$),

$$\int_{\mathbb{R}^d} |\rho^\varepsilon(\mathbf{x})|^2\, d\mathbf{x} \leq C\|\rho^\varepsilon\|_{L^1}^{4/d+2}\|\nabla\rho^\varepsilon\|^{2d/d+2} \leq C + \|\nabla\rho^\varepsilon\|^2.$$

Thus, we conclude that for $\beta = o(\delta^{\frac{2+d}{4+d}})$,

$$E^\varepsilon(\phi^\varepsilon) \geq \int_{\mathbb{R}^d} \left(V(\mathbf{x})|\phi^\varepsilon|^2 + \frac{1}{2}(1 - o(1))|\nabla|\phi^\varepsilon|^2|^2\right) d\mathbf{x} - o(1), \quad \phi^\varepsilon \in S. \tag{3.63}$$

For sufficient small ε, (3.63) gives that for the ground state ϕ_g^ε,

$$E_3(\phi_g^\varepsilon) \leq C, \tag{3.64}$$

and we obtain

$$E^\varepsilon(\phi_g^\varepsilon) \geq E_3(\phi_g^\varepsilon) - o(1). \tag{3.65}$$

Choosing smooth approximations of ϕ_∞ in S if necessary, we could get for any $\eta > 0$,

$$E^\varepsilon(\phi_g^\varepsilon) \leq E_3(\phi_\infty) + \eta + C(\eta)(\varepsilon^4 + o(1)). \tag{3.66}$$

Combining (3.65), (3.66) and the fact that ϕ_∞ minimizes E_3 under the constraint $\|\phi\| = 1$, we find that

$$\lim_{\varepsilon\to 0^+} E_3(\phi_g^\varepsilon) = E_3(\phi_\infty). \tag{3.67}$$

On the other hand, $E_3(\sqrt{(\rho_\infty + s\rho_g^\varepsilon)/(1+s)})$ ($s \geq 0$) reach its minimum at $s = 0$, and

$$\begin{aligned}
0 &\leq \frac{d}{ds}E_3\left(\sqrt{\frac{\rho_\infty + s\rho_g^\varepsilon}{1+s}}\right)\Bigg|_{s=0}\\
&= \int_{\mathbb{R}^d} \left(\rho_g^\varepsilon V(\mathbf{x}) + \nabla\rho_g^\varepsilon \cdot \nabla\rho_\infty\right) d\mathbf{x}\\
&\quad - \int_{\mathbb{R}^d} (\rho_\infty V(\mathbf{x}) + \nabla\rho_\infty \cdot \nabla\rho_\infty)\, d\mathbf{x}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&E_3(\phi_g^\varepsilon) - E_3(\phi_\infty)\\
&= \int_{\mathbb{R}^d} \left((\rho_g^\varepsilon - \rho_\infty)V + \nabla(\rho_g^\varepsilon - \rho_\infty)\cdot\nabla\rho_\infty\right) d\mathbf{x} + \frac{1}{2}\|\nabla\rho_g^\varepsilon - \nabla\rho_\infty\|^2\\
&\geq \frac{1}{2}\|\nabla\rho_g^\varepsilon - \nabla\rho_\infty\|^2.
\end{aligned}$$

The convergence of ρ_g^ε towards ρ_∞ as $\varepsilon \to 0^+$ is then a direct consequence. □

Theorem 3.2 concerns about the case $\beta > 0$. However, as shown in Theorem 2.1, the ground state exists for negative β as long as δ is positive. Now we consider the interesting cases when $\beta \to -\infty$ with $\delta \to +\infty$ in different ways.

Theorem 3.3 (*Negative β limit*)**.** *Let $V(\mathbf{x})$ ($\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3$) be given in (1.4), $\beta < 0$, $\delta > 0$, $\phi_g \in S$ be a nonnegative ground state of (2.1) and $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d/2}\phi_g(\mathbf{x}/\varepsilon) \in S$ for some $\varepsilon > 0$ depending on β and δ.*

(1) For case 1′, i.e. $\beta \to -\infty$, $\delta = o(|\beta|^{\frac{4+d}{2+d}})$ as $|\beta| \to \infty$, let $\varepsilon = |\beta|^{1/2}/\delta^{1/2}$, and it can be checked that, when $\beta \to -\infty$, $\varepsilon \gg 1$ if $\delta = o(\beta)$ and $\varepsilon \ll 1$ if $|\beta| \ll \delta$. Assume the potential $V(\mathbf{x})$ is radially symmetric and increasing in $r = |\mathbf{x}|$, then the ground state $\phi_g \in S$ (ϕ_g^ε) can be chosen as a radially symmetric function, which is decreasing in $r = |\mathbf{x}|$. For $\beta \to -\infty$, we have

$$\rho_g^\varepsilon = |\phi_g^\varepsilon|^2 \to \rho_\infty \text{ in } H^1, \tag{3.68}$$

where ρ_∞ is the unique nonnegative minimizer of the energy (3.42) in Theorem 3.1, which is radially symmetric and increasing in $r = |\mathbf{x}|$.

(2) For case 2′, i.e. $\beta \to -\infty$ and $\lim_{\beta\to-\infty}\delta/|\beta|^{\frac{4+d}{2+d}} = \delta_\infty > 0$, set $\varepsilon = |\beta|^{-\frac{1}{2+d}}$. For $\beta \to -\infty$ ($\varepsilon \to 0^+$), there exists a subsequence $\beta_n \to -\infty$ such that for $\varepsilon_n = |\beta_n|^{-\frac{1}{2+d}} \to 0^+$

$$\rho_g^{\varepsilon_n}(\mathbf{x}) \to \rho_g(\mathbf{x}) \text{ in } H^1, \tag{3.69}$$

where $\rho_g(\mathbf{x})$ is a nonnegative minimizer of the energy (3.41).

(3) For case 3′, i.e. $\beta \to -\infty$ and $\delta/|\beta|^{\frac{4+d}{2+d}} \gg 1$, set $\varepsilon = \delta^{-\frac{1}{4+d}}$. For $\delta \to +\infty$ ($\varepsilon \to 0^+$), we have

$$\rho_g^\varepsilon(\mathbf{x}) = |\phi_g^\varepsilon(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) = |\phi_\infty(\mathbf{x})|^2 \text{ in } H^1, \tag{3.70}$$

where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy (3.40).

Proof. (1) Choosing $\varepsilon = |\beta|^{1/2}/\delta^{1/2}$ in (3.37), we find ϕ_g^ε minimizes the following energy

$$E_\eta(\phi) = \int_{\mathbb{R}^d} \left[\frac{\eta_1}{2}|\nabla\phi|^2 + \eta_2 V(\mathbf{x})|\phi|^2 - \frac{1}{2}|\phi|^4 + \frac{1}{2}\left|\nabla|\phi|^2\right|^2 \right] d\mathbf{x}, \quad \phi \in S, \tag{3.71}$$

with $\eta_1 = \frac{\delta^{\frac{d-2}{2}}}{|\beta|^{d/2}} = o(1)$ and $\eta_2 = \frac{\delta^{\frac{d+2}{2}}}{|\beta|^{\frac{4+d}{2}}} = o(1)$ when $\beta \to -\infty$ and $\delta = o(|\beta|^{\frac{4+d}{2+d}})$. Intuitively, only the leading $O(1)$ terms in (3.71) are important in the limit as $\beta \to -\infty$. Under the hypothesis of a radially increasing potential $V(\mathbf{x})$, we have (regularize $\phi_\infty = \sqrt{\rho_\infty}$ such that $\phi_\infty \in H^1$ if necessary)

$$\begin{aligned} E_{1'}(\sqrt{\rho_\infty}) &\le E_{1'}(\sqrt{\rho_g^\varepsilon}) \le E_\eta(\phi_g^\varepsilon) \le E_\eta(\sqrt{\rho_\infty}) \\ &\le o(1) + E_{1'}(\sqrt{\rho_\infty}), \end{aligned} \tag{3.72}$$

which shows $\lim_{\beta\to-\infty} E_{1'}(\sqrt{\rho_g^\varepsilon}) = E_{1'}(\sqrt{\rho_\infty}) = I_1$. Similar to the proof of part (4) in Theorem 3.1, by using the radially decreasing property of ρ_g^ε which is a minimizing sequence for the energy $E_{1'}$, it is straightforward to check that as $\beta \to -\infty$, ρ_g^ε converges to some radially decreasing function ρ_0 weakly in H^1 and strongly in L^2, $\|\nabla\rho_g^\varepsilon\| \to \|\nabla\rho_0\|$ and $\|\rho_0\|_{L^1} = 1$. Therefore, $\rho_g^\varepsilon \to \rho_0$ in H^1 and ρ_0 is the unique radially decreasing minimizer of energy $E_{1'}$ (3.42).

(2) Let $\varepsilon = |\beta|^{-1/(d+2)}$ and $\rho_g^\varepsilon(\mathbf{x}) = \varepsilon^{-d}|\phi_g(\mathbf{x}/\varepsilon)|^2$ where $\phi_g(\mathbf{x})$ is a ground state of (2.1), then $\sqrt{\rho_g^\varepsilon} \in S$ is a ground state of (3.37). Using Nash inequality with the fact $\sqrt{\rho_g^\varepsilon} \in S$, we can easily find

$$\int_{\mathbb{R}^d} V(\mathbf{x})\rho_g^\varepsilon(\mathbf{x})\,d\mathbf{x} + \|\nabla\rho_g^\varepsilon\| + \|\rho_g^\varepsilon\| \le C. \tag{3.73}$$

We can extract a subsequence $\varepsilon_n \to 0$, such that for some $\rho_0 \in H^1$, we have

$$\begin{aligned} &\rho_g^{\varepsilon_n} \to \rho_0, \quad \text{weakly in } H^1, \quad \text{weakly} - \star \quad \text{in} \\ &L_V^1 = \{\rho | \int_{\mathbb{R}^d} V(\mathbf{x})|\rho|\,dx < +\infty\}, \end{aligned} \tag{3.74}$$

and

$$\begin{aligned} &\int_{\mathbb{R}^d} V(\mathbf{x})\rho_0(\mathbf{x}) + \|\nabla\rho_0\| + \|\rho_0\| \\ &\le \liminf_{\varepsilon_n\to0^+}\left(\int_{\mathbb{R}^d} V(\mathbf{x})\rho_g^{\varepsilon_n}(\mathbf{x}) + \|\nabla\rho_g^{\varepsilon_n}\| + \|\rho_g^{\varepsilon_n}\|\right). \end{aligned}$$

We then show that the convergence is strong in L^2. For any $\eta > 0$, there exists $R > 0$ such that $\int_{|\mathbf{x}|>R} \rho_g^{\varepsilon_n}(\mathbf{x})\,d\mathbf{x} < \eta$ (confining property of $V(\mathbf{x})$). Since $H^1(B_R) \hookrightarrow L^2(B_R)$ is compact, $\int_{|\mathbf{x}|\le R}|\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^2\,d\mathbf{x} \to 0$ and

$$\begin{aligned} &\limsup_{\varepsilon_n\to0}\|\rho_g^{\varepsilon_n} - \rho_0\|^2 \\ &= \limsup_{\varepsilon_n\to0}\int_{|\mathbf{x}|\le R}|\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^2\,d\mathbf{x} \\ &\quad + \limsup_{\varepsilon_n\to0}\int_{|\mathbf{x}|>R}|\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^2\,d\mathbf{x} \\ &\le \limsup_{\varepsilon_n\to0}\left(\int_{|\mathbf{x}|>R}|\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|\,d\mathbf{x}\right)^{\frac{1}{2}} \\ &\quad \times \left(\int_{|\mathbf{x}|>R}|\rho_g^{\varepsilon_n}(\mathbf{x}) - \rho_0(\mathbf{x})|^3\,d\mathbf{x}\right)^{\frac{1}{2}} \\ &\le C\eta^{1/2}. \end{aligned}$$

Hence $\limsup_{\varepsilon_n\to0}\|\rho_g^{\varepsilon_n} - \rho_0\|^2 = 0$ and $\rho_g^{\varepsilon_n} \to \rho_0$ in L^2, which implies that $\rho_0(\mathbf{x}) \ge 0$. Similarly, due to the confining property of $V(\mathbf{x})$, $\|\rho_0\|_{L^1} = 1$. In particular, regularizing the minimizer of $E_{2'}(\cdot)$ (3.41) if necessary, we have

$$E_{2'}(\sqrt{\rho_0}) \le \liminf_{\varepsilon^n\to0} E_{2'}(\sqrt{\rho_g^{\varepsilon_n}}) \le \limsup_{\varepsilon^n\to0} E^{\varepsilon_n}(\sqrt{\rho_g^{\varepsilon_n}}) \le E^{\varepsilon_n}(\sqrt{\rho_0}),$$

and $E^{\varepsilon_n}(\sqrt{\rho_0}) \le E_{2'}(\sqrt{\rho_0}) + o(1)$, which verifies ρ_0 is a minimizer of $E_{2'}(\cdot)$ (3.41) as well as $\|\nabla\rho_g^{\varepsilon_n}\| \to \|\nabla\rho_0\|$. Thus, $\rho_g^{\varepsilon_n} \to \rho_0$ in H^1.

(3) The proof is similar to part (1), in view of the fact that the minimizer of (3.40) is unique. □

3.2. Vanishing higher order effect

In this subsection, we consider the case $\delta \to 0^+$, i.e. the vanishing higher order effects. For fixed β, we denote ϕ_g^δ to be the non-negative ground state corresponding to $\delta > 0$. When $\delta = 0$, the MGPE degenerates to the GPE case, and the ground state exists [6] if $\beta \ge 0$ when $d = 3$, or $\beta > -C_b$ when $d = 2$, or $\beta \in \mathbb{R}$ when $d = 1$, and C_b is defined as [32,40]

$$C_b := \inf_{0\ne f\in H^1(\mathbb{R}^2)} \frac{\|\nabla f\|_{L^2(\mathbb{R}^2)}^2 \|f\|_{L^2(\mathbb{R}^2)}^2}{\|f\|_{L^4(\mathbb{R}^2)}^4} = \pi\cdot(1.86225\ldots). \tag{3.75}$$

It is obvious that, in such cases, there exists a subsequence $\delta_n \to 0$ ($n = 1, 2, \ldots$), such that $\phi_g^{\delta_n}(\mathbf{x}) \to \phi_g(\mathbf{x})$ in H^1, where $\phi_g(\mathbf{x})$ is a nonnegative minimizer of the energy

$$E_{\mathrm{GP}}(\phi) = \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\phi|^2 + V(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4\right]d\mathbf{x}, \quad \|\phi\| = 1 \tag{3.76}$$

Moreover, when $\beta \ge 0$, the nonnegative minimizer ϕ_g of (3.76) is unique and $\phi_g^\delta \to \phi_g$ in H^1 as $\delta \to 0^+$.

A more interesting topic would be to study the cases for β in the regimes where the ground state does not exist when $\delta = 0$. In such cases, it is worth noticing that the ground state profiles will have certain blow-up phenomenon as $\delta \to 0^+$, i.e., the density will concentrate towards a Dirac function. This phenomenon can be characterized by the following theorem.

Theorem 3.4 ($\delta \to 0^+$ *limit*). *Let $V(\mathbf{x})$ ($\mathbf{x} \in \mathbb{R}^d$, $d = 1, 2, 3$) be given in (1.4), $\delta > 0$, $\phi_g^\delta \in S$ be a nonnegative ground state of (2.1).*

(1) When $d = 2$ and $\beta < -C_b$, denoting $\phi_\delta(\mathbf{x}) = \sqrt{\delta}\phi_g^\delta(\sqrt{\delta}\mathbf{x})$, there exists a subsequence $\delta_n \to 0$ such that

$$\phi_{\delta_n}(\mathbf{x}) \to \phi_0(\mathbf{x}) \text{ in } H^1, \tag{3.77}$$

where $\phi_0(\mathbf{x})$ is a nonnegative minimizer of the energy

$$\begin{aligned} &E_\beta(\phi) \\ &= \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\phi|^2 + \frac{\beta}{2}|\phi|^4 + \frac{1}{2}|\nabla|\phi|^2|^2\right]d\mathbf{x}, \ \text{subject to } \|\phi\| = 1. \end{aligned} \tag{3.78}$$

(2) When $d = 3$, $\beta < 0$ and $V(\mathbf{x})$ is radially increasing, the ground state $\phi_g^\delta(\mathbf{x})$ can be chosen as decreasing radially symmetric functions. Let $\rho_\delta(\mathbf{x}) = |\phi_\delta(\mathbf{x})|^2$, where $\phi_\delta(\mathbf{x}) = \delta^{3/4}\phi_g^\delta(\sqrt{\delta}\mathbf{x})$. For $\delta \to 0^+$, we have

$$\rho_\delta \to \rho_0 \text{ in } H^1, \tag{3.79}$$

where ρ_0 is the unique decreasing radially symmetric nonnegative minimizer of the following energy

$$\begin{aligned} &E_r^\beta(\sqrt{\rho}) \\ &= \int_{\mathbb{R}^d}\left[\frac{\beta}{2}|\rho|^2 + \frac{1}{2}|\nabla\rho|^2\right]d\mathbf{x}, \ \text{with } \rho \ge 0 \text{ and } \int_{\mathbb{R}^d}\rho(\mathbf{x})\,d\mathbf{x} = 1. \end{aligned} \tag{3.80}$$

More precisely, $\rho_0 \ge 0$ satisfies the free boundary problem

$$\beta\rho - \Delta\rho = \mu\chi_{\rho>0}, \quad \rho|_{\partial\{\rho>0\}} = |\nabla\rho|\big|_{\partial\{\rho>0\}} = 0, \tag{3.81}$$

where $\mu = 2E_r^\beta(\sqrt{\rho_0})$.

Proof. (1) The existence of the nonnegative minimizer of $E_\beta(\cdot)$ can be proved by a similar argument in Theorem 3.1 for energy $E_{1'}(\cdot)$ and the detail is omitted here. We denote the minimum energy of $E_\beta(\cdot)$ as E_0.

Letting $\varepsilon = \delta^{-1/2}$ in (3.37), it is obvious that $\tilde{\phi}_\delta(\mathbf{x}) \in S$ minimizes the energy

$$\tilde{E}_\delta(\phi) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\phi|^2 + \delta^2 V(\mathbf{x})|\phi|^2 + \frac{\beta}{2}|\phi|^4 + \frac{1}{2}|\nabla|\phi|^2|^2\right] d\mathbf{x}, \quad \phi \in S. \tag{3.82}$$

Now, choosing a ground state $\phi_g \in S$ of (3.78) as a testing state (using a C_0^∞ approximation if necessary for the potential term), we have

$$\delta^2 \int_{\mathbb{R}^d} V(\mathbf{x})|\tilde{\phi}_\delta(\mathbf{x})|^2\, d\mathbf{x} + E_\beta(\tilde{\phi}_\delta) = \tilde{E}_\delta(\tilde{\phi}_\delta) \le \tilde{E}_\delta(\phi_g) \le E_0 + C\delta^2,$$

which implies $\int_{\mathbb{R}^d} V(\mathbf{x})|\tilde{\phi}_\delta(\mathbf{x})|^2\, d\mathbf{x} \le C$. Therefore, we have

$$\int_{\mathbb{R}^d} V(\mathbf{x})|\tilde{\phi}_\delta(\mathbf{x})|^2\, d\mathbf{x} + \|\tilde{\phi}_\delta\|_{H^1} + \|\nabla|\tilde{\phi}_\delta|^2\| \le C.$$

Following the proof in Theorem 2.1, there exist $\phi_0 \in H^1$ with $\|\phi_0\| = 1$ and a subsequence $\delta_n \to 0$ such that $\phi_{\delta_n} \to \phi_0$ strongly in L^2 and weakly in H^1,

$$E_\beta(\phi_0) \le \liminf_{n\to\infty} E_\beta(\tilde{\phi}_{\delta_n}) \le \liminf_{n\to\infty} \tilde{E}_\delta(\tilde{\phi}_{\delta_n}) \le E_0,$$

and ϕ_0 is a minimizer of (3.78). From the above inequality, it is easy to find that $\|\nabla\phi_{\delta_n}\| \to \|\nabla\phi_0\|$ and thus $\phi_{\delta_n} \to \phi_0$ strongly in H^1.

(2) The proof is essentially presented in Theorem 3.3, part (1) and Theorem 3.1, part (4). □

4. Limiting behavior of ground states in bounded domains

In this section, we consider (1.3) defined in a bounded domain $\Omega \subset \mathbb{R}^d$, and the limiting profiles of ground states (2.1) are considered under different sets of parameters δ and β. To simplify the discussion, we choose the external potential as box potential, i.e.

$$V(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in \Omega, \\ +\infty, & \text{otherwise}. \end{cases} \tag{4.83}$$

The energy $E(\cdot)$ (1.6) reduces to

$$E_\Omega(\phi) = \int_\Omega \left[\frac{1}{2}|\nabla\phi|^2 + \frac{\beta}{2}|\phi|^4 + \frac{\delta}{2}\left|\nabla|\phi|^2\right|^2\right] d\mathbf{x}, \tag{4.84}$$

and the ground state ϕ_g is then the minimizer of the energy E_Ω under the constraint $\|\phi\|_{L^2(\Omega)} = 1$. The major difference between the whole space case (Section 3) and the bounded domain case is that the scalings under different sets of parameters are very different. We list the following different regimes for bounded domain:

Case B1: $\beta \to +\infty$ and $\delta = o(\beta)$;
Case B2: $\beta \to +\infty$ and $\lim_{\beta\to+\infty}\delta/\beta = \delta_\infty > 0$;
Case B3: $\beta \to +\infty$ and $\delta/\beta \gg 1$, i.e. $\beta = o(\delta)$ as $\delta \to +\infty$;
and for $\beta \to -\infty$
Case B1′: $\beta \to -\infty$ and $\delta = o(\beta)$;
Case B2′: $\beta \to -\infty$ and $\lim_{\beta\to-\infty}\delta/|\beta| = \delta_\infty > 0$;
Case B3′: $\beta \to -\infty$ and $\delta/|\beta| \gg 1$, i.e. $|\beta| = o(\delta)$ as $\delta \to +\infty$.

Theorem 4.1 (*Thomas–Fermi Limit*). *Let $V(\mathbf{x})$ ($\mathbf{x} \in \Omega$, $d = 1, 2, 3$) be a box potential, $\delta > 0$, and $\phi_g \in S$ be the positive ground state of (2.1).*

(1) For Case B1, i.e. $\beta \to +\infty$ and $\delta = o(\beta)$, we have

$$\rho_g^\beta = |\phi_g(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) := |\phi_\infty(\mathbf{x})|^2 \text{ in } L^2, \tag{4.85}$$

where $\phi_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy

$$E_b(\phi) = \int_\Omega \frac{1}{2}|\phi|^4\, d\mathbf{x} \text{ with } \|\phi\|^2 = 1. \tag{4.86}$$

More precisely, $\rho_\infty = \frac{1}{|\Omega|}$ with $|\Omega|$ being the volume of the domain.

(2) For Case B2, i.e. $\beta \to +\infty$ and $\lim_{\beta\to+\infty}\delta/\beta = \delta_\infty > 0$ for some $\delta_\infty > 0$, we have

$$\rho_g^{\beta,\delta} = |\phi_g(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) \text{ in } H^1, \tag{4.87}$$

where $\rho_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy

$$E_{bd}^+(\sqrt{\rho}) = \int_\Omega \left[\frac{1}{2}|\rho|^2 + \frac{\delta_\infty}{2}|\nabla\rho|^2\right] d\mathbf{x}, \quad \text{where } \rho \ge 0 \text{ and } \int_\Omega \rho(\mathbf{x})\, d\mathbf{x} = 1. \tag{4.88}$$

Moreover, $\rho_\infty \ge 0$ satisfies the equation

$$\rho - \delta_\infty \Delta\rho = 2E_{bd}^+(\sqrt{\rho}) \text{ for } \mathbf{x} \in \Omega, \text{ and } \rho(\mathbf{x})|_{\partial\Omega} = 0. \tag{4.89}$$

(3) For Case B3, i.e. $\delta \to +\infty$ and $\beta = o(\delta)$, we have

$$\rho_g^\delta = |\phi_g(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) \text{ in } H^1, \tag{4.90}$$

where $\rho_\infty(\mathbf{x})$ is the unique nonnegative minimizer of the energy

$$E_d(\sqrt{\rho}) = \int_\Omega \frac{1}{2}|\nabla\rho|^2\, d\mathbf{x}, \text{ where } \rho \ge 0 \text{ and } \int_\Omega \rho(\mathbf{x})\, d\mathbf{x} = 1. \tag{4.91}$$

Moreover, $\rho_\infty \ge 0$ satisfies the equation

$$-\Delta\rho = 2E_d(\sqrt{\rho}) \text{ for } \mathbf{x} \in \Omega, \text{ and } \rho(\mathbf{x})|_{\partial\Omega} = 0. \tag{4.92}$$

Proof. The proofs are similar to those in Theorem 3.2. □

Remark 4.1.

- In Theorem 4.1, part (3) holds true for Case B3′, i.e. $\beta \to -\infty$ and $\delta \gg |\beta|$.
- For Case B2′, i.e. $\beta \to -\infty$ and $\lim_{\beta\to-\infty}\delta/|\beta| = \delta_\infty > 0$ for some $\delta_\infty > 0$, we have a subsequence $\beta_n \to -\infty$ and δ_n such that

$$\rho_g^{\beta_n,\delta_n} = |\phi_g^{\beta_n,\delta_n}(\mathbf{x})|^2 \to \rho_\infty(\mathbf{x}) \text{ in } H^1, \tag{4.93}$$

where $\rho_\infty(\mathbf{x})$ is a nonnegative minimizer of the energy

$$E_{bd}^-(\sqrt{\rho}) = \int_\Omega \left[-\frac{1}{2}|\rho|^2 + \frac{\delta_\infty}{2}|\nabla\rho|^2\right] d\mathbf{x}, \quad \text{where } \rho \ge 0 \text{ and } \int_\Omega \rho(\mathbf{x})\, d\mathbf{x} = 1. \tag{4.94}$$

More precisely, $\rho_\infty \ge 0$ satisfies the equation

$$\rho_\infty - \delta_0 \Delta\rho_\infty = 2E_{bd}^-(\sqrt{\rho_\infty})\chi_{\{\rho_\infty>0\}} \quad \text{for } \mathbf{x} \in \Omega, \text{ and } \rho_\infty(\mathbf{x})|_{\partial\Omega} = 0. \tag{4.95}$$

It remains to consider the last case B1′ as $\beta \to -\infty$ and $\delta = o(|\beta|)$. For simplicity, we assume Ω is a ball in $\mathbb{R}^d$.

Theorem 4.2. *Consider the box potential given in (4.83) with $\Omega = B_R := \{|\mathbf{x}| < R\}$. For case B1′, i.e. $\beta \to -\infty$, $\delta > 0$ and $\delta = o(|\beta|)$, the ground state of (4.84), denoted as $\phi_g^{\beta,\delta} \in H^1(\mathbb{R}^d)$, can be chosen to be a non-increasing radially symmetric function. Let $\phi_g^\varepsilon(\mathbf{x}) = \varepsilon^{d/2}\phi_g^{\beta,\delta}(\mathbf{x}\varepsilon) \in S$ with $\varepsilon = \delta^{1/2}/|\beta|^{1/2}$. Then $\varepsilon \to 0^+$ as $\beta \to -\infty$, and we have*

$$\rho_g^\varepsilon = |\phi_g^\varepsilon|^2 \to \rho_\infty \text{ in } H^1, \tag{4.96}$$

where ρ_∞ is the unique non-increasing radially symmetric minimizer of energy $E_{1'}$ (3.42).

Proof. Let $\Omega^\varepsilon = \{\mathbf{x}/\varepsilon, \mathbf{x} \in \Omega\}$. Since ρ_∞ is compactly supported as shown in Theorem 3.1, for sufficiently small ε, we have $\mathrm{supp}(\rho_\infty) \subset \Omega^\varepsilon$. On the other hand, ϕ_g^ε minimizes the energy

$$E^\eta_{\mathrm{box}}(\phi) = \int_{\mathbb{R}^d} \left[\frac{\eta}{2}|\nabla\phi|^2 - \frac{1}{2}|\phi|^4 + \frac{1}{2}\left|\nabla|\phi|^2\right|^2 \right] d\mathbf{x}, \qquad \phi \in H^1_0(\Omega^\varepsilon), \quad \|\phi\| = 1, \tag{4.97}$$

where $\eta = \frac{\delta^{\frac{d-2}{2}}}{|\beta|^{\frac{d}{2}}} = o(1)$ as $\varepsilon \to 0^+$. We can then proceed as that in Theorem 3.3 and the limit of ρ_g^ε as $\beta \to -\infty$ ($\varepsilon \to 0^+$) follows. $\square$

Similarly, we could extend the $\delta \to 0^+$ limit results in Theorem 3.4 to the bounded domain case here. Since no different scaling is involved, the extension is straightforward and we omit it here.

5. Conclusion

We have analyzed the ground state of a Bose–Einstein condensate in the presence of higher-order interaction (HOI), modeled by a modified Gross–Pitaevskii equation (MGPE). The ground state structures are quite different from the case without HOI. We established the existence and uniqueness as well as non-existence results on ground states in different parameter regimes. The asymptotic profiles of the ground states under different combinations of the HOI and the contact interaction were studied. The limiting profiles were found to be quite interesting and complicated involving free boundary problems.

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