ANALYSIS AND COMPUTATION FOR GROUND STATE SOLUTIONS OF BOSE–FERMI MIXTURES AT ZERO TEMPERATURE

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Abstract. Previous numerical studies on the ground state structure of Bose–Fermi mixtures mostly relied on Thomas–Fermi (TF) approximation for the Fermi gas. In this paper, we establish the existence and uniqueness of ground state solutions of Bose–Fermi mixtures at zero temperature for both a coupled Gross–Pitaevskii (GP) equations model and a model with TF approximation for fermions. To prove the uniqueness, the key is to estimate the $L^\infty$ bounds of the ground state solution. By implementing an efficient method—gradient flow with discrete normalization with backward Euler finite difference discretization—to compute the coupled GP equations, we report extensive numerical results in one and two dimensions. The numerical experiments show that we can also extract many interesting phenomena without reference to TF approximation for the fermions. Finally, we numerically compare the ground state solutions for the coupled GP equations model and the model with TF approximation for fermions as well as for the model with TF approximations for both bosons and fermions.

Key words. coupled Gross–Pitaevskii equations, Bose–Fermi mixtures, gradient flow with discrete normalization, numerical simulation, ground state

AMS subject classifications. 35Q55, 65Z05, 65N06, 81-08

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1. Introduction. The achievement of Bose–Einstein condensation in trapped and dilute alkali gases has stimulated rapidly growing activity in the field of ultracold degenerate quantum Fermi gases, as fermions are the fundamental building blocks of ordinary matter. One recent progress in experiments is creating a degenerate fermionic system by cooling and mixing them with ultracold bosons. Several successful attempts to trap and cool mixtures of a bosonic and a fermionic species were reported. Quantum degeneracy was first reached with mixtures of bosonic $^7$Li and fermionic $^6$Li atoms [30, 32]. More recently, experiments to cool mixtures of different atomic elements, i.e., $^{23}$Na and $^6$Li [13] as well as $^{87}$Rb and $^{40}$K [12, 25, 27], to ultralow temperatures succeeded. These ultracold Bose–Fermi mixtures offer unique possibilities to study the many effects of quantum statistics directly and may be used as an efficient tool to produce a degenerate single-component spin-polarized Fermi gas [28].

Many theories, including the density functional theory, the Bogoliubov approximation, and Hartree Fock theory, have been introduced to study the ground state properties of Bose–Fermi mixtures. However, theoretical studies of these Bose–Fermi mixtures at zero temperature are mostly based on mean-field theory, which is quite...
successful in describing the bosonic condensates. In this mean-field model at extremely low temperatures, for Bose–Fermi mixtures with degenerate nonsuperfluid Fermi gas, the dynamics are governed by coupled Gross–Pitaevskii (GP) equations [1, 2, 10, 11, 33],

\begin{align}
(1.1) \quad i\hbar \frac{\partial}{\partial t} \bar{\psi}_B &= \left( -\frac{\hbar^2 \nabla^2}{2m_B} + V_B(x) + g_{BB} |\bar{\psi}_B|^2 + g_{BF} |\bar{\psi}_F|^2 \right) \bar{\psi}_B, \quad x \in \mathbb{R}^3, \\
(1.2) \quad i\hbar \frac{\partial}{\partial t} \bar{\psi}_F &= \left( -\frac{\hbar^2 \nabla^2}{6m_F} + V_F(x) + g_{BF} |\bar{\psi}_B|^2 + A |\bar{\psi}_F|^4/3 \right) \bar{\psi}_F, \quad x \in \mathbb{R}^3,
\end{align}

where \( \hbar \) is the Planck constant and \( A = \hbar^2 (6\pi^2)^{2/3}/2m_F \), \( \bar{\psi}_B = \bar{\psi}_B(x,t) \) is the condensate wavefunction for bosons with \( m_B \) being the bosonic mass, and \( \bar{\psi}_F = \bar{\psi}_F(x,t) \) is the condensate wavefunction for fermions with \( m_F \) being the fermionic mass. \( g_{BB} = 4\pi \hbar^2 a_{BB}/m_B \) is the strength of internal boson-boson interaction, and \( g_{BF} = 2\pi \hbar^2 a_{BF}/m_B \) is the strength of boson-fermion interaction with the boson-fermion reduced mass defined as \( m_R = m_B m_F/(m_B + m_F) \). \( a_{BB} \) and \( a_{BF} \) are the the s-wave scattering lengths for the boson-fermion and the boson-boson scatterings. When the fermions interact and the Fermigas becomes superfluid, the coefficient in front of the kinetic part \( \nabla^2 \) in (1.2) for Fermigas should be \(-\hbar^2/8m_F\) instead of \(-\hbar^2/6m_F\) [3].

Here, we focus on the degenerate nonsuperfluid Fermi gas case (1.2), and the results can be generalized to the superfluid Fermi gas.

The wavefunctions are normalized according to the number of bosons \( N_B \) and the number of fermions \( N_F \), respectively, i.e.,

\begin{equation}
\int_{\mathbb{R}^3} |\bar{\psi}_B(x,t)|^2 dx = N_B \quad \text{and} \quad \int_{\mathbb{R}^3} |\bar{\psi}_F(x,t)|^2 dx = N_F.
\end{equation}

The trap potentials may be written as \( V_B(x) = \frac{1}{2} m_B \omega_B^2 (\gamma_2 x^2 + \gamma_3 y^2 + \gamma_4 z^2) \) for bosons and \( V_F(x) = \frac{1}{2} m_F \omega_F^2 (\gamma_2 x^2 + \gamma_3 y^2 + \gamma_4 z^2) \) for fermions, where \( \omega_B \) and \( \omega_F \) are the angular frequency.

In experiments and theoretical studies, the confining potentials are usually strongly anisotropic, resulting in a disk-shaped condensate, i.e., \( \gamma_2 \gg \gamma_3, \gamma_4 \), or a cigar-shaped condensate, i.e., \( \gamma_2, \gamma_3 \gg \gamma_4 \). In such cases, the three-dimensional coupled GP equations (1.1)–(1.2) can be reduced to equations in two dimensions [31] and one dimension [17], respectively, which have forms similar to (1.1)–(1.2) [8].

In this paper, after proper nondimensionalization, we consider the dimensionless form of coupled GP equations in \( d \) dimensions \((d = 1, 2, 3)\) for rescaled wavefunctions \( \psi_B := \bar{\psi}_B(x,t) \) and \( \psi_F := \bar{\psi}_F(x,t) \) as

\begin{align}
(1.4) \quad i \frac{\partial}{\partial t} \psi_B &= \left( -\frac{\nabla^2}{2} + V_B(x) + \beta_{11} |\psi_B|^2 + \beta_{12} N_B |\psi_F|^2 \right) \psi_B, \quad x \in \mathbb{R}^d, \\
(1.5) \quad i \frac{\partial}{\partial t} \psi_F &= \left( -\frac{\nabla^2}{6\lambda} + V_F(x) + \beta_{12} N_B |\psi_B|^2 + \beta_{22} |\psi_F|^4/3 \right) \psi_F, \quad x \in \mathbb{R}^d,
\end{align}

where \( \beta_{11} \sim \frac{4\pi a_{BB} N_B}{m_B} \), \( \beta_{12} \sim \frac{2\pi a_{BF}}{m_B/1+\lambda} \), and \( \beta_{22} \sim \frac{(6\pi^2 N_F)^{2/3}}{2\lambda} \) with \( \lambda = m_F/m_B \), and

\begin{equation}
V_k(x) = \begin{cases} \frac{C_0}{2} \gamma_2 x^2, & d = 1, \\ \frac{C_0}{2} (\gamma_2 x^2 + \gamma_3 y^2), & d = 2, \quad \text{where} \quad k = B, F, \\ \frac{C_0}{2} (\gamma_2 x^2 + \gamma_3 y^2 + \gamma_4 z^2), & d = 3, \end{cases}
\end{equation}

and \( C_B = 1, C_F = \lambda \).
In this dimensionless form, coupled GP equations (1.4)–(1.5) conserve the normalizations for the two wavefunctions \( \psi_B \) and \( \psi_F \) as

\[
\int_{\mathbb{R}^d} |\psi_B(x,t)|^2 \, dx = 1, \quad \int_{\mathbb{R}^d} |\psi_F(x,t)|^2 \, dx = 1, \quad t \geq 0,
\]

and the dimensionless energy per particle (the total particle number \( N = N_B + N_F \))

\[
E(\psi_B, \psi_F) = \frac{N_B}{N} \int_{\mathbb{R}^d} \left( \frac{|\nabla \psi_B|^2}{2} + V_B |\psi_B|^2 + \beta_{11} |\psi_B|^4 \right) \, dx
\]

\[
+ \frac{N_F}{N} \int_{\mathbb{R}^d} \left( \frac{|\nabla \psi_F|^2}{6\lambda} + V_F |\psi_F|^2 + \frac{3\beta_{22}}{5} |\psi_F|^4 \right) \, dx + \frac{N_B N_F}{N} \int_{\mathbb{R}^d} \beta_{12} |\psi_F|^2 |\psi_B|^2 \, dx.
\]

A fundamental problem in the study of Bose–Fermi mixtures lies in investigating the properties of the ground state. Mathematically, the ground state solution \((\phi_B^g(x), \phi_F^g(x))\) for the coupled GP equations description (1.4)–(1.5) of Bose–Fermi mixture can be found by minimizing the energy \( E(\phi_B, \phi_F) \) (1.8) under the constraints \( \int_{\mathbb{R}^d} |\phi_j(x)|^2 \, dx = 1, \, j = B, F; \)

(A) Find \((\phi_B^g(x), \phi_F^g(x)) \in S_d\) such that

\[
E(\phi_B^g(x), \phi_F^g(x)) = \min_{(\phi_B, \phi_F) \in S_d} E(\phi_B, \phi_F),
\]

where the nonconvex set \( S_d \) is defined as

\[
S_d = \left\{ (\phi_B, \phi_F) \, | \, \int_{\mathbb{R}^d} |\phi_B(x)|^2 \, dx = 1, \quad \int_{\mathbb{R}^d} |\phi_F(x)|^2 \, dx = 1, \, E(\phi_B, \phi_F) < \infty \right\}.
\]

It is easy to see that the ground state \((\phi_B^g, \phi_F^g)\) solves the nonlinear eigenvalue problem

\[
\mu_B \phi_B = \left( -\frac{\nabla^2}{2} + V_B(x) + \beta_{11} |\phi_B|^2 + \beta_{12} N_F |\phi_F|^2 \right) \phi_B,
\]

\[
\mu_F \phi_F = \left( -\frac{\nabla^2}{6\lambda} + V_F(x) + \beta_{12} N_B |\phi_B|^2 + \beta_{22} |\phi_F|^{4/3} \right) \phi_F,
\]

where

\[
\|\phi_B\|_{L^2(\mathbb{R}^d)} := \int_{\mathbb{R}^d} |\phi_B(x)|^2 \, dx = 1, \quad \|\phi_F\|_{L^2(\mathbb{R}^d)} := \int_{\mathbb{R}^d} |\phi_F(x)|^2 \, dx = 1,
\]

and the eigenvalues (chemical potential) \( \mu_B \) and \( \mu_F \) are given by

\[
\mu_B = \int_{\mathbb{R}^d} \left( \frac{|\nabla \phi_B|^2}{2} + V_B |\phi_B|^2 + \beta_{11} |\phi_B|^4 + \beta_{12} N_F |\phi_F|^2 |\phi_B|^2 \right) \, dx,
\]

\[
\mu_F = \int_{\mathbb{R}^d} \left( \frac{|\nabla \phi_F|^2}{6\lambda} + V_F |\phi_F|^2 + \beta_{12} N_B |\phi_B|^2 |\phi_F|^2 + \beta_{22} |\phi_F|^{10/3} \right) \, dx.
\]

Using the mean-field approximation, the earliest numerical treatment of the ground state of Bose–Fermi mixtures was done by Mølmer [22], where the wavefunctions
for both bosons and fermions are treated with Thomas–Fermi (TF) approximations. Later Nygaard and Mølmer extended their numerical studies on the component separation of Bose–Fermi mixtures [24], where the wavefunction for bosons is governed by a GP equation, while the wavefunction for fermions is still approximated with TF approximations. Based on the mean-field model with fermions approximated by TF approximations, many aspects of the ground state structure of Bose–Fermi mixtures have been intensively studied, including its stability [20, 24, 28], its collapse [9, 21, 26], its separation [19], its collective excitations [10, 18], and its vortex states [35]. In detail, when \( N_p \gg 1 \), we have the TF approximation for the fermions. The ground state solution for the Bose–Fermi mixture \((\phi_B^0(x), \phi_F^0(x))\) in this approximation can be found by minimizing the energy \( E_1(\phi_B, \phi_F) \) (1.16) under the constraints (1.13):

(B) Find \((\phi_B^0(x), \phi_F^0(x)) \in S^1_d\) such that

\[
E_1(\phi_B^0(x), \phi_F^0(x)) = \min_{(\phi_B^0, \phi_F^0) \in S^1_d} E_1(\phi_B, \phi_F).
\]

Here \( E_1(\phi_B, \phi_F) \) is denoted by

\[
E_1(\phi_B, \phi_F) = \frac{N_B}{N} \int_{\mathbb{R}^d} \left( \frac{\nabla \phi_B}{2} + V_B |\phi_B|^2 + \frac{\beta_{11}}{2} |\phi_B|^4 \right) dx
\]

\[
+ \frac{N_B N_F}{N} \int_{\mathbb{R}^d} \beta_{12} |\phi_F|^2 |\phi_B|^2 dx
\]

\[
+ \frac{N_F}{N} \int_{\mathbb{R}^d} \left( V_F |\phi_F|^2 + \frac{3 \beta_{22}}{5} |\phi_F|^4 \right) dx,
\]

and \( S^1_d = \{(\phi_B, \phi_F) | \int_{\mathbb{R}^d} |\phi_B|^2 dx = 1, \int_{\mathbb{R}^d} |\phi_F|^2 dx = 1, E_1(\phi_B, \phi_F) < \infty\}\). In this case, we notice that the ground state solution \((\phi_B^0(x), \phi_F^0(x))\) must satisfy (1.13) and

\[
\mu^1_B \phi_B = \left( -\frac{\nabla^2}{2} + V_B(x) + \beta_{11} |\phi_B|^2 + \beta_{12} N_F |\phi_F|^2 \right) \phi_B,
\]

\[
\mu^1_F \phi_F = \left( V_F(x) + \beta_{12} N_B |\phi_B|^2 + \beta_{22} |\phi_F|^4 / 3 \right) \phi_F,
\]

where \( \mu^1_B \) and \( \mu^1_F \) can be computed as

\[
\mu^1_B = \int_{\mathbb{R}^d} \left( \frac{|\nabla \phi_B|^2}{2} + V_B |\phi_B|^2 + \beta_{11} |\phi_B|^4 + \beta_{12} N_F |\phi_F|^2 |\phi_B|^2 \right) dx,
\]

\[
\mu^1_F = \int_{\mathbb{R}^d} \left( V_F |\phi_F|^2 + \beta_{12} N_B |\phi_F|^2 |\phi_B|^2 + \beta_{22} |\phi_F|^4 / 3 \right) dx.
\]

In this paper, we will study the ground state of Bose–Fermi mixtures analytically and numerically, using the coupled GP model (1.8) and the partial approximation model (1.16). To our knowledge, applying TF approximation for the fermions is the most frequently used approach in previous numerical studies on ground state structure of Bose–Fermi mixtures, and there is no rigorous mathematical analysis on the ground state with (1.8) and (1.16). The use of the coupled GP equations allows one to investigate a system where the TF approximation is not applicable. In addition, without reference to the TF approximation for the fermions, we here show that we can also extract many interesting phenomena similar to those obtained through TF approximation for the fermions.
The rest of this paper is organized as follows. In section 2, we discuss the existence, nonexistence, and uniqueness of the ground state solutions for both models (1.8) and (1.16). In section 3, we introduce the numerical methods for computing the ground state—discretizing normalized gradient flows with backward Euler finite difference schemes. In section 4, we present numerical results on the ground state solution of Bose–Fermi mixtures in one and two dimensions. In section 5, some conclusions are drawn.

2. Ground state. In this section, we will investigate the existence and uniqueness of the ground states for the Bose–Fermi mixture, using definitions (A) (1.9) and (B) (1.14), respectively. We will first consider the coupled GP equations description, i.e., problem (A) (1.9). Let us define the best Sobolev constant \( C_a, C_b \) to be

\[
C_a = \inf_{f \neq 0, f \in H^1(\mathbb{R}^3)} \left\{ \frac{\| \nabla f \|^2_{L^2(\mathbb{R}^3)}}{\| f \|^4/3_{L^6(\mathbb{R}^3)}} \right\}, \quad C_b = \inf_{f \neq 0, f \in H^1(\mathbb{R}^2)} \left\{ \frac{\| \nabla f \|^2_{L^2(\mathbb{R}^2)}}{\| f \|^2_{L^2(\mathbb{R}^2)}} \right\}.
\]

It is well known that \( C_a, C_b \) can be attained at some radially symmetric smooth function.

In practice, we can split the energy (1.8) into the kinetic energy \( E_{\text{kin}} \), the potential energy \( E_{\text{pot}} \), the interaction energy \( E_{\text{int}} \), and the internal-interaction-between-fermions energy \( E_{\text{int}}^F \) as

\[
\begin{align*}
E_{\text{kin}}(\phi_B, \phi_F) &= \frac{N_B}{2N} \int_{\mathbb{R}^d} |\nabla \phi_B|^2 \, dx + \frac{N_F}{6\lambda N} \int_{\mathbb{R}^d} |\nabla \phi_F|^2 \, dx, \\
E_{\text{pot}}(\phi_B, \phi_F) &= \frac{N_B}{N} \int_{\mathbb{R}^d} V_B |\phi_B|^2 \, dx + \frac{N_F}{N} \int_{\mathbb{R}^d} V_F |\phi_F|^2 \, dx, \\
E_{\text{int}}(\phi_B, \phi_F) &= \frac{N_B}{2N} \int_{\mathbb{R}^d} \beta_{11} |\phi_B|^4 \, dx + \frac{N_F}{N} \int_{\mathbb{R}^d} \beta_{12} |\phi_F|^2 |\phi_B|^2 \, dx, \\
E_{\text{int}}^F(\phi_B, \phi_F) &= \frac{3N_F}{5N} \int_{\mathbb{R}^d} \beta_{22} |\phi_F|^4/3 \, dx.
\end{align*}
\]

Then the energy (1.16) in problem (B) can be viewed as (1.8) without the kinetic energy of \( \phi_F \).

2.1. Results for problem (A) (1.9). We have the following results on the existence of the ground states for the minimization problem (A) (1.9).

**Theorem 2.1** (existence and nonexistence). Suppose \( 0 \leq V_B(\mathbf{x}), V_F(\mathbf{x}) \in L_{\text{loc}}(\mathbb{R}^d) \) \((\mathbf{x} \in \mathbb{R}^d)\) satisfies \( \lim_{|\mathbf{x}| \to \infty} V_j(\mathbf{x}) = \infty \) \((j = B, F)\); there exists a ground state \((\phi_B^0, \phi_F^0) \in S_d\) if one of the following holds:

(i) \( d = 3, \beta_{11} \geq 0, \beta_{12} \geq 0, \) and \( \beta_{22} > -\frac{5}{2} C_a \);
(ii) \( d = 2, \beta_{11} < -C_b, \) and \( \beta_{12} > -\sqrt{\frac{C_b (1 + C_a)}{2}} \);
(iii) \( d = 1 \) for all \( \beta_{11}, \beta_{12}, \beta_{22} \in \mathbb{R} \).

Moreover, the ground state can be chosen as \((|\phi_B^0|, |\phi_F^0|)\) and \((\phi_B^0, \phi_F^0) = (e^{i\theta_B} |\phi_B^0|, e^{i\theta_F} |\phi_F^0|)\) for some constants \( \theta_B, \theta_F \in \mathbb{R} \).

In contrast, there exists no ground state, i.e., \( \min_{(\phi_B, \phi_F) \in S_d} E(\phi_B, \phi_F) = -\infty \), if one of the following holds:

(i') \( d = 3, \beta_{11} < 0, \) or \( \beta_{12} < 0 \) or \( \beta_{22} < -\frac{5}{18} C_a \);
(ii') \( d = 2, \beta_{11} < -C_b, \) or \( \beta_{12} < -\frac{5}{2N_F} C_b + \frac{C_b^2}{6\lambda N_B} \).

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Before going to the proof, we first present the following useful lemma. Denote the weighted $L^2$ space for some nonnegative potential $V(x) \geq 0$ as

\[(2.3) \quad L_V = \left\{ \|\phi\|_{L^2_V}^2 = \int_{\mathbb{R}^d} V(x) |\phi(x)|^2 dx < \infty \right\}.\]

Let $X_V = L_V \cap H^1(\mathbb{R}^d)$; then by the standard Sobolev embedding, we know that $X_V \hookrightarrow H^1(\mathbb{R}^d) \hookrightarrow L^p(\mathbb{R}^d)$, where

\[(2.4) \quad p \in [2, \infty] \quad \text{for} \quad d = 1; \quad p \in [2, \infty) \quad \text{for} \quad d = 2; \quad \text{and} \quad p \in [2, 6) \quad \text{for} \quad d = 3.\]

We have the following results.

**Lemma 2.2.** Suppose $V(x) \geq 0$ ($x \in \mathbb{R}^d$) satisfies $\lim_{|x| \to \infty} V(x) = \infty$; the embedding $X_V \hookrightarrow L^p(\mathbb{R}^d)$ is compact, where $p$ satisfies (2.4).

**Proof.** First, it suffices to prove the case $p = 2$, and the case of other $p$ satisfying (2.4) can be then proved by interpolation. For $p = 2$, we only need to prove that any weakly convergent sequence in $X_V$ has a strong convergent subsequence in $L^2(\mathbb{R}^d)$. Taking a sequence $\{\phi^n\}_{n=1}^\infty \subset X_V$ such that

\[(2.5) \quad \phi^n \rightharpoonup \phi \text{ in } X_V,\]

since the weak convergence in $L^2(\mathbb{R}^d)$ is obvious, in order to prove the strong $L^2(\mathbb{R}^d)$ convergence of the sequence, we only need to prove that

\[(2.6) \quad \|\phi^n\|_{L^2(\mathbb{R}^d)} \to \|\phi\|_{L^2(\mathbb{R}^d)}.\]

This can be deduced by the confining condition of $V(x)$ [5, 16], and then the strong convergence in $L^2(\mathbb{R}^d)$ holds true. The conclusion then follows. \[\square\]

**Lemma 2.3.** If $(\phi^0_p, \phi^0_q) \in S_d$ is a ground state, $(|\phi^0_p|, |\phi^0_q|) \in S_d$ is also a ground state, and $(\phi^0_p, \phi^0_q) = (e^{i\theta_p} |\phi^0_p|, e^{i\theta_q} |\phi^0_q|)$ for some constants $\theta_p, \theta_q \in \mathbb{R}$.

**Proof.** Noticing the inequality for $f \in H^1(\mathbb{R}^d)$ ($d \in \mathbb{N}$) [15],

\[(2.7) \quad \|\nabla f\|_{L^2(\mathbb{R}^d)} \leq \|\nabla f\|_{L^2(\mathbb{R}^d)},\]

where the equality holds iff $f = e^{i\theta}|f|$ for some $\theta \in \mathbb{R}$, a direct application implies the conclusion. \[\square\]

**Proof of Theorem 2.1.** We separate the proof into the existence and nonexistence parts.

1. **Existence.** Form Lemmas 2.2 and 2.3, we only need to prove that the energy $E$ is bounded below in the $S_d$ in the corresponding cases. In case (i), it is obvious that $E(\phi^0_p, \phi^0_q) \geq 0$ by noticing the definitions of the best constants $C_d$. In case (ii), the Sobolev inequality implies

\[
\int_{\mathbb{R}^2} |\phi^0_p(x)|^{10/3} dx \leq \left( \int_{\mathbb{R}^2} |\phi^0_p(x)|^2 dx \right)^{1/3} \left( \int_{\mathbb{R}^2} |\phi^0_p(x)|^4 dx \right)^{2/3} \\
\leq \left( \int_{\mathbb{R}^2} |\nabla \phi^0_p(x)|^2 dx \right)^{4/3} \\
\leq \varepsilon \|\nabla \phi^0_p\|_2^2 + C_\varepsilon \quad \text{for} \quad \varepsilon > 0.
\]
Using the Cauchy inequality, we have
\[
\begin{align*}
\frac{\beta_1 N_B}{2N} \int_{\mathbb{R}^d} |\phi_B(x)|^4 \, dx + \frac{\beta_2 N_F}{N} \int_{\mathbb{R}^d} |\phi_F(x)|^2 |\phi_F(x)|^2 \, dx \\
\geq - \frac{C_B N_B}{2N} \int_{\mathbb{R}^d} |\phi_B(x)|^4 \, dx - \frac{C_B N_F}{6AN} \int_{\mathbb{R}^d} |\phi_F(x)|^4 \, dx \\
\geq - \frac{N_B}{2N} \int_{\mathbb{R}^d} |\nabla \phi_B(x)|^2 \, dx - \frac{N_F}{6AN} \int_{\mathbb{R}^d} |\nabla \phi_F(x)|^2 \, dx.
\end{align*}
\]

Then it is easy to see that $E$ is bounded below in this case. In case (iii), using the Sobolev inequality and the Cauchy inequality, we have for any $f \in H^1(\mathbb{R})$ and any $\varepsilon > 0$
\[
(2.8) \quad \|f\|_{L^2(\mathbb{R})}^2 \leq \|f\|_{L^2(\mathbb{R})}^2 \leq \|f\|_{L^2(\mathbb{R})} \leq \varepsilon \|f\|_{L^2(\mathbb{R})}^2 + C_\varepsilon \|f\|_{L^2(\mathbb{R})}^2
\]
and
\[
(2.9) \quad \|f\|_{L^{10/3}(\mathbb{R})} \leq C_1 \|f\|_{L^2(\mathbb{R})} + C_2 \|f\|_{L^4(\mathbb{R})}.
\]

Hence, it is straightforward to see that $E$ is bounded below in case (iii). In summary, for all cases (i), (ii), and (iii), we can take a sequence $(\delta_n, \phi_n)_{n=1}^\infty$ minimizing the energy $E$ in $S_d$, and $\phi_n$ and $\phi_n^\varepsilon$ are uniformly bounded in $H^1 \cap L^q$ and $H^1 \cap L^q_p$, respectively, where $L^q_V = \{ \|f\|_{L^q_V} = \int_{\mathbb{R}^d} |f|^q V \, dx < \infty \}$ ($j = B, F$). Thus, there exists a weakly convergent subsequence (denoted as the original sequence for simplicity) such that
\[
(2.10) \quad \phi_n^\varepsilon \to \phi_\varepsilon^\infty \text{ in } H^1 \cap L^q, \quad \phi_n^\varepsilon \to \phi_\varepsilon^\infty \text{ in } H^1 \cap L^{q_p}.
\]

Lemma 2.2 ensures that $\phi_n^\varepsilon \to \phi_\varepsilon^\infty$ and $\phi_n^\varepsilon \to \phi_n^\infty$ in $L^p$, where $p$ satisfies (2.4). Combining the lower-semicontinuity of the $H^1$ and $L^q_V$ ($j = B, F$), we can conclude that $(\phi_\varepsilon^\infty, \phi_\varepsilon^\infty) \in S_d$ is a ground state [15].

(2) Nonexistence. First, we consider the case $d = 3$, i.e., case (i'). If $\beta_1 < 0$, and let $\phi_B(x) = \pi^{-\frac{d}{2}} e^{-|x|^2/2}$, and $\phi_F(x)$ ($x \in \mathbb{R}^3$) be the smooth, radial symmetric (decreasing) function such that the best constant $C_\varepsilon$ holds in (2.1). Denoting
\[
\phi_\varepsilon^B(x) = \varepsilon^{-3/2} \phi_B(x/\varepsilon), \quad \phi_\varepsilon^F(x) = \delta^{-3/2} \phi_F(x/\delta), \quad \varepsilon, \delta > 0,
\]
we find
\[
(2.11) \quad E(\phi_\varepsilon^B, \phi_\varepsilon^F) = \frac{C_1}{\varepsilon^2} + \frac{\beta_1 C_2}{\varepsilon^3} + C_3 + O(1), \quad C_1, C_2 > 0 \quad \text{as } \varepsilon \to 0^+.
\]

Hence $E(\phi_\varepsilon^B, \phi_\varepsilon^F) \to -\infty$ as $\varepsilon \to 0^+$, which shows that there exists no ground state. If $\beta_{12} < 0$, we first claim that
\[
(2.12) \quad \inf_{(\phi_1, \phi_2) \in S_3} \frac{\int_{\mathbb{R}^3} |\phi_1(x)|^4 \, dx}{\int_{\mathbb{R}^3} |\phi_1(x)|^2 |\phi_2(x)|^2 \, dx} = 0.
\]

This can be seen from the constructions below. For $\varepsilon > 0$, define
\[
(2.13) \quad f_\varepsilon := f_\varepsilon(x) = \begin{cases} 2, & |x| \leq \varepsilon, \\ \varepsilon, & 1 \leq |x| \leq R_\varepsilon, \\ 0 & \text{otherwise}, \end{cases}
\]
where \( R_\varepsilon \geq 0 \) is chosen such that \( \|f_\varepsilon\|_{L^2} = 1 \). It is clear that by letting \( \varepsilon \to 0 \), \( \|f_\varepsilon\|_{L^4} \to 0 \). Using a standard mollifier to mollify \( f_\varepsilon \), we can find \( \tilde{f}_\varepsilon(x) \) such that \( \tilde{f}_\varepsilon \in C_0^\infty \), \( \|\tilde{f}_\varepsilon\|_{L^2} = 1 \), \( \tilde{f}_\varepsilon = \tilde{f}_\varepsilon(x) \geq 1 \) for \( |x| \leq \frac{\varepsilon}{2} \), and \( \|\tilde{f}_\varepsilon\|_{L^4}^4 \to 0 \) as \( \varepsilon \to 0 \). Next, \( |\phi_\delta^B|^2 \) converge to Dirac distribution as \( \delta \to 0^+ \), and

\[
(2.15) \quad \lim_{\delta \to 0^+} \int_{\mathbb{R}^3} |\phi_\delta^B(x)|^2 \left| \tilde{f}_\varepsilon(x) \right|^2 \, dx = \left| \tilde{f}_\varepsilon(0) \right|^2 > 1.
\]

Then choosing \( (\phi_1, \phi_2) = (\tilde{f}_\varepsilon, \phi_\delta^B) \) with sufficiently small \( \varepsilon \) and \( \delta \), we can draw conclusion (2.13). Based on the above discussion, for \( \beta_{12} < 0 \), choose \( (\phi_1^0, \phi_2^0) \in S_3 \) such that

\[
(2.16) \quad C_0 = \frac{\beta_{11}}{2} \int_{\mathbb{R}^3} |\phi_1^0(x)|^4 \, dx \cdot N_B / N + \beta_{12} \int_{\mathbb{R}^3} |\phi_1^0(x)|^2 \left| \phi_2^0(x) \right|^2 \, dx \cdot N_B N_F / N < 0.
\]

Letting \( (\phi_1^\varepsilon(x), \phi_2^\varepsilon(x)) = \varepsilon^{-3/2}(\phi_1^0(x/\varepsilon), \phi_2^0(x/\varepsilon)) \in S_3 \), we then conclude that

\[
(2.17) \quad E(\phi_1^\varepsilon, \phi_2^\varepsilon) = \frac{C_0}{\varepsilon^3} + \frac{C_4}{\varepsilon^2} + C_5 + O(1) \quad \text{as} \ \varepsilon \to 0^+.
\]

Hence \( E(\phi_1^0, \phi_2^0) \to -\infty \) as \( \varepsilon \to 0^+ \), which shows that there exists no ground state in this case. If \( \beta_{22} < -\frac{4}{18} C_6 \), we have

\[
(2.18) \quad E(\phi_1^b, \phi_2^b) = \left( \frac{C_6}{6} + \frac{3}{5} \beta_{22} \right) \delta^{-2} + C_6 + O(1) \quad \text{as} \ \delta \to 0^+.
\]

Then \( E(\phi_1^b, \phi_2^b) \to -\infty \), as \( \varepsilon \to 0^+ \), which shows that there exists no ground state in this case. The case for \( d = 3 \) is complete.

Second, we consider the case \( d = 2 \). Let \( \phi^b(x) (x \in \mathbb{R}^2) \) be the smooth, radial symmetric (decreasing) function such that the best constant \( C_b \) holds in (2.1). If \( \beta_{11} < -C_b \), let \( \phi_2^b(x) = \varepsilon^{-1} \phi^b(x/\varepsilon) (\varepsilon > 0) \), and we have

\[
(2.19) \quad E(\phi_1^b, \phi_2^b) = \frac{\beta_{11} + C_b}{2\varepsilon^2} + C_7 + O(1) \quad \text{as} \ \varepsilon \to 0^+.
\]

Similarly, if \( \beta_{12} < -\frac{\beta_{11} - C_b}{2 N_F} \), we have

\[
(2.20) \quad E(\phi_1^b, \phi_2^b) = \frac{C_8}{2\varepsilon^2} + \frac{C_9}{\varepsilon^4/3} + O(1) \quad \text{as} \ \varepsilon \to 0^+,
\]

where \( C_b < 0 \). Then in both cases, as \( \varepsilon \to 0^+ \), \( E \to -\infty \), and this shows that there exists no ground state. The proof is complete. \( \square \)

From Theorem 2.1, we know that the ground state can always be chosen as the positive one. Now, we want to study the uniqueness of the positive ground state for the case \( \beta_{11}, \beta_{12}, \beta_{22} \geq 0 \). Generally, the uniqueness of the minimizer for problem (A) (1.9) is unknown unless it is a convex problem. But one can transform problem (A) into convex minimization form [16] for the density in the single bosonic condensate case. In a two-component bosonic condensates case [5], the same technique still applies and the convexity depends on the coefficients \( \beta_{jk} (j, k = 1, 2) \), where the interaction energy is a quadratic form for the densities of the two components. However, for the current Bose–Fermi mixture case, the total interaction energy is not a quadratic form on the densities \( |\phi_p|^2 \) and \( |\phi_p|^2 \). Alternatively, we can estimate the \( L^\infty \) bound of the
ground states using the Euler–Lagrange equation (1.11)–(1.12) and then establish the uniqueness.

**Theorem 2.4.** For \( \beta_{11}, \beta_{12}, \beta_{22} \geq 0, 0 \leq V_B(x), V_F(x) \in C^1 \) with \( \lim_{|x| \to \infty} V_j(x) = \infty \) (\( j = B, F \)), denote \( \rho_B(x) := |\phi_B(x)|^2, \rho_F(x) := |\phi_F(x)|^2 \) (\( x \in \mathbb{R}^d, d = 1, 2, 3 \)), \( E_g = \min_{(\phi_B, \phi_F) \in \mathcal{S}_d} E(\phi_B, \phi_F) \); i.e., \( E_g \) is the minimal energy. Then the ground state \((\sqrt{\rho_B}, \sqrt{\rho_F})\) is unique under the following condition:

\[
\beta_{12}^2 \leq \frac{2}{\sqrt{15} N_B \sqrt{N_F^2 N E_g}} \beta_{11} \beta_{22}^{3/2}.
\]

The ground state energy \( E_g \) can be bounded by using any testing functions, e.g., choosing \((\phi_B, \phi_F)\) such that \( \phi_B \phi_F = 0 \). Then there exist constant \( C \) depending on \( V_B \) and \( V_F \), such that

\[
E_g \leq C(1 + \beta_{11} + \beta_{22}).
\]

This upper bound will yield a sufficient condition for the uniqueness of the positive ground state.

**Proof.** The ground state of (1.8) is the minimizer of the energy functional in \( \mathcal{S}_d \). Here, we argue by contradiction. If we have two positive ground states \((\sqrt{\rho_B^1}, \sqrt{\rho_F^1}) = (\phi_B^1, \phi_F^1), (\sqrt{\rho_B^2}, \sqrt{\rho_F^2}) = (\phi_B^2, \phi_F^2)\) of energy (1.8), consider \((\phi_B^\theta, \phi_F^\theta) = (\sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta}) \in \mathcal{S}_d, \theta \in [0, 1], \) defined as

\[
\rho_B^\theta = \theta \rho_B^1 + (1 - \theta) \rho_B^2, \quad \rho_F^\theta = \theta \rho_F^1 + (1 - \theta) \rho_F^2.
\]

Let \( g(\theta) = E(\sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta}), \theta \in [0, 1], \) and

\[
g_1(\theta) = E_{\text{kin}} \left( \sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta} \right) + E_{\text{pot}} \left( \sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta} \right),
\]

\[
g_2(\theta) = E_{\text{int}} \left( \sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta} \right) + E_{\text{F}} \left( \sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta} \right).
\]

Then \( g(\theta) = g_1(\theta) + g_2(\theta) \). Following [16], \( g_1(\theta) \) is convex in \([0, 1]\). For \( g_2(\theta) \), it is easy to see \( g_2 \) is convex if

\[
2N_B N_F \sup_{\theta, x} (\rho_F^\theta(x))^{1/3} \beta_{11} \beta_{22} \geq \beta_{12}^2 \frac{N_B^2 N_F^2}{N^2}.
\]

We can derive some a priori bound for \( \rho_F^\theta(x) \) using the Euler–Lagrange equations for the ground states. Let \( \mu_1^F, \mu_2^F \) and \( \mu_1^B, \mu_2^B \) be the corresponding chemical potentials for \((\sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta})\) and \((\sqrt{\rho_B^\theta}, \sqrt{\rho_F^\theta})\). Following [16], we can show that the two ground states are bounded and belong to the \( C^2 \) function class. Consider the point \( x_0 \) where \( \phi_F^1 \) takes its maximal. We can obtain

\[
\mu_1^F \phi_1^F(x_0) = \left( \frac{\nabla^2}{2a} \phi_1^F + V_F + \beta_{12} N_B |\phi_B^1|^2 + \beta_{22} |\phi_F^1|^{4/3} \right) \phi_1^F(x_0) \geq \left( V_F(x_0) + \beta_{22} |\phi_F^1(x_0)|^{4/3} \right) \phi_1^F(x_0),
\]

and so

\[
\beta_{22} \| \phi_F^1 \|_{L^\infty}^{4/3} \leq \mu_1^F \leq \frac{5}{3} \frac{N}{N_F} E(\phi_B^1, \phi_F^1) = \frac{5}{3} \frac{N}{N_F} E_g.
\]
The same estimates hold for \( \phi^2_p \). Hence,

\[
\| q_p \|^{1/3}_\infty \leq \frac{1}{\sqrt{22}} \sqrt{\frac{5}{3} \frac{N}{N_p} E_g}.
\]

Combined with (2.24), we directly get that \( g_2(\theta) \) is convex if

\[
\beta_{12}^2 \leq \frac{2}{\sqrt{15}N_B \sqrt{N_p NEg}} \beta_{11}^{3/2}.
\]

The conclusion then follows.

In addition, we can obtain the virial identity as follows.

**Theorem 2.5.** Suppose \( V_j(x) \) (\( j = B, F \)) are harmonic potentials. Then for the ground state solution \( (\phi^g_B, \phi^g_F) \), its kinetic energy \( E_{\text{kin}} \), potential energy \( E_{\text{pot}} \), interaction energy \( E_{\text{int}} \), and internal-interaction-between-fermions energy \( E^{\text{F}^2}_{\text{int}} \) must satisfy

\[
2E_{\text{kin}}(\phi^g_B, \phi^g_F) - 2E_{\text{pot}}(\phi^g_B, \phi^g_F) + dE_{\text{int}}(\phi^g_B, \phi^g_F) + \frac{2d}{3} E^{\text{F}^2}_{\text{int}}(\phi^g_B, \phi^g_F) = 0.
\]

**Proof.** The proof follows the analogous proof for the single Bose–Einstein condensate (BEC) case [16].

Equation (2.28) also holds true for the excited state solutions of Bose–Fermi mixtures at extremely low temperature, i.e., the solutions of the nonlinear eigenvalue problem (1.11)-(1.12) with (1.13).

### 2.2 Results for problem (B) (1.14)

Here, we present the results concerning the minimization problem (B) (1.14), i.e., the minimizers of \( E_1 \) (1.14).

**Theorem 2.6.** Suppose that \( 0 \leq V_j(x), V_{\phi}(x) \in L_\infty(\mathbb{R}^d) \) \( (x \in \mathbb{R}^d) \) satisfies \( \lim_{|x| \to \infty} V_j(x) = \infty \) \( (j = B, F) \). There exists a ground state \( (\phi^g_B, \phi^g_F) \) in \( S^1_d \) for problem (B) (1.14) if one of the following holds:

(i) \( d = 3, \beta_{11} \geq 0, \beta_{12} \geq 0, \) and \( \beta_{22} \geq 0; \)

(ii) \( d = 2, \beta_{11} > -C_b, \beta_{12} \geq 0, \) and \( \beta_{22} > 0; \)

(iii) \( d = 1, \beta_{22} > 0. \)

Moreover, the ground state can be chosen as \( (|\phi^g_B|, |\phi^g_F|) \) and \( (\phi^g_B, \phi^g_F) = (e^{i\theta_B} |\phi^g_B|, e^{i\theta_F} |\phi^g_F|) \) for some constant \( \theta_B \in \mathbb{R} \) and real measurable function \( \theta_F(x) \).

In contrast, there exists no ground state, i.e., \( \min_{(\phi_B, \phi_F) \in S^1_d} E_1(\phi_B, \phi_F) = -\infty, \)

if one of the following holds:

(i') \( d = 3, \beta_{11} < 0 \) or \( \beta_{12} < 0 \) or \( \beta_{22} < 0; \)

(ii') \( d = 2, \beta_{11} < -C_b \) or \( \beta_{12} < 0 \) or \( \beta_{22} < 0; \)

(iii') \( d = 1, \beta_{22} < 0. \)

**Proof.** Existence. The proof is quite similar to the proof of Theorem 2.1. Given conditions (i), (ii), and (iii), one can easily show that \( E_1(\phi_B, \phi_F) \) is bounded below in \( S^1_d \). Hence, we can take a minimizing sequence \( \{ (\phi^n_B, \phi^n_F) \}_{n=1}^\infty \subset S^1_d \) of energy \( E_1 \), where \( \phi^n_B \) and \( \phi^n_F \) are chosen as nonnegative functions. In fact, we can choose

\[
\phi^n_F = \arg\min_{||\phi||_{L^2} = 1, \phi \geq 0} E_1(\phi^n_B, \phi), \quad n \geq 1.
\]

It is not difficult to see that such nonnegative \( \phi^n_F \) is uniquely determined by the TF equation (convex minimization) [14]

\[
\mu^n_F \phi^n_F = (V_F + \beta_{12} |\phi^n_B|^2 + \beta_{22} |\phi^n_F|^{4/3}) \phi^n_F \quad \text{and} \quad \phi^n_F = \left( (\mu^n_F - V_F - \beta_{12} |\phi^n_B|^2)^+ \right)^{3/4}.
\]
where \((f)\) is \(\max\{f, 0\}\) and \(\mu^N\) is chosen such that \(\|\phi^N\|_{L^2} = 1\). Similarly to Theorem 2.1, we see that there exist \(\phi^\infty_B \in H^1 \cap L^{V_B}\) and a subsequence (we denote as the original sequence for simplicity) such that

\[
\phi^n_B \rightharpoonup \phi^\infty_B \quad \text{weakly in} \quad H^1 \cap L^{V_B}, \quad \text{and} \quad \phi^n_B \to \phi^\infty_B \quad \text{in} \quad L^p,
\]

where \(p\) is given in (2.4). Noticing the above TF equation, to satisfy the constraint \(\|\phi^\infty_B\|_{L^2} = 1\), we see that as \(n \to \infty\), \(\mu^N\) converges to some \(\mu^\infty_F\), and hence there exists some \(\phi^\infty_F\), such that \(\phi^n_F \to \phi^\infty_F\) in \(L^{2} \cap L^{10/3}\), and \(\|\phi^\infty_F\|_{L^2} = 1\). Making use of the weak convergence and strong convergence as above, one can easily deduce that

\[
E(\phi^n_B, \phi^n_F) \leq \liminf_{n \to \infty} E_1(\phi^n_B, \phi^n_F) = \min_{(\phi_B, \phi_F) \in S^1} E_1(\phi_B, \phi_F),
\]

which implies the existence of ground state.

**Nonexistence.** For the \(d = 3\) case, it is the same as Theorem 2.1. For \(d = 1, 2\), \(\beta_{22} < 0\), choosing \(\phi_F\) as a Dirac distribution, one can get the nonexistence. For \(d = 2, \beta_{22} < 0\), it is similar by choosing \(\phi_F\) as a Dirac distribution; if \(\beta_{11} < -C_n\), it reduces to the case in Theorem 2.1. Then we only consider \(d = 2, \beta_{12} < 0\), in this case, noticing that

\[
\inf_{\phi \in H^1(\mathbb{R}^2), \phi \neq 0} \frac{\|\nabla \phi\|_{L^2(\mathbb{R}^2)}^2 + \|\phi\|_{L^4(\mathbb{R}^2)}^4}{\|\phi\|_{L^\infty(\mathbb{R}^2)}^2} = 0,
\]

which is easily justified by noticing the fact \(H^1(\mathbb{R}^2) \not\subseteq L^\infty(\mathbb{R}^2)\), or if we take \(\phi(x) = |\ln(|x|)|^{1/4} \rho(|x|^2)\) \((x \in \mathbb{R}^2)\), where \(\rho\) is a smooth radial function such that \(\rho(r) = 0\) for \(|r| \geq 1/2\) and \(\rho(r) = 1\) for \(|r| \leq 1/4\). Thus, by choosing \(\phi_F\) sufficiently close to a Dirac distribution (as in the proof of Theorem 2.1), we could find \((\phi_B, \phi_F) \in S^1\) such that

\[
\int_{\mathbb{R}^d} \frac{\|\nabla \phi_B\|^2}{2} d\mathbf{x} + N_B/N + E_{\text{int}}(\phi_B, \phi_F) < 0.
\]

By letting \(\phi^\infty_B = \varepsilon^{-1} \phi_B(\varepsilon^{-1} \mathbf{x})\), \(\phi^\infty_F = \varepsilon^{-1} \phi_F(\varepsilon^{-1} \mathbf{x})\) \((\varepsilon > 0)\), we have \((\phi^\infty_B, \phi^\infty_F) \in S^1\) and

\[
E_1(\phi^\infty_B, \phi^\infty_F) = \frac{C_1}{\varepsilon^2} + \frac{C_2}{\varepsilon^{4/3}} + O(1) \quad \text{as} \quad \varepsilon \to 0^+,
\]

where \(C_1 < 0\). This leads to the nonexistence of the ground state for problem (B) in this case if sending \(\varepsilon \to 0^+\).

Very similarly to Theorem 2.4, we can obtain the uniqueness of the positive ground state for problem (B).

**Theorem 2.7.** For \(\beta_{11}, \beta_{12}, \beta_{22} \geq 0, 0 \leq V_B(x) \in C^1, V_F(x) \in L_{\text{loc}}\) with \(\lim_{|x| \to \infty} V_j(x) = \infty\) \((j = B, F)\), denote \(\rho_B(x) := |\phi_B(x)|^2, \rho_F(x) := |\phi_F(x)|^2\) \((x \in \mathbb{R}^d, d = 1, 2, 3)\), \(E_1 = \min_{(\phi_B, \phi_F) \in S^1} E_1(\phi_B, \phi_F)\); i.e., \(E_1\) is the minimal energy. Then the ground state \((\sqrt{V_B}, \sqrt{V_F})\) is unique under the following condition:

\[
\beta_{12}^2 \leq \frac{2}{\sqrt{15N_B \sqrt{N_F N_E}} \beta_{11} \beta_{22}^{3/2}}.
\]
The ground state energy $E_g$ can be bounded by using any testing functions, e.g., choosing $(\phi_B, \phi_F)$ such that $\phi_B \phi_F = 0$. Then there exists a constant $C$ depending on $V_B$ and $V_F$, such that

\begin{equation}
E_g \leq C(1 + \beta_{11} + \beta_{22}),
\end{equation}

which yields a sufficient condition for the uniqueness of the positive ground state.

### 3. Numerical method for computing the ground state

In this section, we propose an efficient numerical method—gradient flow with discrete normalization (GFDN)—to compute the ground state for coupled GP equation (1.4)–(1.5), i.e., the minimizer of problem (A) (1.9). The GFDN method can be directly extended to find the minimizer of problem (B) (1.14), and we will omit the details.

To compute the ground state of (1.4)–(1.5), we truncate the problem in a bounded domain $\Omega \subset \mathbb{R}^d$ due to the confining potentials, and we evolve the following gradient flow with discrete normalization to reach a steady state [4, 5, 7, 34]:

\begin{align}
\frac{\partial \phi_B}{\partial t} &= \left( \frac{\nabla^2}{2} - V_B(x) - \beta_{11} |\phi_B|^2 - \beta_{12} N_F |\phi_F|^2 \right) \phi_B, \quad t_n < t < t_{n+1}, \\
\frac{\partial \phi_F}{\partial t} &= \left( \frac{\nabla^2}{6\lambda} - V_F(x) - \beta_{12} N_B |\phi_B|^2 - \beta_{22} |\phi_F|^{4/3} \right) \phi_F, \quad t_n < t < t_{n+1}, \\
\phi_k(x, t_{n+1}) &= \frac{\phi_k(x, t_{n+1})}{\|\phi_k(x, t_{n+1})\|}, \quad k = B, F, \ x \in \Omega,
\end{align}

with zero boundary conditions and initial conditions as

\begin{equation}
\phi_B(x, t = 0) = \phi_B^0(x), \ \phi_F(x, t = 0) = \phi_F^0(x).
\end{equation}

Here we denote that $\phi_k(x, t_{n+1})^\pm = \lim_{t \to t_{n+1}^\pm} \phi_k(x, t) \ (k = B, F)$. This GFDN method, also known as the imaginary time method in the physics community, is widely used in the study of the BEC [7].

In practical calculation, we discretize GFDN (3.1)–(3.3) with the central finite difference method in space and the backward-Euler method in time. For simplicity of notation, we will only show the discretization for the case of one space dimension. Generalizations to higher dimensions are straightforward for tensor product grids and the properties remain valid without modifications.

Choose the computational domain as $\Omega = [a, b]$, the spatial mesh size as $\Delta x = \frac{b-a}{M}$, with $M$ being an even positive integer, and the time step $\Delta t > 0$. Denote the grid points $x_j = a + j\Delta x$ ($j = 0, 1, \ldots, M$) and time sequence $t_n = n\Delta t$ ($n = 0, 1, 2, \ldots$). Let $\phi^n_{j,B}$ and $\phi^n_{j,F}$ be the numerical approximations of $\phi_B(x_j, t_n)$ and $\phi_F(x_j, t_n)$, respectively. Write $\phi^n_B$ ($\phi^n_F$) as the solution vector with component $\psi^n_{j,B}$ ($\psi^n_{j,F}$) ($j = 0, 1, \ldots, M$). Denote $V_{j,B} = V_B(x_j)$, $V_{j,F} = V_F(x_j)$.

From $t = t_n$ to $t = t_{n+1}$, the detailed numerical algorithm for equations (3.1)–(3.3) is as follows [4, 7, 23]:

\begin{align}
\phi^*_{j+1,B} - \phi^n_{j,B} &= \frac{\phi^*_{j+1,B} - 2\phi^*_{j,B} + \phi^*_{j-1,B}}{2\Delta x^2} - \left( V_{j,B} + \beta_{11} |\phi^n_{j,B}|^2 + \beta_{12} N_F |\phi^n_{j,F}|^2 \right) \phi^n_{j,B}, \\
\phi^*_{j+1,F} - \phi^n_{j,F} &= \frac{\phi^*_{j+1,F} - 2\phi^*_{j,F} + \phi^*_{j-1,F}}{6\lambda \Delta x^2} - \left( V_{j,F} + \beta_{12} N_B |\phi^n_{j,B}|^2 + \beta_{22} |\phi^n_{j,F}|^{4/3} \right) \phi^n_{j,F},
\end{align}
(3.7) $\phi_{j,B}^{n+1} = \frac{\phi_{j,B}^n}{\|\phi_{j,B}^n\|^2}, \quad \phi_{j,F}^{n+1} = \frac{\phi_{j,F}^n}{\|\phi_{j,F}^n\|^2}$, where $j = 1, 2, \ldots, M - 1$, and the initial and boundary conditions are discretized as

$\phi_{0,B}^0 = \phi_{0}^0(x_j), \quad \phi_{0,F}^0 = \phi_{F}^0(x_j), \quad j = 0, 1, \ldots, M,$

$\phi_{0,B}^{n+1} = \phi_M^{n+1}(x), \quad \phi_{0,F}^{n+1} = \phi_M^{n+1}(x), \quad n = 0, 1, \ldots.$

Here the discrete $l^2$-norm for the solution $\phi_{B}^*$ is defined as $\|\phi_{B}^*\|_2 = \sqrt{\frac{\sum_{j=0}^{M-1} |\phi_{j,B}^*|^2}{M}}$, and the discrete $l^2$-norm for $\phi_{F}^*$ is similarly defined.

The discretized system (3.5)–(3.6) can be solved very efficiently by the Thomas algorithm. In higher dimensions (such as two or three dimensions), the associated discretized system can be solved with iterative methods, for example, the Jacobian iterative method or the Gauss–Seidel iterative method [6, 34].

As stated in the beginning of this section, the above method can be easily extended to find the ground state of model (1.16), where TF approximation is applied to the fermions. In computation, people sometimes use TF approximations for both bosons and fermions, which results in the following energy by neglecting the total kinetic energy part (2.2) in (1.8):

$$E_2(\phi_B, \phi_F) = \int_{\mathbb{R}^d} \left( V_B |\phi_B|^2 + \frac{\beta_{11}}{2} |\phi_B|^4 \right) dx - \frac{N_B}{N_B} + \beta_{12} \int_{\mathbb{R}^d} |\phi_F|^2 |\phi_B|^2 dx - \frac{N_B N_F}{N_B}$$

$$+ \int_{\mathbb{R}^d} \left( V_F |\phi_F|^2 + \frac{3 \beta_{22}}{5} |\phi_F|^4 \right) dx \cdot \frac{N_F}{N_F}.$$  (3.8)

Then finding the ground state of this TF model involves minimizing the energy $E_2(\phi_B, \phi_F)$ under the constraints (1.13):

(3.9) Find $(\phi_B^* (x), \phi_F^* (x)) \in S_d^2$ such that

$$E_2(\phi_B^* (x), \phi_F^* (x)) = \min_{(\phi_B, \phi_F) \in S_d^2} E_2(\phi_B, \phi_F),$$

where $S_d^2$ is defined as

$$S_d^2 = \left\{ (\phi_B, \phi_F) \mid \int_{\mathbb{R}^d} |\phi_B|^2 dx = 1, \quad \int_{\mathbb{R}^d} |\phi_F|^2 dx = 1, \quad E_2(\phi_B, \phi_F) < \infty \right\}.$$  (3.10)

Similarly to problems (A) and (B), it is not difficult to find the Euler–Lagrange equation for the ground state of (3.8), which reduces to an algebraic system. This system is difficult to solve, and most studies with the model (C) are based on numerics. Our GFDN method (3.5) can be easily extended to solve problem (C).

The TF approximation (C) is limited to the nonnegative parameters $\beta_{11}, \beta_{12}, \beta_{22}$. When one of the parameters $\beta_{11}, \beta_{12},$ and $\beta_{22}$ becomes negative, it is easy to show $\inf_{(\phi_B, \phi_F) \in S_d^2} E_2(\phi_B, \phi_F) = -\infty$, which means there is no ground state. However, the ground state may exist in coupled GP model (A) (1.9) (Theorem 2.1). In the next section, we will focus on the numerical study on model (A) (1.9) for the ground states of Bose–Fermi mixtures.

Throughout our computations, the threshold of approaching steady state solutions for the algorithm (3.5) is set as

$$\max_{1 \leq j \leq M-1} |\phi_{j,B}^{n+1} - \phi_{j,B}^n| < \varepsilon, \quad \max_{1 \leq j \leq M-1} |\phi_{j,F}^{n+1} - \phi_{j,F}^n| < \varepsilon$$  (3.11)

for arbitrary step $n$ and small number $\varepsilon$ (typically chosen as $10^{-6}$ or $10^{-7}$).
4. Numerical results. Most previous numerical investigations on the ground state structure of Bose–Fermi mixtures relied on TF approximation for the Fermi gas, and there have been some numerical studies based on coupled GP equations for both bosons and fermions in one [29], two [2], and three dimensions [23]. Here we present numerical results based on efficient computation of coupled GP equations and compare the results with those obtained by TF approximations.

In what follows, we first apply the method (3.7) to investigate the ground state structure of Bose–Fermi mixtures in one and two dimensions, respectively, with the coupled GP equations (1.4)–(1.5). In the last subsection, we will compare the ground states computed from different models (A), (B), and (C).

In all of the numerical computation, the following set of parameters are considered:

\[ \omega_B = \omega_F = 2\pi \times 200 \text{ Hz}, \quad m_B = 7.016 \text{ u}, \quad m_F = 6.0151 \text{ u}, \]

where the atomic unit \( u = 1.6605 \times 10^{-27} \text{ kg} \), the Planck constant \( \hbar = 1.0546 \times 10^{-34} \text{ Js} \), and \( \lambda = m_F/m_B = 0.8573 \). The scattering length \( a_{BB}, a_{BF} \) can be tuned; for example, when \( a_{BF} = a_{BB} = 1 \text{ nm} \) and \( N_B = N_F = 10^4 \), we have \( \beta_{11} = 12.6418, \beta_{12} N_F = 50.7171, \beta_{12} N_B = 50.7171, \) and \( \beta_{22} = 4112.8 \). Unless specified otherwise, in one dimension, we assume \( V_B(x,y) = 0.5x^2 \) and \( V_F(x) = \lambda V_B(x) \) with \( \lambda = 0.8573 \); in two dimensions, we assume \( V_B(x,y) = 0.5(x^2 + y^2) \) and \( V_F(x,y) = \lambda V_B(x,y) \) with \( \lambda = 0.8573 \). We denote the ratio as \( \nu = a_{BF}/a_{BB} \). In most of our computation, we change the ratio \( \nu \) and look into how the ground state solutions change accordingly.

4.1. Numerical results in one dimension. In this subsection, we compute the ground state solutions of Bose–Fermi mixtures in one dimension by solving problem (A).
ANALYSIS AND COMPUTATION FOR BOSE–FERMI MIXTURES

Fig. 4.2. Ground state solutions \( (\phi_B^g(x), \phi_F^g(x)) \) for bosons (solid curves) and fermions (dashed curves), respectively, for different \( \nu \) when a large \( N_b \) is applied in Example 2 for one dimension.

Fig. 4.3. Ground state solutions \( (\phi_B^g(x), \phi_F^g(x)) \) for bosons (solid curves) and fermions (dashed curves), respectively, for different \( \nu \) when a large \( \beta_{11} \) is applied in Example 3 for one dimension.

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Fig. 4.4. Ground state solutions \((\phi^B_g(x), \phi^F_g(x))\) for bosons (solid curves) and fermions (dashed curves), respectively, for different \(\nu\) when large \(N_F\) is applied in Example 4 for one dimension.

Fig. 4.5. Ground state solutions \((\phi^B_g(x), \phi^F_g(x))\) for bosons (solid curves) and fermions (dashed curves), respectively, for different \(\nu\) when large \(\beta_{11}\), large \(N_B\), and large \(N_F\) are applied in Example 5 for one dimension.
Example 1. We take $\beta_{11} = 12.6418$, $\beta_{12} N_F = 12.6418 \times \nu$, $\beta_{12} N_B = 12.6418 \times \nu$, and $\beta_{22} = 4028.2$ ($N_B = N_F = 10^4$). The ratio $\nu$ is changed from big enough (100) to small enough ($-29$). Figure 4.1 shows that the boson condensate lies in a “sea” of fermions at different regimes. However, when $\nu$ becomes negative (i.e., $a_{BF} < 0$), the bosons attract the fermions, which leads to the BEC density increases, and eventually the boson condensate collapses.

Example 2. We take $\beta_{11} = 1264.18$, $\beta_{12} N_F = 1264.18 \times \nu$, $\beta_{12} N_B = 1264.18 \times \nu$, $\beta_{22} = 886.0764$ ($N_B = N_F = 10^6$). The ratio $\nu$ is changed from 0.25 to 20. Figure 4.2 shows that the fermion condensate constitutes a “shell” around the boson condensate after the ratio $\nu$ is increased to 12. Compared with the numerical results presented in Example 1, a much larger $N_B$ is used here.

Example 3. We take $\beta_{11} = 63209$, $\beta_{12} N_F = 63209 \times \nu$, $\beta_{12} N_B = 63209 \times \nu$, and $\beta_{22} = 4028.2$ ($N_B = N_F = 10^4$). The ratio $\nu$ is changed from 0 to 1.25. Figure 4.3 shows that the fermion condensate constitutes a “core” inside the boson condensate after the ratio $\nu$ is increased to 0.75. Compared with the numerical results presented in Example 1, a much larger $\beta_{11}$ (tuned by the scattering length $a_{BB}$) is used.
Fig. 4.7. Surface plots for ground state solutions \((\phi^B_0(x,y), \phi^F_0(x,y))\) of Bose–Fermi mixtures at (a) \(\nu = 0.5\) and (b) \(\nu = 0.75\) when large \(\beta_{11}\) is applied in Example 7 for two dimensions.

4.2. Numerical results in two dimensions. In this subsection, we compute the ground state solutions of Bose–Fermi mixtures in two dimensions by solving problem (A). In most cases, the computation domain is \([-20, 20] \times [-20, 20]\) and the mesh size is \(\frac{40}{12} \times \frac{40}{112}\). We repeat some computations similar to those in the previous subsection.
ANALYSIS AND COMPUTATION FOR BOSE–FERMI MIXTURES 775

Example 6. We take $N_B = 10^6$, $N_F = 10^4$, $\beta_{11} = 12.6418$, $\beta_{12}N_B = 1264.18$, $\beta_{12}N_F = 12.6418$, $\beta_{22} = 4112.8$. Here we choose a larger particle number $N_F$. Figure 4.6 shows the ground state solutions of Bose–Fermi mixtures at zero temperature in two cases: $\nu = 5$ and $\nu = 10$. From these figures, we can see that the Fermi gas may first constitute a “shell” around the boson condensate, and the boson condensate then forms a core in the sea of fermions when larger $\nu$ is tuned.

Example 7. We take $N_B = N_F = 10^4$, $\beta_{11} = 63209$, $\beta_{12}N_B = 63209$, $\beta_{12}N_F = 63209 \times \nu$, $\beta_{22} = 4112.8$. Here a larger scattering length $a_{BB}$ is used, which leads to larger $\beta_{11}$. Figure 4.7 shows the ground state solutions of Bose–Fermi mixtures in this case. From these figures, it can be observed that the boson condensate may first constitute a “shell” around the fermion condensate, and the fermion condensate then forms a core in the sea of bosons when larger $\nu$ is tuned.

Example 8. We take $N_B = 10^4$, $N_F = 10^6$, $\beta_{11} = 12.6418$, $\beta_{12}N_B = 1264.18$, $\beta_{12}N_F = 1264.18 \times \nu$, $\beta_{22} = 88608$. Here we choose a larger particle number $N_F$. Figure 4.8 shows that the boson condensate may be squeezed into one peak in the sea of fermions when larger $\nu$ is tuned.

Fig. 4.8. Surface plots for ground state solutions ($\phi_B^g(x,y), \phi_F^g(x,y)$) of Bose–Fermi mixtures at (a) $\nu = 5$ and (b) $\nu = 50$ when large $N_F$ is applied in Example 8 for two dimensions.
Example 9. We take $N_B = N_F = 10^6$, $\beta_{11} = 126418$, $\beta_{12}N_B = 126418$, $\beta_{12}N_F = 126418 \times \nu$, $\beta_{22} = 88608$. Here much larger $\beta_{11}$, $N_B$, and $N_F$ are used in the computation. Figure 4.9 shows that the boson condensate and the fermion condensate are interwoven when larger $\nu$ is tuned.

4.3. Comparison between different models. Finally, we compare the ground state solutions for all three different models, approximation A, approximation B, and approximation C, which are the minimizers of the minimization problems (A) (1.9), (B) (1.14), and (C) (3.9), respectively.

In the first computation, we compare approximation A with approximation C. We consider $N_B = N_F = N$, $\beta_{11} = 63.209 \times N/10^4$, $\beta_{12}N_B = \beta_{12}N_F = 15.8023 \times N/10^4$, $\beta_{22} = 8.86 \times (N)^{2/3}$. Tables 4.1 and 4.2 list the energies and the chemical potentials obtained by these two approximations (A, C) in one and two dimensions, respectively. From Tables 4.1 and 4.2, we can observe that for smaller $N$ (for example, $N \leq 10^4$), the numerical ground state solutions obtained from these two approximations are quite similar.
Table 4.1
The energy and the chemical potentials calculated by the numerical ground state for the corresponding model for different $N$ in one dimension.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E$</th>
<th>$\mu_B$</th>
<th>$\mu_F$</th>
<th>$E_2$</th>
<th>$\mu^2_B$</th>
<th>$\mu^2_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^4$</td>
<td>13.15</td>
<td>0.38</td>
<td>19.25</td>
<td>12.98</td>
<td>0.25</td>
<td>19.25</td>
</tr>
<tr>
<td>$10^5$</td>
<td>41.35</td>
<td>1.20</td>
<td>60.90</td>
<td>41.28</td>
<td>1.16</td>
<td>60.88</td>
</tr>
<tr>
<td>$10^6$</td>
<td>131.65</td>
<td>5.43</td>
<td>192.6</td>
<td>131.63</td>
<td>5.42</td>
<td>192.61</td>
</tr>
<tr>
<td>$10^7$</td>
<td>421.4</td>
<td>25.37</td>
<td>631.7</td>
<td>427.3</td>
<td>25.47</td>
<td>631.7</td>
</tr>
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</table>

Table 4.2
The energy and the chemical potentials calculated by the numerical ground state for the corresponding model for different $N$ in two dimensions.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E$</th>
<th>$\mu_B$</th>
<th>$\mu_F$</th>
<th>$E_2$</th>
<th>$\mu^2_B$</th>
<th>$\mu^2_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^2$</td>
<td>6.15</td>
<td>0.88</td>
<td>7.62</td>
<td>5.58</td>
<td>0.22</td>
<td>7.60</td>
</tr>
<tr>
<td>$10^3$</td>
<td>15.30</td>
<td>2.37</td>
<td>19.13</td>
<td>14.11</td>
<td>0.72</td>
<td>19.09</td>
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<td>$10^4$</td>
<td>39.27</td>
<td>7.37</td>
<td>48.10</td>
<td>35.76</td>
<td>2.27</td>
<td>47.96</td>
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<tr>
<td>$10^5$</td>
<td>101.98</td>
<td>23.4</td>
<td>121.05</td>
<td>90.83</td>
<td>7.20</td>
<td>120.48</td>
</tr>
<tr>
<td>$10^6$</td>
<td>267.22</td>
<td>74.60</td>
<td>304.97</td>
<td>231.40</td>
<td>22.86</td>
<td>302.88</td>
</tr>
<tr>
<td>$10^7$</td>
<td>707.22</td>
<td>238.18</td>
<td>769.66</td>
<td>641.59</td>
<td>73.09</td>
<td>893.93</td>
</tr>
</tbody>
</table>

Table 4.3
The energy and the chemical potentials calculated by the numerical ground state for the corresponding model for different $N$ in one dimension.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E$</th>
<th>$\mu_B$</th>
<th>$\mu_F$</th>
<th>$E_1$</th>
<th>$\mu^1_B$</th>
<th>$\mu^1_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>73.824</td>
<td>0.0745</td>
<td>110.644</td>
<td>73.822</td>
<td>0.0745</td>
<td>110.652</td>
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<tr>
<td>$10^4$</td>
<td>254.039</td>
<td>0.0118</td>
<td>381.046</td>
<td>254.051</td>
<td>0.0118</td>
<td>381.262</td>
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<td>$10^5$</td>
<td>810.534</td>
<td>0.00328</td>
<td>1215.798</td>
<td>821.952</td>
<td>0.0034</td>
<td>1259.609</td>
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<tr>
<td>$10^6$</td>
<td>2623.535</td>
<td>0.00162</td>
<td>4047.370</td>
<td>3146.391</td>
<td>0.00226</td>
<td>5107.231</td>
</tr>
</tbody>
</table>

Table 4.4
The energy and the chemical potentials calculated by the numerical ground state for the corresponding model for different $N$ in two dimensions.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E$</th>
<th>$\mu_B$</th>
<th>$\mu_F$</th>
<th>$E_1$</th>
<th>$\mu^1_B$</th>
<th>$\mu^1_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$</td>
<td>24.933</td>
<td>0.1713</td>
<td>25.537</td>
<td>24.884</td>
<td>0.1070</td>
<td>25.192</td>
</tr>
<tr>
<td>$10^4$</td>
<td>67.819</td>
<td>0.02278</td>
<td>68.3996</td>
<td>67.8076</td>
<td>0.01411</td>
<td>68.2483</td>
</tr>
<tr>
<td>$10^5$</td>
<td>171.8275</td>
<td>0.00395</td>
<td>172.4296</td>
<td>171.8314</td>
<td>0.0024</td>
<td>172.6034</td>
</tr>
<tr>
<td>$10^6$</td>
<td>431.9868</td>
<td>0.00106</td>
<td>432.5847</td>
<td>432.1101</td>
<td>0.00064</td>
<td>435.6271</td>
</tr>
</tbody>
</table>

In the second computation, we compare approximation A with approximation B. We consider $N_B = 100$, $N_F = N$, $\beta_{11} = 6.3209$, $\beta_{12} = 1.58023$, $\beta_{12}N_B = 1.58023 \times \frac{1}{N^3}$, $\beta_{12}N_F = 8.86 \times (N)^{2/3}$. Tables 4.3 and 4.4 show us the energies and the chemical potentials obtained by these two approximations (A, B) in one and two dimensions.
dimensions, respectively. From Tables 4.3 and 4.4, we can observe that for smaller $N$ (for example, $N \leq 10^4$), the numerical ground state solutions obtained from these two approximations are quite similar.

5. Conclusions. We have rigorously proved the existence and uniqueness of the ground state solutions of Bose–Fermi mixtures, where the Fermi gas is nonsuperfluid degenerate. We have also presented an efficient method—gradient flow with discrete normalization—for computing the ground state structure of Bose–Fermi mixtures at zero temperature. We applied the method to computing the ground state solutions and found various kinds of ground state structure for the Bose–Fermi mixture. Our extensive numerical studies both in one and two dimensions showed that we can extract many similar interesting phenomena such that the Fermi gas may constitute a “shell” around or a “core” inside the Bose condensate in some regimes; the Bose–Fermi mixture may experience collapse if the scattering length $a_{BF}$ is negative and small enough; the large enough ratio $\nu = a_{BF}/a_{BB}$ may bring in either a complete separation or a demixing process of the Bose–Fermi mixture.

Acknowledgment. We would like to thank Professor Weizhu Bao for the very helpful and stimulating discussions on the subject.

REFERENCES


