The L^2-Critical Limiting Behavior of Ground States for Fermionic Quantum Systems

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Abstract

We study ground states of the N coupled fermionic quantum system with the Coulomb potential $V(x)$ in the L^2-critical case, which admits a parameter $a > 0$ to describe the attractive strength of the quantum particles. For any given $N \in \mathbb{N}^+$, we prove that the system admits ground states, if and only if the attractive strength a satisfies $0 < a < a_N^*$, where the critical constant $0 < a_N^* < \infty$ is the same as the best constant of a dual finite-rank Lieb-Thirring inequality. By developing the so-called blow-up analysis of many-body fermionic systems, we also analyze the limiting mass concentration behavior of ground states for the system as $a \nearrow a_N^*$.

Keywords: Fermionic quantum systems; Coulomb potential; L^2-critical case; Limiting behavior

Contents

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1 Introduction

It is known (cf. [11, 13]) that a system of N identical quantum particles with spin s (such as photons, electrons and neutrons) is usually described by an energy functional of the corresponding N-body normalized wave functions $\Psi \in \bigotimes_{i=1}^N L^2(\mathbb{R}^3, \mathbb{C}^{2s+1})$. In this paper we study ground states of N spinless (i.e., $s = 0$) fermions with the Coulomb potential in the L^2-critical case, which can be described by (cf. [11]) the minimizers of the following constraint variational problem

$$E_a(N) := \inf\Big\{\mathcal{E}_a(\Psi) : \ \|\Psi\|_2^2 = 1, \ \Psi \in \wedge^N L^2(\mathbb{R}^3, \mathbb{C}) \cap H^1(\mathbb{R}^{3N}, \mathbb{C})\Big\}, \quad a > 0, \tag{1.1}$$

where the energy functional $\mathcal{E}_a(\Psi)$ satisfies

$$\mathcal{E}_a(\Psi) := \sum_{i=1}^N \int_{\mathbb{R}^{3N}} \Big(|\nabla_{x_i}\Psi|^2 - \sum_{k=1}^K \frac{1}{|x_i - y_k|}|\Psi|^2\Big) dx_1 \cdots dx_N - a\int_{\mathbb{R}^3} \rho_\Psi^{\frac{5}{3}}(x)dx. \tag{1.2}$$

Here $y_1, y_2, \cdots, y_K \in \mathbb{R}^3$ are different from each other, the parameter $a > 0$ represents the attractive strength of the quantum particles, $\wedge^N L^2(\mathbb{R}^3, \mathbb{C})$ is the subspace of $L^2(\mathbb{R}^{3N}, \mathbb{C})$ consisting of all antisymmetric wave functions, and the one-particle density ρ_Ψ of Ψ is defined as

$$\rho_\Psi(x) := N \int_{\mathbb{R}^{3(N-1)}} |\Psi(x, x_2 \cdots, x_N)|^2 dx_2 \cdots dx_N.$$

We refer [4, 7, 11, 13] and the references therein for detailed physical motivations of the variational problem (1.1).

Following the spectral theorem (see [7] and the references therein), we denote the non-negative self-adjoint operator $\gamma = \sum_{i=1}^N n_i|u_i\rangle\langle u_i|$ on $L^2(\mathbb{R}^3, \mathbb{C})$ by

$$\gamma\varphi(x) = \sum_{i=1}^N n_i u_i(x)(\varphi, u_i)_{L^2(\mathbb{R}^3,\mathbb{C})}, \quad \forall\ \varphi \in L^2(\mathbb{R}^3, \mathbb{C}), \tag{1.3}$$

where both $n_i \geq 0$ and $u_i \in L^2(\mathbb{R}^3, \mathbb{C})$ hold for $i = 1, \cdots, N$. Moreover, we use

$$\rho_\gamma(x) = \sum_{i=1}^N n_i|u_i(x)|^2 \tag{1.4}$$

to denote the corresponding density of γ. Similar argument of [1, Appendix A and Lemma 2.3] then yields that the problem (1.1) can be reduced equivalently to the following form

$$\begin{aligned} E_a(N) = \inf\Big\{\mathcal{E}_a(\gamma) : \ &\gamma = \sum_{i=1}^N |u_i\rangle\langle u_i|, \ u_i \in H^1(\mathbb{R}^3, \mathbb{R}), \\ &(u_i, u_j)_{L^2} = \delta_{ij}, \ i, j = 1, \cdots, N\Big\}, \ \ a > 0, \ \ N \in \mathbb{N}^+, \end{aligned} \tag{1.5}$$

where the energy functional $\mathcal{E}_a(\gamma)$ satisfies

$$\mathcal{E}_a(\gamma) := \mathrm{Tr}\big(-\Delta + V(x)\big)\gamma - a\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx, \tag{1.6}$$

and the function $V(x) \le 0$ is the Coulomb potential of the form

$$V(x) := -\sum_{k=1}^{K} \frac{1}{|x - y_k|} \tag{1.7}$$

containing different singular points $y_1, \cdots, y_K \in \mathbb{R}^3$. Throughout the paper we focus on the analysis of the variational problem $E_a(N)$ defined in (1.5), instead of (1.1). As a continuation of [1], which handles the L^2-subcritical case of $E_a(N)$, the main purpose of the present paper is to analyze the limiting concentration behavior of minimizers for $E_a(N)$. As far as we know, this is the first work on investigating the limiting behavior of ground states for L^2-critical many-body fermionic systems.

For any given $N \in \mathbb{N}^+$, we now consider the following minimization problem

$$\begin{aligned} 0 < a_N^* := \inf \Big\{ \frac{\|\gamma\|^{\frac{2}{3}} \mathrm{Tr}(-\Delta\gamma)}{\int_{\mathbb{R}^3} \rho_\gamma^{5/3} dx} :\ \gamma = \sum_{i=1}^{N} n_i |u_i\rangle\langle u_i| \neq 0, \\ u_i \in H^1(\mathbb{R}^3, \mathbb{C}),\ \ (u_i, u_j)_{L^2} = \delta_{ij},\ \ n_i \ge 0 \Big\}, \end{aligned} \tag{1.8}$$

where ρ_γ is as in (1.4), and $\|\gamma\| > 0$ denotes the norm of the operator γ. The proof of [4, Theorem 6] gives essentially that for any $N \in \mathbb{N}^+$, the best constant $a_N^* \in (0, +\infty)$ of (1.8) is attained, and any minimizer $\gamma^{(N)}$ of a_N^* can be written in the form

$$\gamma^{(N)} = \|\gamma^{(N)}\| \sum_{i=1}^{R_N} |Q_i\rangle\langle Q_i|,\ \ (Q_i, Q_j) = \delta_{ij}\ \text{ for }\ i, j = 1, \cdots, R_N, \tag{1.9}$$

where the positive integer $R_N \in [1, N]$, and the orthonormal family $Q_1, \cdots, Q_{R_N}$ solves the following fermionic nonlinear Schrödinger system

$$\Big[-\Delta - \frac{5}{3} a_N^* \Big(\sum_{j=1}^{R_N} |Q_j|^2 \Big)^{\frac{2}{3}} \Big] Q_i = \hat{\mu}_i Q_i \ \text{ in } \mathbb{R}^3,\ \ i = 1, \cdots, R_N. \tag{1.10}$$

Here $\hat{\mu}_1 < \hat{\mu}_2 \le \cdots \le \hat{\mu}_{R_N} < 0$ are the R_N first eigenvalues (counted with multiplicity) of the operator

$$\hat{H}_{\gamma^{(N)}} := -\Delta - \frac{5}{3} a_N^* \Big(\sum_{j=1}^{R_N} |Q_j|^2 \Big)^{\frac{2}{3}} \ \text{ in } \mathbb{R}^3.$$

We note from Mathieu Lewin[1] that any optimizer $\gamma^{(N)}$ of the problem (1.8) is essentially a real-valued operator on $L^2(\mathbb{R}^3, \mathbb{R})$, see Lemma 2.2 below for more details. Moreover, it was proved in [4, Proposition 11] that

$$a_N^* > a_{2N}^* \text{ holds for any } N \in \mathbb{N}^+, \tag{1.11}$$

and thus there exists an infinite sequence of integers $N_1 = 1 < N_2 = 2 < N_3 < \cdots$ such that

$$a_{N_m - 1}^* > a_{N_m}^*,\quad m = 2, 3, 4, \cdots, \tag{1.12}$$

[1]Private communications.

which further implies that any minimizer $\gamma^{(N_m)}$ of $a^*_{N_m}$ satisfying (1.12) must satisfy $\mathrm{Rank}\big(\gamma^{(N_m)}\big) = N_m$. We also comment that the uniqueness of minimizers for a^*_N is still open for any $N \geq 2$.

The minimization problem $E_a(1)$ defined in (1.5) is essentially an L^2-critical constraint variational problem, which was investigated widely over the past few years, starting from the earlier work [8]. Moreover, we expect that for any $N \in \mathbb{N}^+$, the minimizers of $E_a(N)$ are connected with ground states of a fermionic nonlinear Schrödinger system, in the sense that

Definition 1.1. (*Ground states*). A system $(u_1, \cdots, u_N) \in \big(H^1(\mathbb{R}^3)\big)^N$ with $(u_i, u_j)_{L^2} = \delta_{ij}$ is called a ground state of

$$H_V u_i := \Big[-\Delta + V(x) - \frac{5a}{3}\Big(\sum_{j=1}^N |u_j|^2\Big)^{\frac{2}{3}}\Big] u_i = \mu_i u_i \ \text{ in } \ \mathbb{R}^3, \ \ i = 1, \cdots, N, \tag{1.13}$$

if it solves the system (1.13), where $\mu_1 < \mu_2 \leq \cdots \leq \mu_N < 0$ are the N first eigenvalues (counted with multiplicity) of the operator H_V.

1.1 Main results

The purpose of this subsection is to introduce the main results of the present paper. Motivated by [4,8], in this paper we first prove the following existence and nonexistence of minimizers for $E_a(N)$.

Theorem 1.1. *For any fixed $N \in \mathbb{N}^+$, suppose $E_a(N)$ is defined in (1.5), and let $0 < a^*_N < \infty$ be defined by (1.8). Then*

1. *If $0 < a < a^*_N$, then $E_a(N)$ admits at least one minimizer. Moreover, any minimizer γ of $E_a(N)$ can be written as $\gamma = \sum_{i=1}^N |u_i\rangle\langle u_i|$, where $(u_1, \cdots, u_N)$ is a ground state of the following fermionic nonlinear Schrödinger system*

$$H_V u_i := \Big[-\Delta + V(x) - \frac{5a}{3}\Big(\sum_{j=1}^N u_j^2\Big)^{\frac{2}{3}}\Big] u_i = \mu_i u_i \ \text{ in } \ \mathbb{R}^3, \ \ i = 1, \cdots, N. \tag{1.14}$$

   Here the Coulomb potential $V(x) \leq 0$ is as in (1.7), and $\mu_1 < \mu_2 \leq \cdots \leq \mu_N < 0$ are the N first eigenvalues, counted with multiplicity, of the operator H_V in $\mathbb{R}^3$.

2. *If $a \geq a^*_N$, then $E_a(N)$ does not admit any minimizer, and $E_a(N) = -\infty$.*

We remark that for any fixed $N \in \mathbb{N}^+$, Theorem 1.1 provides a complete classification on the existence and nonexistence of minimizers for $E_a(N)$ in terms of $a > 0$. Moreover, the proof of Theorem 1.1 implies that Theorem 1.1 can be naturally extended not only to the general singular potential $V(x) = -\sum_{k=1}^K |x - y_k|^{-s_k}$ with $0 < s_k < 2$, but also to the generally dimensional case $\mathbb{R}^d$ with $d \geq 3$, if the exponent $\frac{5}{3}$ in the last term of (1.6) is replaced by $1 + \frac{2}{d}$. On the other hand, in order to prove Theorem 1.1, in Section 2 we shall derive the boundedness, monotonicity and some other analytical properties of the energy $E_a(N)$ in terms of $N > 0$ and $a > 0$. Furthermore, the existence proof of Theorem 1.1 is based on an adaptation of the classical concentration compactness principle (cf. [14] [15, Section 3.3]). Towards this purpose, the key step is to prove in Subsection 2.1 that the following strict inequality holds for any fixed $0 < \lambda < N$,

$$E_a(N) < E_a(\lambda), \ \text{ if } \ E_a(\lambda) \ \text{admits minimizers,} \tag{1.15}$$

where $E_a(\lambda)$ is defined by (2.1) below, see (2.61) for more details.

By developing the so-called blow-up analysis of many-body fermionic systems, in the following we focus on exploring the limiting concentration behavior of minimizers for $E_a(N)$ as $a \nearrow a_N^*$. For simplicity, we first address the particular case $N = 2$, where $a_1^* > a_2^*$ holds true in view of (1.11).

Theorem 1.2. *Let $\gamma_a = \sum_{i=1}^{2} |u_i^a\rangle\langle u_i^a|$ be a minimizer of $E_a(2)$ for $0 < a < a_2^*$, where the orthonormal system (u_1^a, u_2^a) is a ground state of (1.14). Then for any sequence $\{a_n\}$ satisfying $a_n \nearrow a_2^*$ as $n \to \infty$, there exist a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ and a point $y_{k_*} \in \{y_1, \cdots, y_K\}$ given by (1.7) such that*

$$\begin{aligned} w_i^{a_n}(x) :=\, & \epsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}\big(\epsilon_{a_n} x + y_{k_*}\big) \\ & \to w_i(x) \ \ \textit{strongly in} \ \ H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3) \ \ \textit{as} \ \ n \to \infty, \quad i = 1, 2, \end{aligned} \tag{1.16}$$

and

$$\lim_{n\to\infty} \epsilon_{a_n} E_{a_n}(2) = -\int_{\mathbb{R}^3} \rho_\gamma^{5/3} dx, \tag{1.17}$$

where $\epsilon_{a_n} := a_2^* - a_n > 0$, and $\gamma := \sum_{i=1}^{2} |w_i\rangle\langle w_i|$ satisfying $(w_i, w_j) = \delta_{ij}$ is an optimizer of a_2^*.

Remark 1.1. (1). As a byproduct of Theorem 1.2, we shall derive in (3.57) that the following identities hold true:

$$\frac{1}{a_2^*} \mathrm{Tr}\big(-\Delta\gamma\big) = \int_{\mathbb{R}^3} \rho_\gamma^{5/3} dx = \frac{1}{2} \int_{\mathbb{R}^3} |x|^{-1} \rho_\gamma dx, \tag{1.18}$$

where $\gamma = \sum_{i=1}^{2} |w_i\rangle\langle w_i|$ given by (1.16) is an optimizer of a_2^*.

(2). The proof of Theorem 1.2 shows that Theorem 1.2 actually holds true for any $E_a(N)$, provided that $2 \le N \in \mathbb{N}^+$ satisfies $a_{N-1}^* > a_N^*$, see Remark 3.1 for more details.

(3). The L^∞-uniform convergence (1.16) presents the following mass concentration behavior of minimizers $\gamma_{a_n} = \sum_{i=1}^{2} |u_i^{a_n}\rangle\langle u_i^{a_n}|$ for $E_{a_n}(2)$ as $a_n \nearrow a_2^*$:

$$\gamma_{a_n}(x,y) \approx \big(a_2^* - a_n\big)^{-3} \gamma\Big(\frac{x - y_{k_*}}{a_2^* - a_n}, \frac{y - y_{k_*}}{a_2^* - a_n}\Big) \ \text{ as } \ a_n \nearrow a_2^*, \tag{1.19}$$

where $\gamma(x,y) = \sum_{i=1}^{2} w_i(x) w_i(y)$ denotes the integral kernel of γ, and $y_{k_*} \in \{y_1, \cdots, y_K\}$ is as in Theorem 1.2. This implies that the mass of the minimizers for $E_{a_n}(2)$ as $a_n \nearrow a_2^*$ concentrates at a global minimum point $y_{k_*} \in \{y_1, \cdots, y_K\}$ of the Coulomb potential $V(x) = -\sum_{k=1}^{K} |x - y_k|^{-1}$. It is still interesting to further address the exact point y_{k_*} among the set $\{y_1, \cdots, y_K\}$.

We now follow three steps to explain briefly the general strategy of proving Theorem 1.2:

The first step of proving Theorem 1.2 is to derive the precise upper bound (3.16) of the energy $E_a(2)$ as $a \nearrow a_2^*$, which further implies the estimates of Lemma 3.1. Due to the orthonormal constrained conditions, it however seems difficult to borrow the existing methods (e.g. [8]) of analyzing the L^2-critical variational problems. In order to overcome this difficulty, in Lemma 3.1 we shall construct a new type of test operators involved with the complicated analysis.

As the second step of proving Theorem 1.2, we shall prove Lemma 3.2 on the H^1-uniform convergence of the sequence $\{w_i^{a_n}\}_n$ as $a_n \nearrow a_2^*$ for $i = 1, 2$, where $w_i^{a_n}$ is defined by

$$w_i^{a_n}(x) := \epsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}\big(\epsilon_{a_n} x + y_{k_*}\big), \quad \epsilon_{a_n} := a_2^* - a_n > 0, \tag{1.20}$$

and $\gamma_{a_n} = \sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ is a minimizer of $E_{a_n}(2)$. To reach this aim, in Section 3 we shall apply the following finite-rank Lieb-Thirring inequality

$$L_N^* \int_{\mathbb{R}^3} W^{\frac{5}{2}}(x)dx \geq \sum_{i=1}^N \big|\lambda_i(-\Delta - W(x))\big|, \quad \forall\, 0 \leq W(x) \in L^{\frac{5}{2}}(\mathbb{R}^3)\backslash\{0\}, \tag{1.21}$$

where the best constant $L_N^* \in (0, +\infty)$ is attainable (cf. [5, Corollary 2]), and $\lambda_i\big(-\Delta - W(x)\big) \leq 0$ denotes the ith negative eigenvalue (counted with multiplicity) of $-\Delta - W(x)$ in $L^2(\mathbb{R}^3)$ when it exists, and zero otherwise. We point out that by proving

$$a_N^* \big(L_N^*\big)^{\frac{2}{3}} = \frac{3}{5}\Big(\frac{2}{5}\Big)^{\frac{2}{3}}, \tag{1.22}$$

it was addressed in [3–5] that the corresponding inequality of (1.8) is dual to the finite rank Lieb-Thirring inequality (1.21). Applying the energy estimates of the first step, together with the above dual relationship and the strict inequality $a_1^* > a_2^*$, we shall prove the crucial $L^{\frac{5}{3}}$-uniform convergence of the density sequence $\{\rho_n\} := \big\{\sum_{i=1}^2 |w_i^{a_n}|^2\big\}$ as $a_n \nearrow a_2^*$. Since any minimizer $\gamma^{(2)}$ of a_2^* satisfies $\gamma^{(2)} = \|\gamma^{(2)}\| \sum_{i=1}^2 |Q_i\rangle\langle Q_i|$ with $(Q_i, Q_j) = \delta_{ij}$, in Lemma 3.2 we are then able to establish finally the H^1-uniform convergence of $\{w_i^{a_n}\}_n$ as $a_n \nearrow a_2^*$.

The third step of proving Theorem 1.2 is to establish the energy estimate (1.17) and the L^∞-uniform convergence of $\{w_i^{a_n}\}_n$ as $a_n \nearrow a_2^*$. Actually, employing the energy estimates and the $L^{\frac{5}{3}}$-uniform convergence of the previous two steps, we can analyze the exact leading term of $E_{a_n}(2)$ as $a_n \nearrow a_2^*$, which then helps us prove the energy limit (1.17). On the other hand, to prove the L^∞-uniform convergence of $\{w_i^{a_n}\}_n$, we shall prove the following uniformly exponential decay

$$\Big(|w_1^{a_n}(x)|^2 + |w_2^{a_n}(x)|^2\Big) \leq C(\theta)e^{-\theta|x|} \text{ uniformly in } \mathbb{R}^3 \text{ as } n \to \infty, \tag{1.23}$$

where the constants $\theta > 0$ and $C(\theta) > 0$ are independent of $n > 0$, see Lemma 3.3 for more details. Unfortunately, the exponential decay (1.23) cannot be established by the standard comparison principle, due to the singularity of the Coulomb potential $V(x)$. For this reason, we shall prove (1.23) by employing Green's functions. The complete proof of Theorem 1.2 is given in Section 3.

In order to discuss the general case of $E_a(N)$, we next analyze the limiting concentration behavior of minimizers for $E_a(3)$ as $a \nearrow a_3^*$, where $a_1^* > a_2^* \geq a_3^*$ holds true in view of (1.8) and (1.11).

Theorem 1.3. *Let $\gamma_a = \sum_{i=1}^3 |u_i^a\rangle\langle u_i^a|$ be a minimizer of $E_a(3)$ for $0 < a < a_3^*$, where the orthonormal system (u_1^a, u_2^a, u_3^a) is a ground state of (1.14). Then for any sequence $\{a_n\}$ satisfying $a_n \nearrow a_3^*$ as $n \to \infty$, there exist a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ and a point $y_{k_*} \in \{y_1, \cdots, y_K\}$ given by (1.7) such that*

$$w_i^{a_n}(x) := \epsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}\big(\epsilon_{a_n} x + y_{k_*}\big) \to w_i \text{ strongly in } L^\infty(\mathbb{R}^3) \text{ as } n \to \infty, \ \ i = 1, 2, 3, \quad (1.24)$$

where $\epsilon_{a_n} := a_3^* - a_n > 0$, and $\gamma := \sum_{i=1}^3 |w_i\rangle\langle w_i|$ is an optimizer of a_3^*. Furthermore, we have

1. *If either $a_2^* > a_3^*$, or $a_2^* = a_3^*$ and $Rank(\gamma) = 3$, then $(w_i, w_j) = \delta_{ij}$ holds for $i, j = 1, 2, 3$.*
2. *If $a_2^* = a_3^*$ and $Rank(\gamma) = 2$, then $(w_i, w_j) = \delta_{ij}$ holds for $i, j = 1, 2$, and $w_3(x) \equiv 0$ in $\mathbb{R}^3$.*

Remark 1.2. (1). As for Theorem 1.3 (1), the similar proof of Theorem 1.2 can further yield the H^1-strong convergence of $\{w_i^{a_n}\}$ defined in (1.24) as $n \to \infty$, where $i = 1, 2, 3$.

(2). We expect that the argument of Theorem 1.3 can further yield the following general results: For any given $N \geq 3$, if $\gamma_{a_n} = \sum_{i=1}^N |u_i^{a_n}\rangle\langle u_i^{a_n}|$ is a minimizer of $E_{a_n}(N)$, where the orthonormal system $(u_1^a, \cdots, u_N^a)$ is a ground state of (1.14) and $a_n \nearrow a_N^*$ as $n \to \infty$, then there exist a point $y_{k_*} \in \{y_1, \cdots, y_K\}$ and a minimizer $\gamma := \sum_{i=1}^N |w_i\rangle\langle w_i|$ of a_N^* such that, up to a subsequence if necessary,

$$w_i^{a_n}(x) := \epsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}\big(\epsilon_{a_n} x + y_{k_*}\big) \to w_i \text{ strongly in } L^\infty(\mathbb{R}^3) \text{ as } n \to \infty \quad (1.25)$$

holds for $i = 1, 2, \cdots, N$, where $\mathrm{Rank}(\gamma) = \dim\big(\mathrm{span}\{w_1, \cdots, w_N\}\big) := R_N \in [2, N]$, and $w_{R_N+1}(x) \equiv \cdots \equiv w_N(x) \equiv 0$ in $\mathbb{R}^3$.

We next explain, totally by five steps, the general strategy of proving Theorem 1.3, which can be summarized as *the blow-up analysis of many-body fermionic systems*. The first three steps of proving Theorem 1.3 are similar to those of proving Theorem 1.2, which then yield the L^∞-uniform convergence of (1.24) in view of (1.11). Moreover, since Theorem 1.3 (1) focuses essentially on the cases where $\dim\mathrm{span}\{w_1^{a_n}, w_2^{a_n}, w_3^{a_n}\} = \dim\mathrm{span}\{w_1, w_2, w_3\}$, and $\sum_{i=1}^3 |w_i\rangle\langle w_i|$ is an optimizer of a_3^*, where w_i is as in (1.24), the above analysis procedure also yields that $(w_i, w_j) = \delta_{ij}$, $i, j = 1, 2, 3$, holds in this case. This proves Theorem 1.3 (1).

Since Theorem 1.3 (2) is concerned with the case where $a_2^* = a_3^*$ and $Rank(\gamma) = 2$, we first note that

$$3 = \dim\mathrm{span}\big\{w_1^{a_n}, w_2^{a_n}, w_3^{a_n}\big\} > \dim\mathrm{span}\{w_1, w_2, w_3\} = 2, \quad (1.26)$$

where w_i is given by (1.24), and $\gamma := \sum_{i=1}^3 |w_i\rangle\langle w_i|$ is an optimizer of a_3^*. This implies that there exist two different cases:

$$\text{either } w_i \not\equiv 0 \text{ holds for all } i = 1, 2, 3, \quad (1.27)$$

$$\text{or there exists exactly one } i_* \in \{1, 2, 3\} \text{ such that } w_{i_*} \equiv 0 \text{ in } \mathbb{R}^3. \quad (1.28)$$

The fourth step of proving Theorem 1.3 is to exclude the above case (1.27). Actually, similar to the proof of Theorem 1.2, one can establish the following convergence:

$$\sum_{i=1}^{3}|w_i^{a_n}|^2 \to \sum_{i=1}^{3} w_i^2 \quad \text{strongly in } L^{\frac{5}{3}}(\mathbb{R}^3) \text{ as } n\to\infty, \tag{1.29}$$

where $w_i^{a_n}$ is as in (1.24) and satisfies

$$-\Delta w_i^{a_n} + \epsilon_{a_n}^2 V\big(\epsilon_{a_n}x + y_{k_*}\big)w_i^{a_n} - \frac{5}{3}a_n\Big(\sum_{j=1}^{3}|w_j^{a_n}|^2\Big)^{\frac{2}{3}} w_i^{a_n} = \epsilon_{a_n}^2\mu_i^{a_n} w_i^{a_n} \text{ in } \mathbb{R}^3, \tag{1.30}$$

and $\mu_1^{a_n} < \mu_2^{a_n} \le \mu_3^{a_n} < 0$. Following the facts that $\int_{\mathbb{R}^3} w_1^{a_n} w_i^{a_n} dx = 0$ for $i = 2, 3$, we shall prove in (4.20) that for the case (1.27),

$$w_1 \text{ and } w_i \text{ are linearly independent for } i = 2, 3, \tag{1.31}$$

which further yields from (1.26) that w_2 and w_3 are linearly dependent. On the other hand, since the first eigenvalue of the operator $-\Delta - \frac{5}{3}a_3^*\Big(\sum_{j=1}^3 w_j^2\Big)^{\frac{2}{3}}$ in $\mathbb{R}^3$ is simple, and $\sum_{i=1}^3 |w_i\rangle\langle w_i|$ is an optimizer of a_3^*, we shall prove that once w_2 and w_3 are linearly dependent, then

$$-\infty < \lim_{n\to\infty}\epsilon_{a_n}^2\mu_2^{a_n} = \lim_{n\to\infty}\epsilon_{a_n}^2\mu_3^{a_n} < 0. \tag{1.32}$$

However, the same argument of (1.31) gives from (1.32) that w_2 and w_3 are linearly independent, a contradiction. This finishes the fourth step of proving Theorem 1.3.

The fifth step of proving Theorem 1.3 is to complete the proof of Theorem 1.3 (2). Since it necessarily has (1.28) in view of the previous step, the challenging point of this step is to further show that $w_1(x) \not\equiv 0$ and $w_2(x) \not\equiv 0$ in $\mathbb{R}^3$. We shall prove this result as follows. Similar to the proof of Theorem 1.2, one can establish the following convergence:

$$|\nabla w_i^{a_n}| \to |\nabla w_i| \quad \text{strongly in } L^2(\mathbb{R}^3) \text{ as } n\to\infty, \quad i = 1, 2, 3. \tag{1.33}$$

By contradiction, we next suppose that $w_{i_*}(x) \equiv 0$ in $\mathbb{R}^3$ for some $i_* \in \{1, 2\}$. By deriving some energy estimates of $u_i^{a_n}$ and $\mu_i^{a_n}$ as $n \to \infty$, we shall derive from (1.24), (1.29), (1.30) and (1.33) that

$$\lim_{n\to\infty}\sum_{i=1}^{3}\epsilon_{a_n}^2\mu_i^{a_n} = \lim_{n\to\infty}\sum_{i\neq i_*}^{3}\epsilon_{a_n}^2\mu_i^{a_n}, \quad \lim_{n\to\infty}\epsilon_{a_n}^2\mu_{i_*}^{a_n} < 0, \tag{1.34}$$

a contradiction, which yields that $w_{i_*}(x) \not\equiv 0$ in $\mathbb{R}^3$ for any $i_* \in \{1, 2\}$. This completes the proof of Theorem 1.3 (2). For the detailed proof of Theorem 1.3, we refer the reader to Section 4.

This paper is organized as follows. Section 2 is devoted to the proof of Theorem 1.1 on the existence and nonexistence of minimizers for $E_a(N)$. In Section 3, we shall address Theorem 1.2 on the limiting concentration behavior of minimizers for $E_a(2)$ as $a \nearrow a_2^*$. The proof of Theorem 1.3 is given in Section 4, which is concerned with the limiting concentration behavior of minimizers for $E_a(N)$ in the case $N = 3$.

2 Existence of Minimizers for $E_a(N)$

In this section, we mainly prove Theorem 1.1 on the existence and nonexistence of minimizers for $E_a(N)$ defined by (1.5), where $N \in \mathbb{N}^+$ is arbitrary. Towards this purpose, we need to introduce the following general minimization problem

$$E_a(\lambda) := \inf\Big\{\mathcal{E}_a(\gamma): \ \gamma = \sum_{i=1}^{N'} |u_i\rangle\langle u_i| + (\lambda - N')|u_{N'}\rangle\langle u_{N'}|,$$
$$u_i \in H^1(\mathbb{R}^3, \mathbb{R}),\ (u_i, u_j)_{L^2} = \delta_{ij},\ i, j = 1, \cdots, N'\Big\},\ \ a > 0,\ \ \lambda > 0, \quad (2.1)$$

where the energy functional $\mathcal{E}_a(\gamma)$ is defined by (1.6), and N' is the smallest integer such that $\lambda \leq N'$. One can note that when $\lambda = N' \in \mathbb{N}^+$, (2.1) coincides with $E_a(N')$ defined in (1.5).

We first address the analytical properties of $E_a(\lambda)$. Denoting $\mathcal{B}\big(L^2(\mathbb{R}^3)\big)$ the set of bounded linear operators on $L^2(\mathbb{R}^3)$, we then have the following equivalence of $E_a(\lambda)$.

Lemma 2.1. *Suppose the problem $E_a(\lambda)$ is defined by (2.1) for $a > 0$ and $\lambda > 0$. Then we have*

$$E_a(\lambda) = \inf_{\gamma' \in \mathcal{K}_\lambda} \mathcal{E}_a(\gamma'), \quad (2.2)$$

where the functional $\mathcal{E}_\alpha(\gamma')$ is as in (1.6), and $\mathcal{K}_\lambda$ is defined by

$$\mathcal{K}_\lambda = \big\{\gamma' \in \mathcal{B}\big(L^2(\mathbb{R}^3)\big):\ 0 \leq \gamma' = (\gamma')^* \leq 1,\ \mathrm{Tr}(\gamma') = \lambda,\ \mathrm{Tr}(-\Delta\gamma') < \infty\big\}. \quad (2.3)$$

Moreover, if $\inf_{\gamma' \in \mathcal{K}_\lambda} \mathcal{E}_a(\gamma')$ admits minimizers, then $E_a(\lambda)$ also admits minimizers.

Since Lemma 2.1 can be proved by a similar approach of [7, Lemma 11] and [1, Lemma 2.3], we omit the detailed proof for simplicity. The following lemma, whose proof is due to Mathieu Lewin, shows that even though the minimization problem (1.8) is defined in the complex-valued range, it is essentially attained by the real-valued operators.

Lemma 2.2. *For any $N \in \mathbb{N}^+$, suppose $\gamma^{(N)}$ is an optimizer of the problem* (1.8)*. Then we have $\gamma^{(N)} \in \mathcal{B}(L^2(\mathbb{R}^3, \mathbb{R}))$.*

Proof. For any $N \in \mathbb{N}^+$, since $\gamma^{(N)}$ is an optimizer of the problem (1.8), we obtain from [4, Theorem 6] that $\gamma^{(N)} = \|\gamma^{(N)}\| \sum_{j=1}^{R_N} |Q_j\rangle\langle Q_j|$ holds for some positive integer $R_N \in [1, N]$, where the orthonormal family $Q_1, \cdots, Q_{R_N} \in H^1(\mathbb{R}^3, \mathbb{C})$ satisfies

$$H_{\gamma^{(N)}} Q_k := \Big[-\Delta - \frac{5}{3} a_N^* \Big(\sum_{j=1}^{R_N} |Q_j|^2\Big)^{\frac{2}{3}}\Big] Q_k = \hat{\mu}_k Q_k \ \text{ in } \mathbb{R}^3, \quad k = 1, \cdots, R_N. \quad (2.4)$$

Here $\hat{\mu}_1 < \hat{\mu}_2 \leq \cdots \leq \hat{\mu}_{R_N} < 0$ are the R_N first eigenvalues (counted with multiplicity) of the operator $H_{\gamma^{(N)}}$ in $\mathbb{R}^3$. In order to establish Lemma 2.2, we only need to prove that for any $j \in \{1, \cdots, R_N\}$,

$$\text{either } \mathrm{Re}(Q_j) \equiv 0 \text{ in } \mathbb{R}^3, \ \text{ or } \ \mathrm{Im}(Q_j) \equiv 0 \text{ in } \mathbb{R}^3. \quad (2.5)$$

We next address (2.5) as follows.

If $R_N < N$, then it follows from [4, Theorem 6 (ii)] that the operator $H_{\gamma^{(N)}}$ in $\mathbb{R}^3$ has exactly R_N negative eigenvalues, counted with multiplicity. This thus implies from (2.4) that

$$\dim\Big(\bigcup_{k=1}^{R_N}\ker\big(H_{\gamma^{(N)}}-\hat{\mu}_k I\big)\Big)=R_N, \tag{2.6}$$

where I denotes the identity operator on $L^2(\mathbb{R}^3,\mathbb{C})$. On the contrary, suppose (2.5) is false. Then there exists some $k_*\in\{1,\cdots,R_N\}$ such that $Q_{k_*}=Q_{1k_*}+iQ_{2k_*}$ holds, where $Q_{1k_*},\ Q_{2k_*}\in H^1(\mathbb{R}^3,\mathbb{R})\backslash\{0\}$. We thus deduce from (2.4) that Q_{1k_*} is also an eigenfunction associated to $\hat{\mu}_{k_*}$, where Q_{1k_*} and Q_k are linear independent for any $k\in\{1,\cdots,R_N\}$. This further implies that $\dim\Big(\bigcup_{k=1}^{R_N}\ker\big(H_{\gamma^{(N)}}-\hat{\mu}_k I\big)\Big)>R_N$, which however contradicts with (2.6). Therefore, (2.5) holds true for the case where $R_N<N$.

If $R_N=N$, we denote by $\hat{\mu}_{N+1}$ to be the $(N+1)$th min-max level of the operator $H_{\gamma^{(N)}}$ in $\mathbb{R}^3$. Note from [4, Theorem 6 (ii)] that the function $\frac{5}{3}a_N^*\Big(\sum_{j=1}^N|Q_j|^2\Big)^{2/3}$ is an optimizer of the Lieb-Thirring inequality (1.21). We then deduce from [5, Theorem 3] that $\hat{\mu}_N<\hat{\mu}_{N+1}$, where $\hat{\mu}_N$ is the Nth negative eigenvalue (counted with multiplicity) of $H_{\gamma^{(N)}}$ in $\mathbb{R}^3$. This further yields that (2.6) holds true for $R_N=N$. Thus, the same argument as before also gives that (2.5) holds true for the case where $R_N=N$. This therefore completes the proof of Lemma 2.2. □

Applying the equivalent version (2.2) of $E_a(\lambda)$, one can obtain the following properties of $E_a(\lambda)$.

Lemma 2.3. *For any fixed $N\in\mathbb{N}^+$, suppose the constant $0<a_N^*<\infty$ is defined by* (1.8)*. Then the energy $E_a(\lambda)$ defined in* (2.1) *admits the following properties:*

1. *If $0<a<a_N^*$, then $-\infty<E_a(\lambda)<0$ holds for all $\lambda\in(0,N]$.*
2. *If $0<a\le a_N^*$, then $E_a(\lambda)$ is decreasing in $\lambda\in(0,N]$.*
3. *If $a\ge a_N^*$, then $E_a(N)=-\infty$.*

Proof. 1. For $\lambda\in(0,N]$, set

$$\gamma:=\sum_{i=1}^{N'}|u_i\rangle\langle u_i|+(\lambda-N')|u_{N'}\rangle\langle u_{N'}|,\quad u_i\in H^1(\mathbb{R}^3),\quad (u_i,u_j)_{L^2}=\delta_{ij}, \tag{2.7}$$

where N' is the smallest integer such that $\lambda\le N'$. Since $\lambda\in(0,N]$, we have $N'\le N$. By the definition of a_N^* defined in (1.8), we then get from Lemma 2.2 that

$$\mathrm{Tr}(-\Delta\gamma)\ge\|\gamma\|^{\frac{2}{3}}\mathrm{Tr}(-\Delta\gamma)\ge a_N^*\int_{\mathbb{R}^3}\rho_\gamma^{\frac{5}{3}}dx, \tag{2.8}$$

where ρ_γ, representing the density of γ, is defined by (1.4). By Hardy's inequality, we have

$$|x|^{-1}\le\varepsilon\big(-\Delta\big)+4\varepsilon^{-1},\ \text{ where }\varepsilon>0\ \text{ is arbitrary.} \tag{2.9}$$

It then yields that

$$V(x)=-\sum_{k=1}^{K}|x-y_k|^{-1}\ge-\varepsilon K(-\Delta)-4\varepsilon^{-1}K\ \text{ holds for any }\varepsilon>0. \tag{2.10}$$

For simplicity, we denote $n_1 = \cdots = n_{N'-1} = 1$ and $n_{N'} = \lambda - N' + 1$, so that

$$\gamma = \sum_{i=1}^{N'} n_i |u_i\rangle\langle u_i|, \quad \rho_\gamma = \sum_{i=1}^{N'} n_i u_i^2. \tag{2.11}$$

By the definitions of (1.3) and Trace, it then follows from (2.10) that

$$\begin{aligned} \mathrm{Tr}\big(-\Delta + V(x)\big)\gamma &= \sum_{i=1}^{N'} n_i \Big(\big(-\Delta + V(x)\big)u_i, u_i\Big) \\ &\geq (1-\varepsilon K)\sum_{i=1}^{N'} n_i\big(-\Delta u_i, u_i\big) - 4\varepsilon^{-1}K \sum_{i=1}^{N'} n_i (u_i, u_i) \\ &= (1-\varepsilon K)\mathrm{Tr}(-\Delta\gamma) - 4\varepsilon^{-1}K\lambda, \quad \varepsilon > 0. \end{aligned} \tag{2.12}$$

For $0 \leq a < a_N^*$, taking $\varepsilon > 0$ so that $\varepsilon K = \frac{1}{2}\Big(1 - \frac{a}{a_N^*}\Big) > 0$, we further obtain from (2.8) and (2.12) that

$$\begin{aligned} \mathcal{E}_a(\gamma) =&\mathrm{Tr}\big(-\Delta + V(x)\big)\gamma - a\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx \\ &\geq (1-\varepsilon K)\mathrm{Tr}(-\Delta\gamma) - \frac{a}{a_N^*}\mathrm{Tr}(-\Delta\gamma) - 4\varepsilon^{-1}K\lambda \\ &= \frac{1}{2}\Big(1 - \frac{a}{a_N^*}\Big)\mathrm{Tr}(-\Delta\gamma) - \frac{8\lambda K^2 a_N^*}{a_N^* - a} \geq -\frac{8\lambda K^2 a_N^*}{a_N^* - a}. \end{aligned} \tag{2.13}$$

Since γ is arbitrary, we obtain from (2.13) that $E_a(\lambda) > -\infty$ holds for any $0 < \lambda \leq N$ and $0 \leq a < a_N^*$.

Associated to (2.7), we define

$$\gamma_t := \sum_{i=1}^{N'} t^3 |u_i(t\cdot)\rangle\langle u_i(t\cdot)| + (\lambda - N')t^3 |u_{N'}(t\cdot)\rangle\langle u_{N'}(t\cdot)|, \quad t > 0. \tag{2.14}$$

Similar to the first identity of (2.12), one can calculate from (1.7) that

$$\mathcal{E}_a(\gamma_t) = t^2 \mathrm{Tr}(-\Delta\gamma) - at^2 \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx - t\sum_{k=1}^{K}\int_{\mathbb{R}^3} |x - ty_k|^{-1}\rho_\gamma dx, \tag{2.15}$$

where γ and ρ_γ are as in (2.11). Since

$$\lim_{t\to 0}\int_{\mathbb{R}^3} |x - ty_k|^{-1}\rho_\gamma dx = \int_{\mathbb{R}^3} |x|^{-1}\rho_\gamma dx > 0, \quad k = 1, \cdots, K,$$

we obtain from (2.15) that if $0 \leq a < a_N^*$ and $0 < \lambda \leq N$, then $\mathcal{E}_a(\gamma_t) < 0$ holds for sufficiently small $t > 0$. This further implies that $E_a(\lambda) < 0$ holds for any $0 \leq a < a_N^*$ and $0 < \lambda \leq N$.

2. For any given $0 < \lambda_1 < \lambda \leq N$, consider any operators γ_1 and γ_2 satisfying the following constraint conditions

$$\begin{aligned} \gamma_1 := \sum_{i=1}^{N_1} |\varphi_i\rangle\langle\varphi_i| + (\lambda_1 - N_1)|\varphi_{N_1}\rangle\langle\varphi_{N_1}|, \quad \varphi_i \in H^1(\mathbb{R}^3), \\ (\varphi_i, \varphi_{i'})_{L^2} = \delta_{ii'}, \quad i, i' = 1, 2, \cdots, N_1, \end{aligned} \tag{2.16}$$

$$\gamma_2 := \sum_{j=1}^{N_2} |\psi_j\rangle\langle\psi_j| + (\lambda - \lambda_1 - N_2)|\psi_{N_2}\rangle\langle\psi_{N_2}|, \quad \psi_j \in H^1(\mathbb{R}^3),$$
$$(\psi_j, \psi_{j'})_{L^2} = \delta_{jj'}, \quad j, j' = 1, 2, \cdots, N_2, \tag{2.17}$$

where $N_1, N_2 \in \mathbb{N}^+$ are the smallest integers such that $\lambda_1 \le N_1$ and $\lambda - \lambda_1 \le N_2$, respectively. For any fixed $\tau > 0$, we define

$$\psi_j^\tau(x) := \psi_j(x - \tau e_1), \quad j = 1, \cdots, N_2, \quad e_1 = (1, 0, 0),$$

and consider the Gram matrix G_τ of the family $\varphi_1, \cdots, \varphi_{N_1}, \psi_1^\tau, \cdots, \psi_{N_2}^\tau$, i.e.,

$$G_\tau := \begin{pmatrix} \mathbb{I}_{N_1} & A_\tau \\ A_\tau^* & \mathbb{I}_{N_2} \end{pmatrix}, \quad A_\tau = (a_{ij}^\tau)_{N_1 \times N_2}, \quad a_{ij}^\tau = (\varphi_i, \psi_j^\tau), \tag{2.18}$$

where $\mathbb{I}_{N_i}$ denotes the N_i-order identity matrix.

Since

$$a_\tau := \max_{i,j} |(\varphi_i, \psi_j^\tau)| = o(1) \quad \text{as} \quad \tau \to \infty, \tag{2.19}$$

it yields that G_τ is positive definite for sufficiently large $\tau > 0$. Hence, the identity

$$\mathbb{I}_{N_1+N_2} = G_\tau^{-\frac{1}{2}} \begin{pmatrix} \mathbb{I}_{N_1} & A_\tau \\ A_\tau^* & \mathbb{I}_{N_2} \end{pmatrix} G_\tau^{-\frac{1}{2}} \tag{2.20}$$

holds for sufficiently large $\tau > 0$. We next set

$$(\tilde{\varphi}_1^\tau, \cdots, \tilde{\varphi}_{N_1}^\tau, \tilde{\psi}_1^\tau, \cdots, \tilde{\psi}_{N_2}^\tau) := (\varphi_1, \cdots, \varphi_{N_1}, \psi_1^\tau, \cdots, \psi_{N_2}^\tau) G_\tau^{-\frac{1}{2}}, \quad \tau > 0, \tag{2.21}$$

and

$$\begin{aligned} \gamma_\tau := &\sum_{i=1}^{N_1} |\tilde{\varphi}_i^\tau\rangle\langle\tilde{\varphi}_i^\tau| + (\lambda_1 - N_1)|\tilde{\varphi}_{N_1}^\tau\rangle\langle\tilde{\varphi}_{N_1}^\tau| \\ &+ \sum_{j=1}^{N_2} |\tilde{\psi}_j^\tau\rangle\langle\tilde{\psi}_j^\tau| + (\lambda - \lambda_1 - N_2)|\tilde{\psi}_{N_2}^\tau\rangle\langle\tilde{\psi}_{N_2}^\tau|, \quad \tau > 0. \end{aligned} \tag{2.22}$$

It then follows from (2.20) that the system $(\tilde{\varphi}_1^\tau, \cdots, \tilde{\varphi}_{N_1}^\tau, \tilde{\psi}_1^\tau, \cdots, \tilde{\psi}_{N_2}^\tau)$ is an orthonormal family in $L^2(\mathbb{R}^3)$ for sufficiently large $\tau > 0$, and hence $\gamma_\tau \in \mathcal{K}_\lambda$ defined by (2.3) holds for sufficiently large $\tau > 0$.

We now calculate $\mathcal{E}_a(\gamma_\tau)$ as $\tau \to \infty$. Since it follows from (2.18) and (2.19) that

$$G_\tau^{-\frac{1}{2}} = \begin{pmatrix} \mathbb{I}_{N_1} & 0 \\ 0 & \mathbb{I}_{N_2} \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 & A_\tau \\ A_\tau^* & 0 \end{pmatrix} + O(a_\tau^2) \quad \text{as} \quad \tau \to \infty, \tag{2.23}$$

one can calculate from (2.21) and (2.22) that

$$\gamma_\tau = \gamma_1 + \gamma_2^\tau - \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} a_{ij}^\tau \left(|\varphi_i\rangle\langle\psi_j^\tau| + |\psi_j^\tau\rangle\langle\varphi_i| \right)$$

$$
\begin{aligned}
&-\frac{1}{2}(\lambda_1 - N_1)\sum_{j=1}^{N_2} a^\tau_{N_1 j}\left(|\varphi_{N_1}\rangle\langle\psi^\tau_j| + |\psi^\tau_j\rangle\langle\varphi_{N_1}|\right) \\
&-\frac{1}{2}(\lambda - \lambda_1 - N_2)\sum_{i=1}^{N_1} a^\tau_{iN_2}\left(|\varphi_i\rangle\langle\psi^\tau_{N_2}| + |\psi^\tau_{N_2}\rangle\langle\varphi_i|\right) \\
&+O(a^2_\tau) \quad \text{as} \quad \tau\to\infty,
\end{aligned} \tag{2.24}
$$

where γ_1 is as in (2.16), and $\gamma^\tau_2 = \sum_{j=1}^{N_2}|\psi^\tau_j\rangle\langle\psi^\tau_j| + (\lambda-\lambda_1-N_2)|\psi^\tau_{N_2}\rangle\langle\psi^\tau_{N_2}|$. We thus deduce from (2.19) that

$$
\mathrm{Tr}(-\Delta\gamma_\tau) = \mathrm{Tr}(-\Delta\gamma_1) + \mathrm{Tr}(-\Delta\gamma_2) + o(1) \quad \text{as} \quad \tau\to\infty, \tag{2.25}
$$

and

$$
\int_{\mathbb{R}^3}\left|\rho_{\gamma_\tau} - \rho_{\gamma_1} - \rho_{\gamma_2}(x-\tau e_1)\right|dx = o(1) \quad \text{as} \quad \tau\to\infty, \tag{2.26}
$$

where $\rho_{\gamma_2}(x-\tau e_1) = \rho_{\gamma^\tau_2}(x)$. Recall (cf. [10]) the following Hoffmann-Ostenhof inequality

$$
\mathrm{Tr}(-\Delta\gamma_\tau) \geq \int_{\mathbb{R}^3}|\nabla\sqrt{\rho_{\gamma_\tau}}|^2dx. \tag{2.27}
$$

Applying Sobolev's embedding theorem, we then get from (2.25) that $\{\rho_{\gamma_\tau}\}$ is bounded uniformly in $L^r(\mathbb{R}^3)$ for all $r\in[1,3]$ as $\tau\to\infty$. Combining this with (2.26), one can deduce from the interpolation inequality that

$$
\rho_{\gamma_\tau}(x) - \rho_{\gamma_1}(x) - \rho_{\gamma_2}(x-\tau e_1) \to 0 \quad \text{strongly in} \quad L^r(\mathbb{R}^3) \quad \text{as} \quad \tau\to\infty, \quad r\in[1,3),
$$

which further implies from (1.7) that

$$
\begin{aligned}
\lim_{\tau\to\infty}\int_{\mathbb{R}^3}V(x)\rho_{\gamma_\tau}dx &= \lim_{\tau\to\infty}\int_{\mathbb{R}^3}V(x)\Big(\rho_{\gamma_1}(x) + \rho_{\gamma_2}(x-\tau e_1)\Big)dx \\
&= \int_{\mathbb{R}^3}V(x)\rho_{\gamma_1}dx,
\end{aligned} \tag{2.28}
$$

and

$$
\begin{aligned}
\lim_{\tau\to\infty}\int_{\mathbb{R}^3}\rho^{\frac{5}{3}}_{\gamma_\tau}dx &= \lim_{\tau\to\infty}\int_{\mathbb{R}^3}\Big(\rho_{\gamma_1}(x) + \rho_{\gamma_2}(x-\tau e_1)\Big)^{\frac{5}{3}}dx \\
&= \int_{\mathbb{R}^3}\Big(\rho^{\frac{5}{3}}_{\gamma_1} + \rho^{\frac{5}{3}}_{\gamma_2}\Big)dx.
\end{aligned} \tag{2.29}
$$

Applying Lemma 2.1, we now conclude from (2.25), (2.28) and (2.29) that

$$
\begin{aligned}
E_a(\lambda) = \inf_{\gamma'\in\mathcal{K}_\lambda}\mathcal{E}_a(\gamma') &\leq \lim_{\tau\to\infty}\mathcal{E}_a(\gamma_\tau) \\
&= \mathcal{E}_a(\gamma_1) + \mathrm{Tr}(-\Delta\gamma_2) - a\int_{\mathbb{R}^3}\rho^{\frac{5}{3}}_{\gamma_2}dx.
\end{aligned} \tag{2.30}
$$

Since γ_1 and γ_2 are arbitrary, the above inequality further implies that

$E_a(\lambda)$

$$
\begin{aligned}
\le & E_a(\lambda_1) + \inf \Big\{ \mathrm{Tr}(-\Delta\gamma) - a\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx : \gamma = \sum_{i=1}^{N_2} |u_i\rangle\langle u_i| + (\lambda-\lambda_1-N_2)|u_{N_2}\rangle\langle u_{N_2}|, \\
& \qquad u_i \in H^1(\mathbb{R}^3),\ (u_i,u_j)_{L^2} = \delta_{ij},\ i,j=1,\cdots,N_2 \Big\} \\
:= & E_a(\lambda_1) + E_a^\infty(\lambda-\lambda_1) \qquad (2.31)
\end{aligned}
$$

holds for any $0<\lambda_1<\lambda\le N$.

For fixed $0\le a\le a_N^*$, it then follows from (1.8) that $E_a^\infty(\lambda-\lambda_1)\ge 0$. Similar to (2.14) and (2.15), where γ_t is replaced by $(\gamma_2)_t$, we obtain that

$$
E_a^\infty(\lambda-\lambda_1) \le \lim_{t\to 0} t^2\Big(\mathrm{Tr}(-\Delta\gamma_2) - a\int_{\mathbb{R}^3} \rho_{\gamma_2}^{\frac{5}{3}} dx\Big) = 0, \quad 0<\lambda_1<\lambda\le N,
$$

and hence $E_a^\infty(\lambda-\lambda_1)=0$. Together with (2.31), this shows that if $0\le a\le a_N^*$, then $E_a(\lambda)\le E_a(\lambda_1)$ holds for any $0<\lambda_1<\lambda\le N$. Therefore, if $0\le a\le a_N^*$, then $E_a(\lambda)$ is decreasing in $\lambda\in(0,N]$.

3. Following (1.9), let $\gamma^{(N)}=\sum_{i=1}^{R_N}|Q_i\rangle\langle Q_i|$ be a minimizer of a_N^*, where $N\ge R_N\in\mathbb{N}^+$, and the system $(Q_1,\cdots,Q_{R_N})$ satisfies $(Q_i,Q_j)=\delta_{ij}$. Since the above analysis gives that $E_{a_N^*}(\lambda)$ is decreasing in $\lambda\in(0,N]$, we have

$$
\begin{aligned}
E_{a_N^*}(N) \le E_{a_N^*}(R_N) &\le \lim_{t\to\infty} \mathcal{E}_{a_N^*}\big(\gamma_t^{(N)}\big) \\
&\le -\lim_{t\to\infty} t\int_{\mathbb{R}^3} |x|^{-1}\rho_{\gamma^{(N)}} dx = -\infty,
\end{aligned}
$$

where

$$
\gamma_t^{(N)} := \sum_{i=1}^{R_N} t^3 \big|Q_i\big(t(\cdot-y_1)\big)\big\rangle\big\langle Q_i\big(t(\cdot-y_1)\big)\big|,
$$

and $y_1\in\mathbb{R}^3$ is given in (1.7). By the definition of $E_a(N)$, we then deduce from above that

$$
E_a(N) \le E_{a_N^*}(N) \le -\infty, \quad \forall\ a\ge a_N^*,
$$

which completes the proof of Lemma 2.3. □

Remark 2.1. Consider any fixed $N\ge 2$, so that $0<a_N^*<a_1^*$ holds in view of [4]: If $a>0$ satisfies $(a_N^*<)a<a_1^*$, then it follows from Lemma 2.3 (1) that $-\infty<E_a(\lambda)<0$ holds for $\lambda=1<N$; If $a>0$ satisfies $a>a_1^*>a_N^*$, then it follows from Lemma 2.3 (3) that $E_a(\lambda)=-\infty$ holds for $\lambda=1<N$. On the other hand, consider $N=3$ and let $a>0$ be fixed so that $a_3^*\le a_2^*<a<a_1^*$: We obtain from Lemma 2.3 (1) that $-\infty<E_a(\lambda)<0$ holds for any $0<\lambda\le 1<N$; it however follows from Lemma 2.3 (3) that $E_a(\lambda)=-\infty$ holds for $\lambda=2<N$. These examples show that for any given $N\in\mathbb{N}^+$, if $a\ge a_N^*$ and $\lambda\in(0,N)$, then $E_a(\lambda)$ can be either bounded or unbounded, which depends on the exact values of a and $\lambda\in(0,N)$.

Applying Lemmas 2.1 and 2.3, one can obtain the following analytical properties of minimizers for $E_a(\lambda)$.

Lemma 2.4. *For any fixed $N\in\mathbb{N}^+$, let $E_a(\lambda)$ be defined by (2.1), where $a\in\big(0,a_N^*\big)$, $\lambda\in(0,N]$, and $V(x)<0$ is as in (1.7). Suppose γ is a minimizer of $E_a(\lambda)$. Then we have*

1. The minimizer γ can be written as $\gamma = \sum_{i=1}^{N'} |u_i\rangle\langle u_i| + (\lambda - N')|u_{N'}\rangle\langle u_{N'}|$, where N' denotes the smallest integer such that $\lambda \le N'$, and $(u_1, \cdots, u_{N'})$ is a ground state of the following system

$$\Big[-\Delta + V(x) - \frac{5}{3}a\Big(\sum_{j=1}^{N'} u_j^2 + (\lambda - N')u_{N'}^2\Big)^{\frac{2}{3}}\Big] u_i = \mu_i u_i \quad in\ \mathbb{R}^3, \quad i = 1, \cdots, N'.$$

Here $\mu_1 < \mu_2 \le \cdots \le \mu_{N'} < 0$ are the N' first eigenvalues, counted with multiplicity, of the operator

$$H_V := -\Delta + V(x) - \frac{5}{3}a\Big(\sum_{j=1}^{N'} u_j^2 + (\lambda - N')u_{N'}^2\Big)^{\frac{2}{3}} \quad in\ \mathbb{R}^3.$$

2. $(u_1, \cdots, u_{N'})$ decays exponentially in the sense that

$$C^{-1}(1+|x|)^{-1} e^{-\sqrt{|\mu_1|}|x|} \le u_1(x) \le C(1+|x|)^{\frac{K}{\sqrt{|\mu_1|}}-1} e^{-\sqrt{|\mu_1|}|x|} \quad in\ \mathbb{R}^3, \tag{2.32}$$

and

$$|u_i(x)| \le C(1+|x|)^{\frac{K}{\sqrt{|\mu_i|}}-1} e^{-\sqrt{|\mu_i|}|x|} \quad in\ \mathbb{R}^3, \quad i = 2, \cdots, N', \tag{2.33}$$

where the constant $K > 0$ is as in (1.7), and $C > 0$ depends on $\|\rho_\gamma\|_{L^3(\mathbb{R}^3)}$.

Since the proof of Lemma 2.4 is similar to that of [1, Lemma 2.3], we omit the details for simplicity.

2.1 Proof of Theorem 1.1

This subsection is devoted to the proof of Theorem 1.1, for which we shall make full use of Lemmas 2.3 and 2.4.

Proof of Theorem 1.1. In view of Lemmas 2.3 and 2.4, we only need to prove the existence of minimizers for $E_a(N)$, where $N \in \mathbb{N}^+$ and $0 < a < a_N^*$.

Consider any fixed $N \in \mathbb{N}^+$ and $0 < a < a_N^*$. It follows from Lemma 2.3 that $E_a(N)$ is finite. Let $\{\gamma_n\}$ be a minimizing sequence of $E_a(N)$ with $\gamma_n = \sum_{i=1}^{N} |u_i^n\rangle\langle u_i^n|$, where $(u_i^n, u_j^n)_{L^2} = \delta_{ij}, \ \ i, j = 1, 2, \cdots, N$. The inequality (2.13) yields that the sequence

$$\big\{\mathrm{Tr}(-\Delta\gamma_n)\big\} = \Big\{\sum_{i=1}^{N} \int_{\mathbb{R}^3} |\nabla u_i^n|^2 dx\Big\}$$

is bounded uniformly in n, and thus $\{u_i^n\}_{n=1}^{\infty}$ is bounded uniformly in $H^1(\mathbb{R}^3)$ for all $i = 1, \cdots, N$. Hence, one can assume that, up to a subsequence if necessary, there exists $u_i \in H^1(\mathbb{R}^3)$ such that

$$u_i^n \rightharpoonup u_i \ \text{ weakly in } \ H^1(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \quad i = 1, \cdots, N, \tag{2.34}$$

and

$$\rho_{\gamma_n} = \sum_{i=1}^{N} |u_i^n|^2 \to \rho_\gamma := \sum_{i=1}^{N} u_i^2 \ \text{ strongly in } \ L^r_{loc}(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \quad 1 \le r < 3, \tag{2.35}$$

where $\gamma = \sum_{i=1}^N |u_i\rangle\langle u_i|$.

We first claim that if

$$\rho_{\gamma_n} \to \rho_\gamma \ \text{ strongly in } L^1(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \tag{2.36}$$

then γ is a minimizer of $E_a(N)$. Actually, using the weak lower semicontinuity, together with the fact that $(u_i^n, u_j^n) = \delta_{ij}$, $i, j = 1, \cdots, N$, we deduce from (2.36) that

$$u_i^n \to u_i \ \text{ strongly in } L^2(\mathbb{R}^3) \text{ as } n \to \infty, \ \text{ and } \ (u_i, u_j) = \delta_{ij}, \ i, j = 1, \cdots, N, \tag{2.37}$$

which yields that

$$\mathcal{E}_a(\gamma) \geq E_a(N), \quad \text{where } \gamma = \sum_{i=1}^N |u_i\rangle\langle u_i|.$$

Using the interpolation inequality and the boundedness of $\{\rho_{\gamma_n}\}$ in $L^3(\mathbb{R}^3)$, we derive from (2.36) that

$$\rho_{\gamma_n} \to \rho_\gamma \ \text{ strongly in } \ L^r(\mathbb{R}^3) \text{ as } n \to \infty, \ 1 \leq r < 3.$$

Therefore, we have

$$\begin{aligned} E_a(N) &= \liminf_{n\to\infty} \mathcal{E}_a(\gamma_n) \\ &\geq \mathrm{Tr}(-\Delta\gamma) + \int_{\mathbb{R}^3} V(x)\rho_\gamma dx - a\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx \\ &= \mathcal{E}_a(\gamma) \geq E_a(N), \end{aligned}$$

which implies that γ is a minimizer of $E_a(N)$.

As a consequence, in order to prove Theorem 1.1, the rest is to prove (2.36). Applying the Brézis-Lieb Lemma (cf. [17]), we note from (2.34) that if $\int_{\mathbb{R}^3} \rho_\gamma dx = N$, then (2.36) holds true. Therefore, the rest proof of Theorem 1.1 is to prove by two steps that the case $\lambda := \int_{\mathbb{R}^3} \rho_\gamma dx \in [0, N)$ cannot occur. We shall denote $\rho_n := \rho_{\gamma_n}$ for convenience.

Step 1. We first prove that the case $\lambda := \int_{\mathbb{R}^3} \rho_\gamma dx = 0$ cannot occur. On the contrary, suppose $\lambda = 0$. It then follows from (2.35) that

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} V(x)\rho_n dx = -\sum_{k=1}^K \lim_{n\to\infty} \int_{\mathbb{R}^3} |x - y_k|^{-1}\rho_n dx = 0.$$

We thus get from (1.8) that

$$\begin{aligned} E_a(N) &= \lim_{n\to\infty} \mathcal{E}_a(\gamma_n) \\ &= \lim_{n\to\infty} \Big[\mathrm{Tr}(-\Delta\gamma_n) - a\int_{\mathbb{R}^3} \rho_n^{\frac{5}{3}} dx\Big] + \lim_{n\to\infty} \int_{\mathbb{R}^3} V(x)\rho_n dx \\ &\geq \Big(1 - \frac{a}{a_N^*}\Big) \liminf_{n\to\infty} \mathrm{Tr}(-\Delta\gamma_n) \geq 0, \end{aligned}$$

which however contradicts with Lemma 2.3 (1). Thus, the case $\lambda = 0$ cannot occur.

Step 2. We next prove that the case $0 < \lambda := \int_{\mathbb{R}^3} \rho_\gamma dx < N$ cannot occur, either. By contradiction, suppose $0 < \int_{\mathbb{R}^3} \rho_\gamma dx = \lambda < N$. By an adaptation of the classical dichotomy result (cf. [15, Section 3.3]), up to a subsequence of $\{\rho_n\}$ if necessary, then there exists a sequence $\{R_n\}$ with $R_n \to \infty$ as $n \to \infty$ such that

$$0 < \lim_{n\to\infty} \int_{|x|\le R_n} \rho_n dx = \int_{\mathbb{R}^3} \rho_\gamma dx < N, \quad \lim_{n\to\infty} \int_{R_n \le |x| \le 6R_n} \rho_n dx = 0. \tag{2.38}$$

Choose $\chi \in C_0^\infty(\mathbb{R}^3, [0,1])$ satisfying $\chi(x) = 1$ for $|x| \le 1$ and $\chi(x) = 0$ for $|x| \ge 2$, and define $\chi_{R_n}(x) := \chi(x/R_n)$, $\eta_{R_n}(x) := \sqrt{1 - \chi^2_{R_n}(x)}$,

$$u_i^{1n} := \chi_{R_n} u_i^n, \quad u_i^{2n} := \eta_{R_n} u_i^n, \quad i = 1, \cdots, N, \tag{2.39}$$

and

$$\gamma_{1n} := \sum_{i=1}^N |u_i^{1n}\rangle\langle u_i^{1n}|, \quad \gamma_{2n} := \sum_{i=1}^N |u_i^{2n}\rangle\langle u_i^{2n}|. \tag{2.40}$$

We now follow above to estimate the energy $\mathcal{E}_a(\gamma_n)$ as $n \to \infty$. It is easy to verify from (2.34) and (2.39) that

$$u_i^{1n} \rightharpoonup u_i \text{ weakly in } H^1(\mathbb{R}^3) \text{ as } n \to \infty, \quad i = 1, \cdots, N. \tag{2.41}$$

Using the weak lower semicontinuity of norm, together with the Brézis-Lieb Lemma (cf. [17]), one can deduce from (2.38) and (2.41) that

$$\liminf_{n\to\infty} \operatorname{Tr}(-\Delta\gamma_{1n}) \ge \operatorname{Tr}(-\Delta\gamma), \tag{2.42}$$

and

$$\rho_{1n} := \rho_{\gamma_{1n}} \to \rho_\gamma \text{ strongly in } L^1(\mathbb{R}^3) \text{ as } n \to \infty. \tag{2.43}$$

Moreover, we have

$$\rho_n = \chi^2_{R_n}\rho_n + \eta^2_{R_n}\chi^2_{3R_n}\rho_n + \eta^2_{3R_n}\rho_n, \tag{2.44}$$

and

$$\eta^2_{R_n}\chi^2_{3R_n}\rho_n \to 0 \quad \text{strongly in } L^1(\mathbb{R}^3) \text{ as } n \to \infty, \tag{2.45}$$

due to the estimate (2.38). Following the uniform boundedness of $\{\rho_n\}$ in $L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$, we derive from (2.43) and (2.45) that

$$\rho_{1n} := \rho_{\gamma_{1n}} \to \rho_\gamma, \quad \eta^2_{R_n}\chi^2_{3R_n}\rho_n \to 0 \text{ strongly in } L^r(\mathbb{R}^3) \text{ as } n \to \infty, \quad r \in [1,3). \tag{2.46}$$

We thus obtain from (2.44) and (2.46) that for $\rho_{2n} := \rho_{\gamma_{2n}}$,

$$\begin{aligned} \int_{\mathbb{R}^3} V(x)\rho_n dx &= \int_{\mathbb{R}^3} V(x)\rho_{1n} dx + \int_{\mathbb{R}^3} V(x)\rho_{2n} dx \\ &= \int_{\mathbb{R}^3} V(x)\rho_\gamma dx + o(1) \quad \text{as } n \to \infty, \end{aligned} \tag{2.47}$$

and

$$\begin{aligned} \int_{\mathbb{R}^3} \rho_n^{\frac{5}{3}} dx &= \int_{\mathbb{R}^3} \left(\chi^2_{R_n}\rho_n + \eta^2_{3R_n}\rho_n\right)^{\frac{5}{3}} dx + o(1) \\ &= \int_{\mathbb{R}^3} \Big[\left(\chi^2_{R_n}\rho_n\right)^{\frac{5}{3}} + \left(\eta^2_{3R_n}\rho_n\right)^{\frac{5}{3}} \Big] dx + o(1) \\ &= \int_{\mathbb{R}^3} \Big[\left(\chi^2_{R_n}\rho_n\right)^{\frac{5}{3}} + \left(\eta^2_{R_n}\chi^2_{3R_n}\rho_n + \eta^2_{3R_n}\rho_n\right)^{\frac{5}{3}} \Big] dx + o(1) \\ &= \int_{\mathbb{R}^3} \Big(\rho_\gamma^{\frac{5}{3}} + \rho_{2n}^{\frac{5}{3}}\Big) dx + o(1) \quad \text{as } n \to \infty. \end{aligned} \tag{2.48}$$

Since it follows from [2, Theorem 3.1] that

$$-\Delta = \chi_{R_n}(-\Delta)\chi_{R_n} + \eta_{R_n}(-\Delta)\eta_{R_n} - |\nabla\chi_{R_n}|^2 - |\nabla\eta_{R_n}|^2,$$

we have

$$\begin{aligned}\mathrm{Tr}(-\Delta\gamma_n) &= \mathrm{Tr}(-\Delta\gamma_{1n}) + \mathrm{Tr}(-\Delta\gamma_{2n}) - \int_{\mathbb{R}^3}(|\nabla\chi_{R_n}|^2 + |\nabla\eta_{R_n}|^2)\rho_n dx \\ &\geq \mathrm{Tr}(-\Delta\gamma_{1n}) + \mathrm{Tr}(-\Delta\gamma_{2n}) - CR_n^{-2}N,\end{aligned} \tag{2.49}$$

where $C > 0$ is independent of $n > 0$. We therefore conclude from (2.42) and (2.47)–(2.49) that

$$E_a(N) = \lim_{n\to\infty} \mathcal{E}_a(\gamma_n) \geq \mathcal{E}_a(\gamma) + \liminf_{n\to\infty}\Big(\mathrm{Tr}(-\Delta\gamma_{2n}) - a\int_{\mathbb{R}^3}\rho_{2n}^{\frac{5}{3}}dx\Big). \tag{2.50}$$

Note from (2.35) that $\gamma = \sum_{i=1}^N |u_i\rangle\langle u_i| \in \mathcal{K}_\lambda$, where $\lambda = \int_{\mathbb{R}^3}\rho_\gamma dx$ and $\mathcal{K}_\lambda$ is defined by Lemma 2.1. We thus get from Lemma 2.1 that

$$\mathcal{E}_a(\gamma) \geq \inf_{\gamma'\in\mathcal{K}_\lambda} \mathcal{E}_a(\gamma') = E_a(\lambda). \tag{2.51}$$

Applying Lemma 2.3 (2), we further obtain from (2.50) and (2.51) that

$$\begin{aligned}E_a(\lambda) \geq E_a(N) &\geq \mathcal{E}_a(\gamma) + \liminf_{n\to\infty}\Big(\mathrm{Tr}(-\Delta\gamma_{2n}) - a\int_{\mathbb{R}^3}\rho_{2n}^{\frac{5}{3}}dx\Big) \\ &\geq \inf_{\gamma'\in\mathcal{K}_\lambda} \mathcal{E}_a(\gamma') + \liminf_{n\to\infty}\Big(\mathrm{Tr}(-\Delta\gamma_{2n}) - a\int_{\mathbb{R}^3}\rho_{2n}^{\frac{5}{3}}dx\Big) \\ &= E_a(\lambda) + \liminf_{n\to\infty}\Big(\mathrm{Tr}(-\Delta\gamma_{2n}) - a\int_{\mathbb{R}^3}\rho_{2n}^{\frac{5}{3}}dx\Big) \\ &\geq E_a(\lambda) + \liminf_{n\to\infty}\Big(1 - \frac{a\|\gamma_{2n}\|^{\frac{2}{3}}}{a_N^*}\Big)\mathrm{Tr}(-\Delta\gamma_{2n}) \\ &\geq E_a(\lambda) + \Big(1 - \frac{a}{a_N^*}\Big)\liminf_{n\to\infty}\mathrm{Tr}(-\Delta\gamma_{2n}),\end{aligned} \tag{2.52}$$

where the last inequality follows from the fact that $\|\gamma_{2n}\| \leq \|\gamma_n\| = 1$. Thus, if $\liminf_{n\to\infty}\mathrm{Tr}(-\Delta\gamma_{2n}) > 0$, then we get a contradiction from (2.52), and thus the case $0 < \lambda := \int_{\mathbb{R}^3}\rho_\gamma dx < N$ cannot occur, which therefore completes the proof of Theorem 1.1.

If $\liminf_{n\to\infty}\mathrm{Tr}(-\Delta\gamma_{2n}) = 0$, we derive from (2.52) that

$$E_a(\lambda) = E_a(N), \tag{2.53}$$

and γ is a minimizer of $\inf_{\gamma'\in\mathcal{K}_\lambda} \mathcal{E}_a(\gamma')$. This further implies from Lemma 2.1 that $E_a(\lambda)$ possesses minimizers, where $0 < \lambda := \int_{\mathbb{R}^3}\rho_\gamma dx < N$. We next consider two different cases.

Case 1: $N = 1$. For the case $N = 1$, since $\int_{\mathbb{R}^3}\rho_\gamma dx = \int_{\mathbb{R}^3}u_1^2 dx = \lambda$, we deduce from (2.53) that for $\varphi := \lambda^{-\frac{1}{2}}u_1$,

$$E_a(1) = E_a(\lambda) = \inf_{\gamma'\in\mathcal{K}_\lambda} \mathcal{E}_a(\gamma') = \mathcal{E}_a(\gamma)$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^3} \Big(|\nabla u_1|^2 + V(x)u_1^2 - a u_1^{\frac{10}{3}} \Big) dx \\
&= \lambda \int_{\mathbb{R}^3} \Big(|\nabla \varphi|^2 + V(x)\varphi^2 - a\lambda^{\frac{2}{3}} \varphi^{\frac{10}{3}} \Big) dx \\
&= \lambda \mathcal{E}_a(|\varphi\rangle\langle\varphi|) + a\lambda\big(1-\lambda^{\frac{2}{3}}\big) \int_{\mathbb{R}^3} \varphi^{\frac{10}{3}} dx \\
&\geq \lambda E_a(1) + a\lambda\big(1-\lambda^{\frac{2}{3}}\big) \int_{\mathbb{R}^3} \varphi^{\frac{10}{3}} dx.
\end{aligned}
$$

If $0 < \lambda := \int_{\mathbb{R}^3} \rho_\gamma dx < 1 = N$, then one has $E_a(1) > \lambda E_a(1)$, which however contradicts with the fact that $E_a(1) < 0$. Therefore, if $N = 1$, then $0 < \lambda := \int_{\mathbb{R}^3} \rho_\gamma dx < N$ cannot occur.

Case 2: $N \geq 2$. As for the case $2 \leq N \in \mathbb{N}^+$, there exists an integer $N' \in [1, N]$ such that $\lambda \in [N'-1, N')$. Let

$$
\gamma_1 := \sum_{i=1}^{N'} |\varphi_i\rangle\langle\varphi_i| + (\lambda - N')|\varphi_{N'}\rangle\langle\varphi_{N'}| \tag{2.54}
$$

be a minimizer of $E_a(\lambda)$, where $(\varphi_i, \varphi_j) = \delta_{ij}$. Consider

$$
\gamma_2 := \sum_{j=1}^{N-N'+1} |\psi_j\rangle\langle\psi_j| + (N' - \lambda - 1)|\psi_{N-N'+1}\rangle\langle\psi_{N-N'+1}|,
$$

where the functions $\psi_1, \cdots, \psi_{N-N'+1} \in C_0^\infty(\mathbb{R}^3, [0,1])$ satisfy $(\psi_i, \psi_j) = \delta_{ij}$. Denote

$$
\psi_j^\tau(x) := \tau^{-3/2}\psi_j(\tau^{-1}x), \quad \text{where} \quad \tau > 0, \quad j = 1, \cdots, N - N' + 1. \tag{2.55}
$$

Since γ_1 is a minimizer of $E_a(\lambda)$, it follows from (2.54) and Lemma 2.4 that there exist constants $C > 0$ and $\theta > 0$ such that

$$
|\varphi_i(x)| \leq Ce^{-\theta|x|} \quad \text{in} \quad \mathbb{R}^3, \quad i = 1, \cdots, N', \tag{2.56}
$$

which yields from (2.55) that

$$
0 \leq a_\tau := \max_{i,j} \big\{ |(\varphi_i, \psi_j^\tau)| \big\} \leq C_1 \tau^{-\frac{3}{2}} \quad \text{as} \quad \tau \to \infty, \tag{2.57}
$$

where $C_1 > 0$ is independent of $\tau > 0$. We thus can define the same operator $\gamma_\tau \in \mathcal{K}_N$ as in (2.22), where $\tau > 0$ is sufficiently large.

Similar to (2.24), one can get that

$$
\begin{aligned}
\gamma_\tau = \gamma_1 + \gamma_2^\tau &- \sum_{i=1}^{N'} \sum_{j=1}^{N-N'+1} a_{ij}^\tau \big(|\varphi_i\rangle\langle\psi_j^\tau| + |\psi_j^\tau\rangle\langle\varphi_i| \big) \\
&- \frac{1}{2}(\lambda - N') \sum_{j=1}^{N-N'+1} a_{N'j}^\tau \big(|\varphi_{N'}\rangle\langle\psi_j^\tau| + |\psi_j^\tau\rangle\langle\varphi_{N'}| \big) \\
&- \frac{1}{2}(N' - \lambda - 1) \sum_{i=1}^{N'} a_{i,N-N'+1}^\tau \big(|\varphi_i\rangle\langle\psi_{N-N'+1}^\tau| + |\psi_{N-N'+1}^\tau\rangle\langle\varphi_i| \big) + O(a_\tau^2)
\end{aligned} \tag{2.58}
$$

$$:= \gamma_1 + \gamma_2^\tau - \gamma_{A_\tau} \quad \text{as} \quad \tau \to \infty,$$

where $a_{ij}^\tau := (\varphi_i, \psi_j^\tau)$, $a_\tau := \max_{i,j} \big\{ |(\varphi_i, \psi_j^\tau)| \big\}$ and

$$\gamma_2^\tau := \sum_{j=1}^{N-N'+1} |\psi_j^\tau\rangle\langle\psi_j^\tau| + (N' - \lambda - 1)|\psi_{N-N'+1}^\tau\rangle\langle\psi_{N-N'+1}^\tau|.$$

Applying Lemma 2.4, we thus deduce from (2.56)–(2.58) that

$$\begin{aligned} \mathrm{Tr}(-\Delta + V(x))\gamma_\tau &= \mathrm{Tr}(-\Delta + V(x))(\gamma_1 + \gamma_2^\tau) + O(a_\tau^2) \\ &= \mathrm{Tr}(-\Delta + V(x))\gamma_1 + \tau^{-2}\mathrm{Tr}(-\Delta\gamma_2) \\ &\quad - \tau^{-1}\sum_{k=1}^{K} \int_{\mathbb{R}^3} \big|x - \tau^{-1}y_k\big|^{-1} \rho_{\gamma_2} dx + O(a_\tau^2) \\ &\le \mathrm{Tr}(-\Delta + V(x))\gamma_1 - C_2\tau^{-1} \quad \text{as} \quad \tau \to \infty, \end{aligned} \tag{2.59}$$

and

$$\begin{aligned} \int_{\mathbb{R}^3} \rho_{\gamma_\tau}^{5/3} dx &\ge \int_{\mathbb{R}^3} \Big(\rho_{\gamma_1} - |\rho_{\gamma_{A_\tau}}|\Big)^{5/3} dx \\ &= \int_{\mathbb{R}^3} \rho_{\gamma_1}^{5/3} dx - \frac{5}{3}\big(1 + o(1)\big) \int_{\mathbb{R}^3} \rho_{\gamma_1}^{2/3} |\rho_{\gamma_{A_\tau}}| dx \\ &= \int_{\mathbb{R}^3} \rho_{\gamma_1}^{5/3} dx - O(a_\tau^2) \ge \int_{\mathbb{R}^3} \rho_{\gamma_1}^{5/3} dx - C_2\tau^{-3} \quad \text{as} \quad \tau \to \infty, \end{aligned} \tag{2.60}$$

where $C_2 > 0$ is independent of $\tau > 0$, and the operator γ_{A_τ} is defined in (2.58). As a consequence, we conclude from (2.2), (2.59) and (2.60) that

$$E_a(N) = \inf_{\gamma' \in \mathcal{K}_N} \mathcal{E}_a(\gamma') \le \mathcal{E}_a(\gamma_\tau) \le E_a(\lambda) - \frac{C_2}{2}\tau^{-1} < E_a(\lambda) \quad \text{as} \quad \tau \to \infty, \tag{2.61}$$

which however contradicts with the identity (2.53). This shows that if $N \ge 2$, then $0 < \lambda := \int_{\mathbb{R}^3} \rho_\gamma dx < N$ cannot occur, either. The proof of Theorem 1.1 is therefore complete. □

3 $N = 2$: Limiting Behavior of Minimizers as $a \nearrow a_2^*$

In this section, we address the proof of Theorem 1.2 on the limiting concentration behavior of minimizers for $E_a(N)$ with $N = 2$ as $a \nearrow a_2^*$, where $a_2^* > 0$ is defined by (1.8). Towards this purpose, we shall employ the first three steps from the so-called blow-up analysis of many-body fermionic systems, which is described in Subsection 1.1.

Throughout the rest part of this paper, we follow Lemma 2.2 and [4, Theorem 6 and Proposition 11] to suppose that

$$\gamma^{(2)} = \sum_{i=1}^{2} |Q_i\rangle\langle Q_i| \quad \text{with} \quad (Q_i, Q_j) = \delta_{ij} \tag{3.1}$$

is an optimizer of a_2^*, where $Q_i \in C^\infty(\mathbb{R}^3, \mathbb{R})$ satisfies

$$|\nabla Q_i(x)|, \quad |Q_i(x)| = O(e^{-\sqrt{|\hat{\mu}_i|}|x|}) \quad \text{as } |x| \to \infty, \quad i = 1, 2, \tag{3.2}$$

and $(\hat{\mu}_i, Q_i)$ denotes the ith eigenpair (counted with multiplicity) of $-\Delta - \frac{5}{3}a_2^*\Big(\sum_{j=1}^2 Q_j^2\Big)^{2/3}$ in $\mathbb{R}^3$.

We start with the following energy estimates of $E_a(2)$ as $a \nearrow a_2^*$.

Lemma 3.1. *Suppose γ_a is a minimizer of $E_a(2)$ defined by (1.5), where $0 < a < a_2^*$. Then there exist some constants $0 < M_1 < M_2$, $0 < M_1' < M_2'$, $0 < M_1''$ and $0 < M_1'''$, independent of $0 < a < a_2^*$, such that*

$$M_1 \le -\epsilon_a E_a(2) \le M_2, \quad M_1' \le -\epsilon_a \int_{\mathbb{R}^3} V(x)\rho_{\gamma_a} dx \le M_2' \quad \text{as} \quad a \nearrow a_2^*, \tag{3.3}$$

and

$$0 \le \epsilon_a^2 \mathrm{Tr}(-\Delta\gamma_a) \le M_1'', \quad 0 \le \epsilon_a^2 \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}} dx \le M_1''' \quad \text{as} \quad a \nearrow a_2^*, \tag{3.4}$$

where $\epsilon_a := a_2^* - a > 0$, and the potential $V(x) = -\sum_{k=1}^K |x - y_k|^{-1} < 0$ is as in (1.7).

Proof. Take a cut-off function $\varphi \in C_0^\infty(\mathbb{R}^3, [0,1])$ satisfying $\varphi(x) = 1$ for $|x| \le 1$ and $\varphi(x) = 0$ for $|x| \ge 2$. Define for $\tau > 0$,

$$Q_i^\tau(x) := A_i^\tau \tau^{\frac{3}{2}} \varphi(x - y_1) Q_i\big(\tau(x - y_1)\big), \quad i = 1, 2, \tag{3.5}$$

where $Q_i \in C^\infty(\mathbb{R}^3)$ and $y_1 \in \mathbb{R}^3$ are given by (3.1) and (1.7), respectively, and $A_i^\tau > 0$ is chosen such that $\int_{\mathbb{R}^3} |Q_i^\tau(x)|^2 dx = 1,\ i = 1, 2$. The exponential decay of Q_i in (3.2) then gives that

$$A_i^\tau = 1 + o(\tau^{-\infty}) \quad \text{and} \quad a_\tau := \big(Q_1^\tau, Q_2^\tau\big) = o(\tau^{-\infty}) \quad \text{as} \ \ \tau \to \infty, \tag{3.6}$$

where $o(\tau^{-\infty})$ means $\lim\limits_{\tau\to\infty} o(\tau^{-\infty})\tau^s = 0$ for any $s \ge 0$. This implies that the following Gram matrix

$$G_\tau := \begin{pmatrix} Q_1^\tau \\ Q_2^\tau \end{pmatrix} \big(Q_1^\tau, Q_2^\tau\big) = \begin{bmatrix} 1 & \big(Q_1^\tau, Q_2^\tau\big) \\ \big(Q_2^\tau, Q_1^\tau\big) & 1 \end{bmatrix} = \begin{bmatrix} 1 & a_\tau \\ a_\tau & 1 \end{bmatrix} \tag{3.7}$$

is positive definite for sufficiently large $\tau > 0$.

We now define for $\tau > 0$,

$$\big(\tilde{Q}_1^\tau, \tilde{Q}_2^\tau\big) := \big(Q_1^\tau, Q_2^\tau\big) G_\tau^{-\frac{1}{2}}. \tag{3.8}$$

It then follows from (3.7) that for sufficiently large $\tau > 0$,

$$\big(\tilde{Q}_i^\tau, \tilde{Q}_j^\tau\big) = \delta_{ij}, \quad i, j = 1, 2. \tag{3.9}$$

Similar to (2.23), one can obtain from (3.7) the Taylor's expansion of G_τ as $\tau \to \infty$. Thus we also derive from (3.8) that

$$\big(\tilde{Q}_1^\tau, \tilde{Q}_2^\tau\big) = \big(Q_1^\tau, Q_2^\tau\big) - \frac{1}{2} a_\tau \big(Q_2^\tau, Q_1^\tau\big) + O(a_\tau^2) \quad \text{as} \ \ \tau \to \infty. \tag{3.10}$$

Setting

$$\tilde{\gamma}_\tau^{(2)} := \sum_{i=1}^2 |\tilde{Q}_i^\tau\rangle\langle\tilde{Q}_i^\tau|,$$

we can compute from (3.6) and (3.10) that

$$\begin{aligned}
\mathcal{E}_a(\tilde{\gamma}_\tau^{(2)}) =& \mathrm{Tr}\big(-\Delta+V(x)\big)\tilde{\gamma}_\tau^{(2)} - a\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_\tau^{(2)}}^{\frac{5}{3}}dx\\
=&\sum_{i=1}^2\int_{\mathbb{R}^3}|\nabla\tilde{Q}_i^\tau|^2dx+\sum_{i=1}^2\int_{\mathbb{R}^3}V(x)|\tilde{Q}_i^\tau|^2dx - a\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|\tilde{Q}_i^\tau|^2\Big)^{\frac{5}{3}}dx\\
=&\sum_{i=1}^2\int_{\mathbb{R}^3}|\nabla Q_i^\tau|^2dx+\sum_{i=1}^2\int_{\mathbb{R}^3}V(x)|Q_i^\tau|^2dx - a\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|Q_i^\tau|^2\Big)^{\frac{5}{3}}dx\\
&-2a_\tau\int_{\mathbb{R}^3}\nabla Q_1^\tau\cdot\nabla Q_2^\tau dx - 2a_\tau\int_{\mathbb{R}^3}V(x)Q_1^\tau Q_2^\tau dx \qquad (3.11)\\
&+\frac{10}{3}aa_\tau\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|Q_i^\tau|^2\Big)^{\frac{2}{3}}Q_1^\tau Q_2^\tau dx + O(a_\tau^2)\\
=&\sum_{i=1}^2\int_{\mathbb{R}^3}|\nabla Q_i^\tau|^2dx+\sum_{i=1}^2\int_{\mathbb{R}^3}V(x)|Q_i^\tau|^2dx - a\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|Q_i^\tau|^2\Big)^{\frac{5}{3}}dx\\
&+o(\tau^{-\infty}) \quad \text{as} \quad \tau\to\infty,
\end{aligned}$$

where the second identity follows from the orthonormality of (3.9).

To estimate the right hand side of (3.11), we calculate from (3.2) and (3.5) that

$$\begin{aligned}
\sum_{i=1}^2\int_{\mathbb{R}^3}|\nabla Q_i^\tau|^2dx =& \sum_{i=1}^2|A_i^\tau|^2\tau^3\int_{\mathbb{R}^3}\Big|Q_i\big(\tau(x-y_1)\big)\nabla\varphi(x-y_1)\\
&+\tau\varphi(x-y_1)\nabla Q_i\big(\tau(x-y_1)\big)\Big|^2dx \qquad (3.12)\\
=&\tau^5\sum_{i=1}^2\int_{\mathbb{R}^3}\varphi^2(x-y_1)\big|\nabla Q_i\big(\tau(x-y_1)\big)\big|^2dx+o(\tau^{-\infty})\\
=&\tau^2\sum_{i=1}^2\int_{\mathbb{R}^3}\big|\nabla Q_i(x)\big|^2dx+o(\tau^{-\infty}) \quad \text{as} \quad \tau\to\infty,
\end{aligned}$$

and

$$\begin{aligned}
\sum_{i=1}^2\int_{\mathbb{R}^3}V(x)|Q_i^\tau|^2dx \le& -\sum_{i=1}^2\int_{\mathbb{R}^3}|x-y_1|^{-1}|Q_i^\tau|^2dx\\
=&-\tau\sum_{i=1}^2\int_{\mathbb{R}^3}|x|^{-1}|A_i^\tau|^2\varphi^2(\tau^{-1}x)Q_i^2(x)dx \qquad (3.13)\\
=&-\tau\sum_{i=1}^2\int_{\mathbb{R}^3}|x|^{-1}Q_i^2(x)dx+o(\tau^{-\infty}) \quad \text{as} \quad \tau\to\infty.
\end{aligned}$$

As for the nonlinear term, one has

$$
\begin{aligned}
\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|Q_i^\tau|^2\Big)^{\frac53}dx =&\tau^2\int_{\mathbb{R}^3}\varphi^{\frac{10}{3}}(\tau^{-1}x)\Big(\sum_{i=1}^2|A_i^\tau|^2Q_i^2(x)\Big)^{\frac53}dx\\
=&\tau^2\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|A_i^\tau|^2Q_i^2(x)\Big)^{\frac53}dx\\
&-\tau^2\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|A_i^\tau|^2Q_i^2(x)\Big)^{\frac53}\Big[1-\varphi^{\frac{10}{3}}(\tau^{-1}x)\Big]dx\\
=&\tau^2\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2|A_i^\tau|^2Q_i^2(x)\Big)^{\frac53}dx+o(\tau^{-\infty})\\
=&\tau^2\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2Q_i^2(x)\Big)^{\frac53}dx+o(\tau^{-\infty})\quad\text{as}\ \ \tau\to\infty.
\end{aligned}\tag{3.14}
$$

Consequently, we obtain from (3.11)–(3.14) that

$$
\begin{aligned}
\mathcal{E}_a(\tilde\gamma_\tau^{(2)})\le&\tau^2\sum_{i=1}^2\int_{\mathbb{R}^3}\big|\nabla Q_i(x)\big|^2dx-\tau\sum_{i=1}^2\int_{\mathbb{R}^3}|x|^{-1}Q_i^2(x)dx\\
&-a\tau^2\int_{\mathbb{R}^3}\Big(\sum_{i=1}^2Q_i^2(x)\Big)^{\frac53}dx+o(\tau^{-\infty})\\
=&\tau^2\mathrm{Tr}(-\Delta\gamma^{(2)})-\tau\int_{\mathbb{R}^3}|x|^{-1}\rho_{\gamma^{(2)}}dx-a\tau^2\int_{\mathbb{R}^3}\rho_{\gamma^{(2)}}^{\frac53}dx+o(\tau^{-\infty})\\
=&\tau^2\big(a_2^*-a\big)\int_{\mathbb{R}^3}\rho_{\gamma^{(2)}}^{\frac53}dx-\tau\int_{\mathbb{R}^3}|x|^{-1}\rho_{\gamma^{(2)}}dx+o(\tau^{-\infty})\quad\text{as}\ \ \tau\to\infty,
\end{aligned}\tag{3.15}
$$

where the last identity follows from the fact that $\gamma^{(2)}$ given in (3.1) is an optimizer of a_2^*.

Taking

$$\tau=t\epsilon_a^{-1}:=t(a_2^*-a)^{-1},\quad t>0,$$

we then conclude from (3.15) that

$$
\begin{aligned}
\lim_{a\nearrow a_2^*}\epsilon_aE_a(2)\le\lim_{a\nearrow a_2^*}\epsilon_a\mathcal{E}_a(\tilde\gamma_\tau^{(2)})&\le\inf_{t>0}\int_{\mathbb{R}^3}\Big(t^2\rho_{\gamma^{(2)}}^{\frac53}-t|x|^{-1}\rho_{\gamma^{(2)}}\Big)dx\\
&=-\frac14\Big(\int_{\mathbb{R}^3}\rho_{\gamma^{(2)}}^{\frac53}dx\Big)^{-1}\Big(\int_{\mathbb{R}^3}|x|^{-1}\rho_{\gamma^{(2)}}dx\Big)^2:=-2M_1<0,
\end{aligned}\tag{3.16}
$$

and hence,

$$-M_1\epsilon_a^{-1}\ge E_a(2)=\mathcal{E}_a(\gamma_a)\ge\int_{\mathbb{R}^3}V(x)\rho_{\gamma_a}(x)dx\quad\text{as}\ \ a\nearrow a_2^*,\tag{3.17}$$

where $\gamma_a=\sum_{i=1}^2|u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$. Moreover, similar to (2.13), we have

$$
\begin{aligned}
E_a(2)+\int_{\mathbb{R}^3}V(x)\rho_{\gamma_a}dx&=\mathcal{E}_a(\gamma_a)+\int_{\mathbb{R}^3}V(x)\rho_{\gamma_a}dx\\
&\ge\ \frac{a_2^*-a}{2a_2^*}\mathrm{Tr}(-\Delta\gamma_a)-\frac{64K^2a_2^*}{a_2^*-a}\quad\text{as}\ \ a\nearrow a_2^*,
\end{aligned}\tag{3.18}
$$

where $K \in \mathbb{N}^+$ is given by (1.7). It then follows from (3.17) and (3.18) that

$$\begin{aligned} -M_1\epsilon_a^{-1} &\geq \int_{\mathbb{R}^3} V(x)\rho_{\gamma_a}dx \geq E_a(2) + \int_{\mathbb{R}^3} V(x)\rho_{\gamma_a}dx \\ &\geq \frac{\epsilon_a}{2a_2^*}\mathrm{Tr}(-\Delta\gamma_a) - 64K^2a_2^*\epsilon_a^{-1} \\ &\geq \frac{1}{2}\epsilon_a \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}dx - 64K^2a_2^*\epsilon_a^{-1} \\ &\geq - 64K^2a_2^*\epsilon_a^{-1} \quad \text{as} \quad a \nearrow a_2^*. \end{aligned} \tag{3.19}$$

Together with (3.16) and (3.17), this completes the proof of Lemma 3.1. □

Let $\gamma_{a_n} = \sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ be a minimizer of $E_{a_n}(2)$, where $a_n \nearrow a_2^*$ as $n \to \infty$. Note from (3.4) that the sequence $\{\epsilon_{a_n}^2 \mathrm{Tr}(-\Delta\gamma_{a_n})\} = \{\epsilon_{a_n}^2 \sum_{i=1}^2 \int_{\mathbb{R}^3} |\nabla u_i^{a_n}|^2dx\}$ is bounded uniformly in n, where $\epsilon_{a_n} := a_2^* - a_n > 0$. This yields that the sequence $\{\epsilon_{a_n}^{3/2} u_i^{a_n}(\epsilon_{a_n}x)\}_{n=1}^\infty$ is bounded uniformly in $H^1(\mathbb{R}^3)$, which thus admits a weak limit $w_i \in H^1(\mathbb{R}^3)$ for $i = 1, 2$. The following lemma shows that, after suitable transformations, the operator $|w_1\rangle\langle w_1| + |w_2\rangle\langle w_2|$ is actually a minimizer of a_2^*.

Lemma 3.2. *Let $\gamma_{a_n} = \sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ be a minimizer of $E_{a_n}(2)$, where the system $(u_1^{a_n}, u_2^{a_n})$ satisfies (1.14), and $a_n \nearrow a_2^*$ as $n \to \infty$. Then there exist a subsequence, still denoted by $\{u_i^{a_n}\}_{n=1}^\infty$, of $\{u_i^{a_n}\}_{n=1}^\infty$ and a point $y_{k_*} \in \{y_1, \cdots, y_K\}$ given by (1.7) such that for $i = 1, 2$,*

$$w_i^{a_n}(x) := \epsilon_{a_n}^{3/2} u_i^{a_n}(\epsilon_{a_n}x + y_{k_*}) \to w_i(x) \ \ \text{strongly in} \ \ H^1(\mathbb{R}^3) \ \ \text{as} \ \ n \to \infty, \tag{3.20}$$

where $\epsilon_{a_n} := a_2^* - a_n > 0$, and $\gamma := \sum_{i=1}^2 |w_i\rangle\langle w_i|$ is a minimizer of a_2^*.

Proof. We shall carry out the proof by three steps.

Step 1. In this step, we mainly establish the weak convergence (3.26) of $\{u_i^{a_n}\}_{n=1}^\infty$ after transformations, where $i = 1, 2$.

Note from (1.7) and (3.3) that

$$\epsilon_{a_n} \sum_{k=1}^K \int_{\mathbb{R}^3} |x - y_k|^{-1}\rho_{\gamma_{a_n}}dx = -\epsilon_{a_n}\int_{\mathbb{R}^3} V(x)\rho_{\gamma_{a_n}}dx \geq M_1' > 0 \quad \text{as} \ \ n \to \infty.$$

This gives that there exists some point $y_{k_*} \in \{y_1, \cdots, y_K\}$ such that

$$\epsilon_{a_n} \int_{\mathbb{R}^3} |x - y_{k_*}|^{-1}\rho_{\gamma_{a_n}}dx \geq \frac{M_1'}{K} > 0 \quad \text{as} \ \ n \to \infty. \tag{3.21}$$

Set

$$w_i^{a_n}(x) := \epsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}(\epsilon_{a_n}x + y_{k_*}), \quad \tilde{\gamma}_{a_n} := \sum_{i=1}^2 |w_i^{a_n}\rangle\langle w_i^{a_n}|, \quad \epsilon_{a_n} := a_2^* - a_n > 0, \tag{3.22}$$

where the point $y_{k_*} \in \{y_1, \cdots, y_K\}$ is as in (3.21). We then have $(w_i^{a_n}, w_j^{a_n}) = \delta_{ij}$,

$$\mathrm{Tr}(-\Delta\tilde{\gamma}_{a_n}) = \sum_{i=1}^2 \int_{\mathbb{R}^3} |\nabla w_i^{a_n}|^2dx = \epsilon_{a_n}^2 \mathrm{Tr}(-\Delta\gamma_{a_n}), \tag{3.23}$$

and

$$\int_{\mathbb{R}^3} \rho_{\tilde{\gamma}_{a_n}}^{\frac{5}{3}} dx = \int_{\mathbb{R}^3} \Big(\sum_{i=1}^{2} |w_i^{a_n}|^2 \Big)^{\frac{5}{3}} dx = \epsilon_{a_n}^2 \int_{\mathbb{R}^3} \rho_{\gamma_{a_n}}^{\frac{5}{3}} dx. \tag{3.24}$$

By the uniform boundedness of the sequence $\big\{\epsilon_{a_n}^2 \operatorname{Tr}(-\Delta\gamma_{a_n})\big\}$ in $n > 0$, we obtain from (3.23) that

$$\big\{w_i^{a_n}\big\}_{n=1}^{\infty} \text{ is bounded uniformly in } H^1(\mathbb{R}^3), \quad i = 1, 2. \tag{3.25}$$

Hence, up to a subsequence if necessary, there exists $w_i \in H^1(\mathbb{R}^3)$ such that

$$w_i^{a_n} \rightharpoonup w_i \text{ weakly in } H^1(\mathbb{R}^3) \text{ as } n \to \infty, \ i = 1, 2, \tag{3.26}$$

and

$$\rho_{\tilde{\gamma}_{a_n}} \to \rho_\gamma := w_1^2 + w_2^2 \text{ strongly in } L^r_{loc}(\mathbb{R}^3) \text{ as } n \to \infty, \ 1 \le r < 3, \tag{3.27}$$

where $\gamma := \sum_{i=1}^2 |w_i\rangle\langle w_i|$. We thus deduce from (3.21), (3.22) and (3.27) that, up to a subsequence if necessary,

$$0 < \lim_{n\to\infty} \epsilon_{a_n} \int_{\mathbb{R}^3} |x - y_{k_*}|^{-1} \rho_{\gamma_{a_n}} dx = \lim_{n\to\infty} \int_{\mathbb{R}^3} |x|^{-1} \rho_{\tilde{\gamma}_{a_n}} dx = \int_{\mathbb{R}^3} |x|^{-1} \rho_\gamma dx, \tag{3.28}$$

which indicates that $\int_{\mathbb{R}^3} \rho_\gamma^{5/3} dx > 0$.

Step 2. This step is to prove that

$$\rho_{\tilde{\gamma}_{a_n}} \to \rho_\gamma \text{ strongly in } L^{\frac{5}{3}}(\mathbb{R}^3) \text{ as } n \to \infty, \tag{3.29}$$

By the Brézis-Lieb Lemma (cf. [17]), we only need to prove that $\lim\limits_{n\to\infty} \int_{\mathbb{R}^3} \rho_{\tilde{\gamma}_{a_n}}^{5/3} dx = \int_{\mathbb{R}^3} \rho_\gamma^{5/3} dx$.

We first claim that

$$\{W_n\} := \Big\{ \frac{5}{3} a_2^* \rho_{\tilde{\gamma}_{a_n}}^{2/3} \Big\} \text{ is a maximizing sequence of the best constant } L_2^*, \tag{3.30}$$

where

$$L_2^* := \sup_{0 \le W \in L^{5/2}(\mathbb{R}^3)\setminus\{0\}} \frac{\sum_{j=1}^2 |\lambda_j(-\Delta - W)|}{\int_{\mathbb{R}^3} W^{5/2}(x) dx} \tag{3.31}$$

is attainable (cf. [5, Corollary 2]). Here $\lambda_j(-\Delta - W) \le 0$ denotes the ith negative eigenvalue (counted with multiplicity) of $-\Delta - W(x)$ in $L^2(\mathbb{R}^3)$ when it exists, and zero otherwise. Recall from Theorem 1.1 that the function $u_i^{a_n}$ satisfies

$$H_V^{a_n} u_i^{a_n} := \Big[-\Delta + V(x) - \frac{5}{3} a_n \Big(\sum_{j=1}^2 |u_j^{a_n}|^2 \Big)^{\frac{2}{3}} \Big] u_i^{a_n} = \mu_i^{a_n} u_i^{a_n} \quad \text{in } \mathbb{R}^3, \quad i = 1, 2,$$

where $\mu_i^{a_n} < 0$ is the ith eigenvalue (counted with multiplicity) of the operator $H_V^{a_n}$. We thus deduce from (3.22) that $w_i^{a_n}$ solves the following system

$$-\Delta w_i^{a_n} + \epsilon_{a_n}^2 V\big(\epsilon_{a_n} x + y_{k_*}\big) w_i^{a_n} - \frac{5}{3} a_n \Big(\sum_{j=1}^2 |w_j^{a_n}|^2 \Big)^{\frac{2}{3}} w_i^{a_n} = \epsilon_{a_n}^2 \mu_i^{a_n} w_i^{a_n} \text{ in } \mathbb{R}^3, \tag{3.32}$$

where $i = 1, 2$. Applying Lemma 3.1, we derive from (3.32) that

$$\mathrm{Tr}\big(-\Delta\tilde{\gamma}_{a_n}\big) - \frac{5}{3}a_2^*\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{\frac{5}{3}}dx = \sum_{i=1}^{2}\epsilon_{a_n}^2\mu_i^{a_n} + o(1) \quad \text{as} \quad n\to\infty, \tag{3.33}$$

where $\tilde{\gamma}_{a_n} = \sum_{i=1}^2 |w_i^{a_n}\rangle\langle w_i^{a_n}|$ is defined by (3.22). Moreover, it follows from (3.3), (3.23) and (3.24) that

$$\begin{aligned} o(1) &= \epsilon_{a_n}^2\Big(E_{a_n}(2) - \int_{\mathbb{R}^3}V(x)\rho_{\gamma_{a_n}}dx\Big) \\ &= \mathrm{Tr}\big(-\Delta\tilde{\gamma}_{a_n}\big) - a_n\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{\frac{5}{3}}dx \quad \text{as} \quad n\to\infty. \end{aligned} \tag{3.34}$$

We thus conclude from (3.33) and (3.34) that

$$\liminf_{n\to\infty}\Big(-\sum_{i=1}^{2}\epsilon_{a_n}^2\mu_i^{a_n}\Big) = \frac{2}{3}a_2^*\liminf_{n\to\infty}\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{\frac{5}{3}}dx \geq C\int_{\mathbb{R}^3}\rho_{\gamma}^{\frac{5}{3}}dx > 0, \tag{3.35}$$

where $C > 0$ is independent of $n > 0$. Thus, up to a subsequence if necessary, by the min-max principle of [12, Sect. 12.1], we deduce from (3.33) that

$$\begin{aligned} \sum_{j=1}^{2}\lambda_j\big(-\Delta - W_n\big) &\leq \sum_{j=1}^{2}\Big(\big(-\Delta - W_n\big)w_j^{a_n},\ w_j^{a_n}\Big) \\ &= \sum_{j=1}^{2}\epsilon_{a_n}^2\mu_j^{a_n} + o(1) \\ &= -\frac{2}{3}a_2^*\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{\frac{5}{3}}dx + o(1) \quad \text{as} \quad n\to\infty, \end{aligned}$$

where $W_n = \frac{5}{3}a_2^*\rho_{\tilde{\gamma}_{a_n}}^{2/3}$ is defined by (3.30). This further indicates that

$$\begin{aligned} \frac{\sum_{j=1}^2|\lambda_j(-\Delta - W_n)|}{\int_{\mathbb{R}^3}W_n^{5/2}dx} &= \Big(\frac{5}{3}a_2^*\Big)^{-\frac{5}{2}}\frac{\sum_{j=1}^2|\lambda_j(-\Delta - W_n)|}{\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{5/3}dx} \\ &\geq \frac{2}{5}\Big(\frac{3}{5}\Big)^{\frac{3}{2}}\big(a_2^*\big)^{-\frac{3}{2}} + o(1) \\ &= L_2^* + o(1) \quad \text{as} \quad n\to\infty, \end{aligned}$$

where the last identity follows from (1.22). By the definition of L_2^* in (3.31), we then obtain that $\{W_n\} = \big\{\frac{5}{3}a_2^*\rho_{\tilde{\gamma}_{a_n}}^{2/3}\big\}$ is a maximizing sequence of L_2^*, and the claim (3.30) is thus established.

We now denote

$$\alpha := \lim_{n\to\infty}\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{5/3}dx \quad \text{and} \quad \beta := \int_{\mathbb{R}^3}\rho_{\gamma}^{5/3}dx,$$

where $\alpha \geq \beta > 0$ holds true in view of (3.28). To establish Step 2, on the contrary, suppose that $\alpha > \beta > 0$. By an adaptation of the classical dichotomy result (cf. [15, Sect.

3.3]), there exist a subsequence, still denoted by $\{\rho_{\tilde{\gamma}_{a_n}}\}$, of $\{\rho_{\tilde{\gamma}_{a_n}}\}$ and a sequence $\{R_n\}$ with $R_n \to \infty$ as $n \to \infty$ such that

$$0 < \lim_{n\to\infty} \int_{|x|\le R_n} \rho^{\frac{5}{3}}_{\tilde{\gamma}_{a_n}} dx = \beta, \qquad \lim_{n\to\infty} \int_{R_n\le|x|\le 2R_n} \rho^{\frac{5}{3}}_{\tilde{\gamma}_{a_n}} dx = 0.$$

Thus, the argument of [5, Lemma 17] yields that there exists some $s \in \{0,\ 1,\ 2\}$ such that

$$\begin{aligned}\sum_{j=1}^{2} \big|\lambda_j(-\Delta - W_n)\big| =& \sum_{j=1}^{s} \big|\lambda_j\big(-\Delta - W_n \mathbf{1}_{B_{R_n}}\big)\big| \\ &+ \sum_{j=1}^{2-s} \big|\lambda_j\big(-\Delta - W_n \mathbf{1}_{\mathbb{R}^3\setminus B_{2R_n}}\big)\big| + o(1) \quad \text{as} \ \ n \to \infty,\end{aligned} \tag{3.36}$$

where $W_n = \frac{5}{3} a_2^* \rho^{2/3}_{\tilde{\gamma}_{a_n}}$ for all $n > 0$. Recall from (1.21) that the best constant L_s^* of the finite rank Lieb-Thirring inequality is defined as

$$L_s^* := \sup_{0\le W\in L^{5/2}(\mathbb{R}^3)\setminus\{0\}} \frac{\sum_{j=1}^{s} |\lambda_j(-\Delta - W)|}{\int_{\mathbb{R}^3} W^{5/2}(x)dx}, \quad \forall\ s \in \mathbb{N}.$$

According to the above definition, it is obvious that L_s^* is increasing in $s > 0$. Together with (3.36), one hence gets from the claim (3.30) that for some $s \in \{0,\ 1,\ 2\}$,

$$\begin{aligned}\Big(\frac{5}{3}a_2^*\Big)^{\frac{5}{2}} \alpha L_2^* &= L_2^* \lim_{n\to\infty} \int_{\mathbb{R}^3} W_n^{\frac{5}{2}}(x)dx \\ &= \lim_{n\to\infty} \sum_{j=1}^{2} \big|\lambda_j\big(-\Delta - W_n\big)\big| \\ &\le L_s^* \lim_{n\to\infty} \int_{\mathbb{R}^3} \big(W_n \mathbf{1}_{B_{R_n}}\big)^{\frac{5}{2}} dx + L_{2-s}^* \lim_{n\to\infty} \int_{\mathbb{R}^3} \big(W_n \mathbf{1}_{\mathbb{R}^3\setminus B_{2R_n}}\big)^{\frac{5}{2}} dx \\ &= \Big(\frac{5}{3}a_2^*\Big)^{\frac{5}{2}} \Big[L_s^*\beta + L_{2-s}^*(\alpha - \beta)\Big] \le \Big(\frac{5}{3}a_2^*\Big)^{\frac{5}{2}} \alpha L_2^*,\end{aligned} \tag{3.37}$$

where the last inequality follows from the fact that $L_{2-s}^* \le L_2^*$ and $L_s^* \le L_2^*$ hold for $s \in \{0,1,2\}$. Since $\alpha > \beta > 0$, we obtain from (3.37) that $L_s^* = L_{2-s}^* = L_2^*$, where $s \in \{0,1,2\}$ is as in (3.37). However, recalling from (1.12) (or see [4, Theorem 6]) that $a_1^* > a_2^* > 0$, one can conclude from (1.22) that $0 < L_1^* < L_2^*$, which gives that $s \ne 1$. Moreover, because $L_0^* = 0$, it further yields that $s \ne 0, 2$. These thus lead to a contradiction, if $\alpha > \beta > 0$. This implies that $\lim\limits_{n\to\infty} \int_{\mathbb{R}^3} \rho^{5/3}_{\tilde{\gamma}_{a_n}} dx = \int_{\mathbb{R}^3} \rho_\gamma^{5/3} dx$, and Step 2 is therefore established.

Step 3. Since Step 2 gives that $\rho_{\tilde{\gamma}_{a_n}} \to \rho_\gamma$ strongly in $L^{\frac{5}{3}}(\mathbb{R}^3)$ as $n \to \infty$, we derive from (3.26) and (3.34) that

$$\begin{aligned}a_2^* \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx = a_2^* \lim_{n\to\infty} \int_{\mathbb{R}^3} \rho^{\frac{5}{3}}_{\tilde{\gamma}_{a_n}} dx &= \liminf_{n\to\infty} \mathrm{Tr}(-\Delta \tilde{\gamma}_{a_n}) \\ &\ge \mathrm{Tr}(-\Delta\gamma) \ge a_2^* \|\gamma\|^{-\frac{2}{3}} \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx\end{aligned} \tag{3.38}$$

$$\geq a_2^* \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx,$$

where we have used the definition of a_2^*, together with the fact that $\|\gamma\| \leq \liminf_{n\to\infty} \|\tilde{\gamma}_{a_n}\| = 1$. This further shows that $\|\gamma\| = 1$, γ is an optimizer of a_2^*, and

$$|\nabla w_i^{a_n}| \to |\nabla w_i| \quad \text{strongly in } L^2(\mathbb{R}^3) \text{ as } n \to \infty, \; i = 1, 2. \tag{3.39}$$

Since γ is an optimizer of a_2^*, using again the fact (cf. [4, Proposition 11]) that $0 < a_2^* < a_1^*$, we obtain that Rank(γ) = 2. This further implies from (1.9) that

$$\int_{\mathbb{R}^3} \rho_\gamma dx = \|\gamma\| \,\text{Rank}(\gamma) = 2. \tag{3.40}$$

We thus deduce from (3.26) and (3.40) that

$$\rho_{\tilde{\gamma}_{a_n}} = \sum_{i=1}^{2} |w_i^{a_n}|^2 \to \rho_\gamma = \sum_{i=1}^{2} w_i^2 \quad \text{strongly in } L^1(\mathbb{R}^3) \text{ as } n \to \infty, \tag{3.41}$$

where $\gamma = \sum_{i=1}^2 |w_i\rangle\langle w_i|$ is a minimizer of a_2^*. Using again the Brézis-Lieb Lemma (cf. [17]), one can deduce from (3.26) and (3.41) that

$$w_i^{a_n} \to w_i \quad \text{strongly in } L^2(\mathbb{R}^3) \text{ as } n \to \infty, \; i = 1, 2. \tag{3.42}$$

Together with (3.39), this proves the H^1-convergence of (3.20), and we are therefore done. □

3.1 Proof of Theorem 1.2

The main purpose of this subsection is to complete the proof of Theorem 1.2. We first establish the following uniformly exponential decay of the sequence $\{w_i^{a_n}\}_{n=1}^\infty$ as $n \to \infty$ for $i = 1, 2$.

Lemma 3.3. *Suppose that the system* $\left(w_1^{a_n}, w_2^{a_n}\right)$ *is given by Lemma 3.2. Then there exist constants* $\theta > 0$ *and* $C(\theta) > 0$*, which are independent of* $n > 0$*, such that for sufficiently large* $n > 0$*,*

$$|w_i^{a_n}(x)| \leq C(\theta) e^{-\theta|x|} \quad \textit{uniformly in } \mathbb{R}^3, \; i = 1, 2. \tag{3.43}$$

Proof. By the uniform boundedness (3.25) of $\{w_i^{a_n}\}_{n=1}^\infty$ in $H^1(\mathbb{R}^3)$ for $i = 1, 2$, and the strong convergence (3.29) of $\{\rho_{\tilde{\gamma}_{a_n}}\} = \left\{ \sum_{j=1}^2 |w_j^{a_n}|^2 \right\}$ in $L^{\frac{5}{3}}(\mathbb{R}^3)$, we first claim that, up to a subsequence if necessary,

$$\sup_{n>0} \|\rho_{\tilde{\gamma}_{a_n}}\|_\infty := \sup_{n>0} \Big\| \sum_{i=1}^{2} |w_i^{a_n}|^2 \Big\|_\infty < +\infty, \tag{3.44}$$

and

$$\lim_{|x|\to\infty} \rho_{\tilde{\gamma}_{a_n}}(x) = \lim_{|x|\to\infty} \sum_{i=1}^{2} |w_i^{a_n}|^2 = 0 \quad \text{uniformly for sufficiently large } n > 0, \tag{3.45}$$

where $\tilde\gamma_{a_n}=\sum_{i=1}^2|w_i^{a_n}\rangle\langle w_i^{a_n}|$.

Actually, note from (3.32) that the function $w_i^{a_n}$ satisfies

$$\big(-\Delta-c_{a_n}(x)\big)w_i^{a_n}=\epsilon_{a_n}^2\mu_i^{a_n}w_i^{a_n}\quad\text{in }\ \mathbb{R}^3,\ \ i=1,\,2,\tag{3.46}$$

where

$$c_{a_n}(x)=\epsilon_{a_n}\sum_{k=1}^K\big|x-\epsilon_{a_n}^{-1}(y_k-y_{k_*})\big|^{-1}+\frac{5}{3}a_n\Big(\sum_{j=1}^2|w_j^{a_n}|^2\Big)^{2/3},$$

and $\mu_1^{a_n}<\mu_2^{a_n}<0$ holds for all $n>0$. We then obtain from Kato's inequality (cf. [16, Theorem X.27]) that

$$\big(-\Delta-c_{a_n}(x)\big)|w_i^{a_n}|\le 0\quad\text{ in }\ \mathbb{R}^3,\ \ i=1,2.\tag{3.47}$$

Following the uniform boundedness (3.25) of $\{w_i^{a_n}\}_{n=1}^\infty$ in $H^1(\mathbb{R}^3)$ for $i=1,2$, one can verify that

$$\|c_{a_n}(x)\|_{L^r(B_2(y))}\le C\quad\text{holds for any }\ y\in\mathbb{R}^3,$$

where $r\in\big(3/2,3\big)$, and $C>0$ is independent of $n>0$ and $y\in\mathbb{R}^3$. Thus, applying De Giorgi-Nash-Moser theory (cf. [9, Theorem 4.1]), we immediately conclude from (3.47) that

$$\begin{aligned}\|w_i^{a_n}\|_{L^\infty(B_1(y))}&\le C_1\|w_i^{a_n}\|_{L^{10/3}(B_2(y))}\\&\le C_1\|\rho_{\tilde\gamma_{a_n}}\|^{1/2}_{L^{5/3}(B_2(y))}\quad\text{ for any }\ y\in\mathbb{R}^3,\quad i=1,2,\end{aligned}\tag{3.48}$$

where $\rho_{\tilde\gamma_{a_n}}=\sum_{i=1}^2|w_i^{a_n}|^2$, and $C_1>0$ is independent of $n>0$ and $y\in\mathbb{R}^3$. By the strong convergence (3.29) of $\rho_{\tilde\gamma_{a_n}}$ in $L^{\frac53}(\mathbb{R}^3)$, we thus obtain from (3.48) that both (3.44) and (3.45) hold true, and the above claim is therefore proved.

Furthermore, it follows from (3.46) that

$$\begin{aligned}\sum_{i=1}^2\epsilon_{a_n}^2\mu_i^{a_n}&=\mathrm{Tr}(-\Delta\tilde\gamma_{a_n})-\frac{5}{3}a_n\int_{\mathbb{R}^3}\rho^{\frac53}_{\tilde\gamma_{a_n}}dx\\&\quad-\epsilon_{a_n}\sum_{k=1}^K\int_{\mathbb{R}^3}\big|x-\epsilon_{a_n}^{-1}(y_k-y_{k_*})\big|^{-1}\rho_{\tilde\gamma_{a_n}}dx,\end{aligned}\tag{3.49}$$

and

$$w_i^{a_n}(x)=\int_{\mathbb{R}^3}G_i^{a_n}(x-y)\Big[\epsilon_{a_n}\sum_{k=1}^K\big|y-\epsilon_{a_n}^{-1}(y_k-y_{k_*})\big|^{-1}+\frac{5}{3}a_n\rho^{\frac23}_{\tilde\gamma_{a_n}}(y)\Big]w_i^{a_n}(y)dy,\tag{3.50}$$

where $\rho_{\tilde\gamma_{a_n}}=\sum_{j=1}^2|w_j^{a_n}|^2$, and $G_i^{a_n}(x)$ denotes the Green's function of the operator

$$-\Delta-\epsilon_{a_n}^2\mu_i^{a_n}\quad\text{in }\ \mathbb{R}^3.$$

Using again the uniform boundedness of $\{w_i^{a_n}\}_{n=1}^\infty$ in $H^1(\mathbb{R}^3)$ for $i=1,2$, we derive from (3.49) that the sequence $\big\{\sum_{i=1}^2\epsilon_{a_n}^2\mu_i^{a_n}\big\}$ is bounded uniformly in $n>0$. Since $\mu_1^{a_n}<\mu_2^{a_n}<0$, this implies that

$$\big\{\epsilon_{a_n}^2\mu_i^{a_n}\big\}_{n=1}^\infty\ \text{is also bounded uniformly in }n>0,\ \ i=1,2.\tag{3.51}$$

Thus, up to a subsequence if necessary, we can assume that

$$\lim_{n\to\infty} \epsilon_{a_n}^2 \mu_i^{a_n} = \hat{\mu}_i \le 0.$$

Passing to the limit on both hand sides of (3.46) as $n\to\infty$, we then obtain from Lemma 3.2 that

$$-\Delta w_i - \frac{5}{3} a_2^* \Big(\sum_{j=1}^{2} w_j^2\Big)^{\frac{2}{3}} w_i = \hat{\mu}_i w_i \quad \text{in } \mathbb{R}^3,\ \ i=1,2, \tag{3.52}$$

where w_i is the strong limit of $w_i^{a_n}$ in $H^1(\mathbb{R}^3)$. Recall from Lemma 3.2 that the functions w_1 and w_2 satisfy $(w_i, w_j)=\delta_{ij}$, and $\gamma := \sum_{i=1}^2 |w_i\rangle\langle w_i|$ is a minimizer of a_2^*. We then conclude from (1.10) (or [4, Theorem 6]) that $\hat{\mu}_i<0$ holds for $i=1,2$. As a consequence, employing the fact (cf. [12, Theorem 6.23]) that

$$G_i^{a_n}(x) = \frac{1}{4\pi|x|} e^{-\sqrt{|\epsilon_{a_n}^2 \mu_i^{a_n}|}|x|} \quad \text{in } \mathbb{R}^3,$$

we deduce from (3.50) that for any sufficiently large $n>0$,

$$\begin{aligned} |w_i^{a_n}(x)| \le C \int_{\mathbb{R}^3} & |x-y|^{-1} e^{-\theta|x-y|} |w_i^{a_n}(y)| \\ & \cdot \Big(\epsilon_{a_n} \sum_{k=1}^{K} \big|y-\epsilon_{a_n}^{-1}(y_k-y_{k_*})\big|^{-1} + \frac{5}{3} a_2^* \rho_{\tilde{\gamma}_{a_n}}^{\frac{2}{3}}(y)\Big) dy \ \text{ in } \mathbb{R}^3,\ i=1,2, \end{aligned} \tag{3.53}$$

where $\theta := \frac{1}{2}\min\big\{\sqrt{|\hat{\mu}_1|}, \sqrt{|\hat{\mu}_2|}\big\} > 0$, and $C>0$ is independent of $n>0$.

Following (3.44), (3.45) and (3.53), the exponential decay of (3.43) can be proved in a similar way of [1, Lemma 3.3], and we omit the detailed proof for simplicity. This ends the proof of Lemma 3.3. □

Proof of Theorem 1.2. Let $\gamma_{a_n} = \sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ be a minimizer of $E_{a_n}(2)$, and suppose

$$\tilde{\gamma}_{a_n} := \sum_{i=1}^{2} |w_i^{a_n}\rangle\langle w_i^{a_n}| := \sum_{i=1}^{2} \epsilon_{a_n}^3 \big|u_i^{a_n}(\epsilon_{a_n}\cdot + y_{k_*})\big\rangle\big\langle u_i^{a_n}(\epsilon_{a_n}\cdot + y_{k_*})\big|$$

is as in Lemma 3.2, where $\epsilon_{a_n} = a_2^* - a_n > 0$ and $a_n \nearrow a_2^*$ as $n\to\infty$. The H^1-uniform convergence of (1.16) then follows directly from Lemma 3.2.

We now prove the energy estimate (1.17). Indeed, by the definition of a_2^*, it follows from (3.29) that

$$\begin{aligned} \epsilon_{a_n} E_{a_n}(2) =& \epsilon_{a_n} \mathcal{E}_{a_n}(\gamma_{a_n}) \\ \ge& \epsilon_{a_n}\big(a_2^*-a\big) \int_{\mathbb{R}^3} \rho_{\gamma_{a_n}}^{\frac{5}{3}} dx - \epsilon_{a_n} \int_{\mathbb{R}^3} \sum_{k=1}^{K} |x-y_k|^{-1} \rho_{\gamma_{a_n}} dx \\ =& \int_{\mathbb{R}^3} \rho_{\tilde{\gamma}_{a_n}}^{\frac{5}{3}} dx - \int_{\mathbb{R}^3} \sum_{k=1}^{K} \big|x+\epsilon_{a_n}^{-1}(y_{k_*}-y_k)\big|^{-1} \rho_{\tilde{\gamma}_{a_n}} dx \\ =& \int_{\mathbb{R}^3} \rho_{\gamma}^{\frac{5}{3}} dx - \int_{\mathbb{R}^3} |x|^{-1} \rho_{\gamma} dx + o(1) \quad \text{as } n\to\infty, \end{aligned} \tag{3.54}$$

where $y_{k_*} \in \{y_1, \cdots, y_K\}$ and $\gamma = \sum_{i=1}^{2} |w_i\rangle\langle w_i|$ are as in Lemma 3.2. Since $\gamma = \sum_{i=1}^{2} |w_i\rangle\langle w_i|$ satisfying $(w_i, w_j) = \delta_{ij}$ is a minimizer of a_2^*, we obtain from (3.16) and (3.54) that

$$\int_{\mathbb{R}^3} \Big(\rho_\gamma^{\frac{5}{3}} - |x|^{-1}\rho_\gamma\Big)dx = \lim_{n\to\infty} \epsilon_{a_n} E_{a_n}(2) = \inf_{t>0} \int_{\mathbb{R}^3} \Big(t^2\rho_\gamma^{\frac{5}{3}} - t|x|^{-1}\rho_\gamma\Big)dx. \tag{3.55}$$

Note that the right-hand side of (3.55) has exactly one optimizer

$$t_{min} = \Big(2\int_{\mathbb{R}^3} \rho_\gamma^{5/3}dx\Big)^{-1} \int_{\mathbb{R}^3} |x|^{-1}\rho_\gamma dx.$$

We thus conclude from (3.55) that

$$1 = \Big(2\int_{\mathbb{R}^3} \rho_\gamma^{5/3}dx\Big)^{-1} \int_{\mathbb{R}^3} |x|^{-1}\rho_\gamma dx, \tag{3.56}$$

which further yields in turn that

$$\lim_{n\to\infty} \epsilon_{a_n} E_{a_n}(2) = -\frac{1}{2}\int_{\mathbb{R}^3} |x|^{-1}\rho_\gamma dx = -\int_{\mathbb{R}^3} \rho_\gamma^{5/3}dx = -\frac{1}{a_2^*}\mathrm{Tr}\big(-\Delta\gamma\big). \tag{3.57}$$

Here we have used $\|\gamma\| = 1$ and the fact that γ is a minimizer of a_2^*. This proves (1.17).

We next prove the L^∞-uniform convergence (1.16) of $w_i^{a_n}$ as $n \to \infty$, i.e.,

$$w_i^{a_n} \to w_i \quad \text{strongly in } \ L^\infty(\mathbb{R}^3) \ \text{ as } \ n\to\infty, \ \ i = 1, 2, \tag{3.58}$$

where the system $(w_1^{a_n}, w_2^{a_n})$ is defined by Lemma 3.2. Note from (3.46) that $w_i^{a_n}$ satisfies

$$\begin{aligned}
-\Delta w_i^{a_n} =&\epsilon_{a_n}\sum_{k=1}^{K}\big|x - \epsilon_{a_n}^{-1}(y_k - y_{k_*})\big|^{-1} w_i^{a_n} \\
&+ \frac{5}{3}a_n\Big(\sum_{j=1}^{2}|w_j^{a_n}|^2\Big)^{\frac{2}{3}} w_i^{a_n} + \epsilon_{a_n}^2\mu_i^{a_n} w_i^{a_n} \\
:=&f_i^n(x) \quad \text{in } \ \mathbb{R}^3, \ \ i = 1, 2,
\end{aligned} \tag{3.59}$$

and the sequence $\{f_i^n(x)\}_{n=1}^\infty$ is bounded uniformly in $L^2_{loc}(\mathbb{R}^3)$ for $i = 1, 2$ in view of (3.25), (3.44) and (3.51). One hence gets from (3.59) and [6, Theorem 8.8] that for any fixed $R > 0$,

$$\|w_i^{a_n}\|_{W^{2,2}(B_R)} \le C\Big(\|w_i^{a_n}\|_{H^1(B_{R+1})} + \|f_i^n\|_{L^2(B_{R+1})}\Big), \quad i = 1, 2,$$

where $C > 0$ is independent of $n > 0$. This implies that $\{w_i^{a_n}\}_{n=1}^\infty$ is bounded uniformly in $W^{2,2}(B_R)$ for $i = 1, 2$. Consequently, by the compact embedding theorem (cf. [6, Theorem 7.26]) from $W^{2,2}(B_R)$ into $L^\infty(B_R)$, we obtain that there exists a subsequence, still denoted by $\{w_i^{a_n}\}_{n=1}^\infty$, of $\{w_i^{a_n}\}_{n=1}^\infty$ such that for any fixed $R > 0$,

$$w_i^{a_n} \to w_i \ \text{ strongly in } \ L^\infty(B_R) \ \text{ as } n\to\infty, \ \ i = 1, 2. \tag{3.60}$$

On the other hand, since $\sum_{i=1}^2 |w_i\rangle\langle w_i|$ is a minimizer of a_2^*, we get from (3.45) and the exponential decay (3.2) that for any $\varepsilon > 0$, there exists a sufficiently large constant $R := R(\varepsilon) > 0$, which is independent of $n > 0$, such that for sufficiently large $n > 0$,

$$|w_i(x)|, \quad |w_i^{a_n}(x)| < \frac{\varepsilon}{4} \text{ in } \mathbb{R}^3 \backslash B_R, \quad i = 1, 2, \tag{3.61}$$

and hence,

$$\sup_{|x| \geq R} \big| w_i^{a_n}(x) - w_i(x) \big| \leq \sup_{|x| \geq R} \big(|w_i^{a_n}(x)| + |w_i(x)| \big) < \frac{\varepsilon}{2}, \quad i = 1, 2. \tag{3.62}$$

Together with (3.60), we obtain from (3.62) that the convergence of (3.58) is true, and the proof of Theorem 1.2 is therefore complete. □

Remark 3.1. Generally, suppose there exists an integer $2 \leq N \in \mathbb{N}^+$ such that $a_{N-1}^* > a_N^*$ holds, which is true at least for $N = 2$. It then follows from (1.9) that any minimizer $\gamma^{(N)}$ of a_N^* can be written in the form $\gamma^{(N)} = \|\gamma^{(N)}\| \sum_{i=1}^N |Q_i\rangle\langle Q_i|$, where $(Q_i, Q_j) = \delta_{ij},\ i, j = 1, \cdots, N$. Since $a_k^* > a_{2k}^*$ holds for any $k \in \mathbb{N}^+$ (see [4, Proposition 11]), the same argument of proving Theorem 1.2 yields that Theorem 1.2 essentially holds true for any $E_a(N)$, as soon as $2 \leq N \in \mathbb{N}^+$ satisfies $a_{N-1}^* > a_N^*$.

4 $N = 3$: Limiting Behavior of Minimizers as $a \nearrow a_3^*$

In this section, we prove Theorem 1.3 on the limiting behavior of minimizers for $E_a(3)$ as $a \nearrow a_3^*$. Recall that the positive constants a_2^* and a_3^* are given by (1.8). The main idea of the proof is called the blow-up analysis of many-body fermionic systems, which is explained briefly in Subsection 1.1. We start with the following $L^\infty-$convergence of minimizers as $a \nearrow a_3^*$.

Proposition 4.1. *Under the assumptions of Theorem 1.3, the $L^\infty-$convergence (1.24) holds true.*

Proof. One can note from (1.8) that $a_2^* \geq a_3^*$. If $a_2^* > a_3^*$, then it follows from Remark 3.1 that

$$\text{Theorem 1.2 holds true for } E_a(3). \tag{4.1}$$

Thus, in the following it suffices to focus on the case where $a_2^* = a_3^*$.

Suppose $a_2^* = a_3^*$, and let $\gamma_{a_n} = \sum_{i=1}^3 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ be a minimizer of $E_{a_n}(3)$ with $a_n \nearrow a_3^*$ as $n \to \infty$, where the orthonormal family $(u_1^{a_n}, u_2^{a_n}, u_3^{a_n})$ satisfies (1.14). Recall from (3.16) that

$$\lim_{a \nearrow a_2^*} (a_2^* - a) E_a(2) \leq \inf_{t > 0} \int_{\mathbb{R}^3} \Big(t^2 \rho_{\gamma^{(2)}}^{\frac{5}{3}} - t|x|^{-1} \rho_{\gamma^{(2)}} \Big) dx := -2M_1 < 0, \tag{4.2}$$

where $M_1 > 0$ is independent of $a \in (0, a_2^*)$, and $\gamma^{(2)}$ is a minimizer of a_2^*. Since we consider the case where $a_2^* = a_3^*$, by Lemma 2.3 (2), we obtain from (1.8) and (4.2) that

$$-M_1 \epsilon_{a_n}^{-1} \geq E_{a_n}(2) \geq E_{a_n}(3) = \mathcal{E}_{a_n}(\gamma_{a_n}) \geq \int_{\mathbb{R}^3} V(x) \rho_{\gamma_{a_n}} dx \quad \text{as } n \to \infty, \tag{4.3}$$

where $\epsilon_{a_n} := a_3^* - a_n = a_2^* - a_n > 0$ and $\rho_{\gamma_{a_n}} = \sum_{i=1}^3 |u_i^{a_n}|^2$. Thus, similar to (3.18) and (3.19), we can deduce from (4.3) that the estimates of Lemma 3.1 are also applicable to γ_{a_n} as $n \to \infty$, and thus we particularly have

$$0 < M_1 \leq -\epsilon_{a_n} \int_{\mathbb{R}^3} V(x)\rho_{\gamma_{a_n}} dx \leq M_2 \quad \text{as} \quad n \to \infty, \tag{4.4}$$

where $0 < M_1 < M_2$ are independent of $n > 0$.

Therefore, using again the fact (cf. [4, Proposition 11]) that $a_k^* > a_{2k}^*$ holds for any $k \in \mathbb{N}^+$, the same arguments of proving (3.29) and (3.39) yield that, up to a subsequence if necessary, there exist a point $y_{k_*} \in \{y_1, \cdots, y_K\}$ and $w_i \in H^1(\mathbb{R}^3)$ such that for $\epsilon_{a_n} := a_3^* - a_n > 0$,

$$w_i^{a_n} := \epsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}(\epsilon_{a_n} x + y_{k_*}) \rightharpoonup w_i \ \text{ weakly in } H^1(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \ i = 1, 2, 3, \tag{4.5}$$

$$\rho_{\tilde{\gamma}_{a_n}} = \sum_{i=1}^3 |w_i^{a_n}|^2 \to \rho_\gamma = \sum_{i=1}^3 w_i^2 \quad \text{strongly in } \ L^{\frac{5}{3}}(\mathbb{R}^3) \ \text{ as } n \to \infty, \tag{4.6}$$

and

$$|\nabla w_i^{a_n}| \to |\nabla w_i| \quad \text{strongly in } \ L^2(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \quad i = 1, 2, 3, \tag{4.7}$$

where $\tilde{\gamma}_{a_n} := \sum_{i=1}^3 |w_i^{a_n}\rangle\langle w_i^{a_n}|$, and

$$\gamma := \sum_{i=1}^3 |w_i\rangle\langle w_i| \ \text{ satisfying } \|\gamma\| = 1 \text{ is an optimizer of } a_3^*. \tag{4.8}$$

Similar to (3.45) and (3.58), applying the uniform boundedness of $\{w_i^{a_n}\}_{n=1}^\infty$ in $H^1(\mathbb{R}^3)$ for $i = 1, 2, 3$, one can further derive from (4.6) that

$$\lim_{|x|\to\infty} \rho_{\tilde{\gamma}_{a_n}}(x) = \lim_{|x|\to\infty} \sum_{i=1}^2 |w_i^{a_n}|^2 = 0 \quad \text{uniformly for sufficiently large } n > 0, \tag{4.9}$$

and thus

$$w_i^{a_n} \to w_i \quad \text{strongly in } \ L^\infty(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \ \ i = 1, 2, 3. \tag{4.10}$$

This proves (1.24), and Proposition 4.1 is therefore proved. □

Applying Proposition 4.1, we are now ready to finish the proof of Theorem 1.3.

Proof of Theorem 1.3. In order to complete the proof of Theorem 1.3, we follow Proposition 4.1 to get that the rest proof is to address the limiting function (w_1, w_2, w_3). If $a_2^* > a_3^*$, then the same argument of Theorem 1.2 yields that Theorem 1.3 (1) holds true. If $a_2^* = a_3^*$ and $\gamma = \sum_{i=1}^3 |w_i\rangle\langle w_i|$ is an optimizer of a_3^*, then we conclude from (1.11) that either Rank$(\gamma) = 3$ or Rank$(\gamma) = 2$. We next discuss separately the following two different situations:

1. $a_2^*=a_3^*$ and Rank$(\gamma)=3$. In this situation, we deduce from (1.9) and (4.8) that

$$\begin{aligned}\int_{\mathbb{R}^3}\rho_{\tilde\gamma_{a_n}}dx&=\sum_{i=1}^3\int_{\mathbb{R}^3}|w_i^{a_n}|^2dx=\sum_{i=1}^3\int_{\mathbb{R}^3}|u_i^{a_n}|^2dx\\&=3=\|\gamma\|\,\mathrm{Rank}(\gamma)=\int_{\mathbb{R}^3}\rho_\gamma dx=\sum_{i=1}^3\int_{\mathbb{R}^3}w_i^2dx.\end{aligned}\tag{4.11}$$

We thus obtain from (4.5), (4.7) and (4.11) that

$$w_i^{a_n}\to w_i\quad\text{strongly in }\ H^1(\mathbb{R}^3)\ \text{ as }\ n\to\infty,\quad i=1,2,3,\tag{4.12}$$

which then implies from (1.5) that the functions w_1,w_2 and w_3 satisfy $(w_i,w_j)=\delta_{ij}$. This therefore proves Theorem 1.3 (1).

2. $a_2^*=a_3^*$ and Rank$(\gamma)=2$. In this situation, recall from Theorem 1.1 and (4.5) that $u_i^{a_n}$ satisfies

$$H_V^{a_n}u_i^{a_n}:=\Big[-\Delta+V(x)-\frac{5}{3}a_n\Big(\sum_{j=1}^3|u_j^{a_n}|^2\Big)^{\frac23}\Big]u_i^{a_n}=\mu_i^{a_n}u_i^{a_n}\quad\text{in }\ \mathbb{R}^3,\ \ i=1,2,3,\tag{4.13}$$

and hence for $i=1,2,3$,

$$-\Delta w_i^{a_n}+\epsilon_{a_n}^2V\big(\epsilon_{a_n}x+y_{k_*}\big)w_i^{a_n}-\frac{5}{3}a_n\Big(\sum_{j=1}^3|w_j^{a_n}|^2\Big)^{\frac23}w_i^{a_n}=\epsilon_{a_n}^2\mu_i^{a_n}w_i^{a_n}\ \text{ in }\ \mathbb{R}^3,\tag{4.14}$$

where $\mu_1^{a_n}<\mu_2^{a_n}\le\mu_3^{a_n}<0$ are the 3-first eigenvalues (counted with multiplicity) of $H_V^{a_n}$ in $\mathbb{R}^3$.

Similar to (3.35) and (3.52), we then deduce from (4.5) and (4.14) that

$$\hat H_\gamma w_i:=\Big[-\Delta-\frac{5}{3}a_3^*\Big(\sum_{j=1}^3w_j^2\Big)^{\frac23}\Big]w_i=\hat\mu_iw_i\quad\text{in }\ \mathbb{R}^3,\ \ i=1,2,3,\tag{4.15}$$

where $\hat\mu_i$ satisfies, up to a subsequence if necessary,

$$\hat\mu_i=\lim_{n\to\infty}\epsilon_{a_n}^2\mu_i^{a_n}\ \text{ for }\ i=1,2,3,\quad\hat\mu_1\le\hat\mu_2\le\hat\mu_3\le0\quad\text{and}\quad\sum_{i=1}^3\hat\mu_i<0.\tag{4.16}$$

As a consequence of (4.15), we conclude that for any $i\in\{1,2,3\}$,

$$\text{either }\ w_i(x)\equiv0\ \text{ in }\ \mathbb{R}^3\quad\text{or}\quad(\hat\mu_i,w_i)\ \text{ is an eigenpair of }\hat H_\gamma.\tag{4.17}$$

Since

$$2=\mathrm{Rank}(\gamma)=\mathrm{Rank}\Big(\sum_{i=1}^3|w_i\rangle\langle w_i|\Big)=\dim\big(\mathrm{span}\{w_1,w_2,w_3\}\big),\tag{4.18}$$

we next proceed the proof by the following two steps:

Step 1. We prove that there exists exactly one $i_* \in \{1,2,3\}$ such that $w_{i_*}(x) \equiv 0$ in $\mathbb{R}^3$. Arguing by contradiction, we suppose from (4.18) that

$$w_i \not\equiv 0 \ \text{ in } \ \mathbb{R}^3 \ \text{ for all } i = 1,2,3. \tag{4.19}$$

We first claim that

$$w_1 \ \text{ and } \ w_i \ \text{ are linearly independent for } i = 2,3. \tag{4.20}$$

Actually, note from (4.16) that $\hat{\mu}_1 < 0$. Using this fact and a similar argument of [1, Lemma 3.3], we can deduce from (4.9) and (4.14) that there exist constants $0 < \theta < \sqrt{|\hat{\mu}_1|}$ and $C(\theta) > 0$, which are independent of $n > 0$, such that for sufficiently large $n > 0$,

$$|w_1^{a_n}(x)| \le C(\theta)e^{-\theta|x|} \quad \text{uniformly in } \mathbb{R}^3. \tag{4.21}$$

Thus, if $w_1 \equiv t_{i_*} w_{i_*} \not\equiv 0$ in $\mathbb{R}^3$ for some $i_* \in \{2,3\}$ and $t_{i_*} \in \mathbb{R}\backslash\{0\}$, then it follows from (4.5), (4.10) and (4.21) that

$$\begin{aligned} 0 &= \lim_{R\to\infty}\lim_{n\to\infty}\int_{\mathbb{R}^3} w_1^{a_n} w_{i_*}^{a_n} dx \\ &= \lim_{R\to\infty}\lim_{n\to\infty}\int_{B_R} w_1^{a_n} w_{i_*}^{a_n} dx + \lim_{R\to\infty}\lim_{n\to\infty}\int_{B_R^c} w_1^{a_n} w_{i_*}^{a_n} dx \\ &= t_{i_*}\int_{\mathbb{R}^3} w_{i_*}^2 dx \neq 0, \end{aligned} \tag{4.22}$$

a contradiction. This proves the claim (4.20).

Since $u_1^{a_n}$ is the first eigenfunction of the operator $H_V^{a_n}$ defined in (4.13), and it follows from (4.5) that

$$w_1(x) = \lim_{n\to\infty} \epsilon_{a_n}^{\frac{3}{2}} u_1^{a_n}(\epsilon_{a_n} x + y_{k_*}) \ \text{ a.e. in } \mathbb{R}^3,$$

we derive that $w_1(x) \ge 0$ in $\mathbb{R}^3$. Since the first eigenvalue of the operator $\hat{H}_\gamma$ defined in (4.15) is simple, we deduce from (4.15) and [12, Theorem 11.8] that $(\hat{\mu}_1, w_1)$ is the first eigenpair of $\hat{H}_\gamma$ in $\mathbb{R}^3$. Using again the simplicity of $\hat{\mu}_1$, we then conclude from (4.15) and (4.20) that

$$(w_1, w_2) = (w_1, w_3) = 0. \tag{4.23}$$

We thus obtain from (4.18) and (4.23) that under the assumption (4.19), we have

$$w_3(x) \equiv t w_2(x) \not\equiv 0 \ \text{ in } \mathbb{R}^3 \text{ for some } t \in \mathbb{R}\backslash\{0\}. \tag{4.24}$$

Setting

$$\tilde{w}_1 := w_1, \quad \tilde{w}_2 := \sqrt{1+t^2}\, w_2, \tag{4.25}$$

we then derive from (4.8) and (4.23) that

$$\gamma = \sum_{i=1}^{2} |\tilde{w}_i\rangle\langle\tilde{w}_i| \quad \text{and} \quad 1 = \|\gamma\| = \max\Big\{\|\tilde{w}_1\|_2^2, \ \|\tilde{w}_2\|_2^2\Big\}. \tag{4.26}$$

On the other hand, since $\mathrm{Rank}(\gamma) = 2$, we further deduce from (1.9), (4.8) and (4.26) that

$$2 = \|\gamma\|\mathrm{Rank}(\gamma) = \int_{\mathbb{R}^3} \rho_\gamma dx = \int_{\mathbb{R}^3} \big(\tilde{w}_1^2 + \tilde{w}_2^2\big) dx. \tag{4.27}$$

We thus derive from (4.26) and (4.27) that

$$1 = \|\gamma\| = \|\tilde{w}_1\|_2^2 = \|\tilde{w}_2\|_2^2, \tag{4.28}$$

which yields that $(\tilde{w}_i, \tilde{w}_j) = \delta_{ij}$ for $i, j = 1, 2$. As a consequence, since $\gamma = \sum_{i=1}^2 |\tilde{w}_i\rangle\langle\tilde{w}_i|$ is an optimizer of a_3^*, together with [4, Theorem 6], we deduce from (4.15) and (4.25) that

$$\hat{\mu}_1 < \hat{\mu}_2 = \hat{\mu}_3 < 0. \tag{4.29}$$

Similar to (4.22), we therefore derive from (4.24) and (4.29) that

$$\begin{aligned}
0 &= \lim_{R\to\infty} \lim_{n\to\infty} \int_{\mathbb{R}^3} w_2^{a_n} w_3^{a_n} dx \\
&= \lim_{R\to\infty} \lim_{n\to\infty} \int_{B_R} w_2^{a_n} w_3^{a_n} dx + \lim_{R\to\infty} \lim_{n\to\infty} \int_{B_R^c} w_2^{a_n} w_3^{a_n} dx \\
&= t \int_{\mathbb{R}^3} w_2^2 dx \neq 0,
\end{aligned}$$

a contradiction, which indicates that (4.19) cannot occur. Because $\mathrm{Rank}(\gamma) = 2$, this completes the proof of Step 1.

Step 2. We prove that $(w_i, w_j) = \delta_{ij}$ holds for $i, j \in \{1, 2\}$, and $w_3(x) \equiv 0$ in $\mathbb{R}^3$. Since Step 1 gives that there exists exactly one $i_* \in \{1, 2, 3\}$ such that $w_{i_*}(x) \equiv 0$ in $\mathbb{R}^3$, we derive from (1.9), (4.5), (4.8) and (4.18) that

$$0 < \|w_i\|_2^2 \leq 1 \quad \text{for} \quad i \neq i_*, \quad \text{and} \quad \sum_{i\neq i_*}^3 \int_{\mathbb{R}^3} w_i^2 dx = \int_{\mathbb{R}^3} \rho_\gamma dx = \|\gamma\| \,\mathrm{Rank}(\gamma) = 2,$$

which yield that $\|w_i\|_2^2 = 1$ holds for all $i \neq i_*$. Together with (4.7), one gets that

$$w_i^{a_n} \to w_i \;\text{ strongly in } H^1(\mathbb{R}^3) \;\text{ as }\; n \to \infty, \quad i \neq i_*,$$

and hence

$$(w_i, w_j) = \delta_{ij} \quad \text{for} \quad i, j \in \{1, 2, 3\}\backslash\{i_*\}. \tag{4.30}$$

We now prove that $i_* \neq 2$ holds for (4.30). On the contrary, suppose $i_* = 2$. Then it implies that $w_2(x) \equiv 0$ in $\mathbb{R}^3$. This implies from (4.18) that $\gamma = |w_1\rangle\langle w_1| + |w_3\rangle\langle w_3|$ is a minimizer of a_3^* and satisfies $(w_i, w_j) = \delta_{ij}$ for $i, j = 1, 3$. We thus obtain from [4, Theorem 6] that $\hat{\mu}_1 < \hat{\mu}_3 < 0$, and $\hat{\mu}_1$, $\hat{\mu}_3$ are the first two eigenvalues of the operator $\hat{H}_\gamma = -\Delta - \frac{5}{3} a_3^* \Big(\sum_{j\neq 2}^3 w_j^2\Big)^{2/3}$ in $\mathbb{R}^3$. Together with (4.16), we further derive that $\hat{\mu}_2 < 0$, and hence

$$\sum_{i=1}^3 \hat{\mu}_i < \sum_{i\neq 2}^3 \hat{\mu}_i. \tag{4.31}$$

On the other hand, we calculate from (4.4), (4.14) and (4.16) that

$$\begin{aligned}\sum_{i=1}^{3}\hat{\mu}_i &= \lim_{n\to\infty}\sum_{i=1}^{3}\epsilon_{a_n}^2\mu_i^{a_n}\\ &= \lim_{n\to\infty}\Big[\sum_{i=1}^{3}\int_{\mathbb{R}^3}|\nabla w_i^{a_n}|^2dx-\frac{5}{3}a_n\int_{\mathbb{R}^3}\Big(\sum_{i=1}^{3}|w_i^{a_n}|^2\Big)^{\frac{5}{3}}dx\Big],\end{aligned}\tag{4.32}$$

and

$$\begin{aligned}&\sum_{i\neq 2}^{3}\hat{\mu}_i = \lim_{n\to\infty}\sum_{i\neq 2}^{3}\epsilon_{a_n}^2\mu_i^{a_n}\\ =&\lim_{n\to\infty}\Big[\sum_{i\neq 2}^{3}\int_{\mathbb{R}^3}|\nabla w_i^{a_n}|^2dx-\frac{5}{3}a_n\int_{\mathbb{R}^3}\Big(\sum_{i=1}^{3}|w_i^{a_n}|^2\Big)^{\frac{2}{3}}\Big(|w_1^{a_n}|^2+|w_3^{a_n}|^2\Big)dx\Big]\\ =&\lim_{n\to\infty}\Big[\sum_{i\neq 2}^{3}\int_{\mathbb{R}^3}|\nabla w_i^{a_n}|^2dx-\frac{5}{3}a_n\int_{\mathbb{R}^3}\Big(\sum_{i=1}^{3}|w_i^{a_n}|^2\Big)^{\frac{5}{3}}dx\\ &+\frac{5}{3}a_n\int_{\mathbb{R}^3}\Big(\sum_{i=1}^{3}|w_i^{a_n}|^2\Big)^{\frac{2}{3}}|w_2^{a_n}|^2dx\Big].\end{aligned}\tag{4.33}$$

Since $w_2(x)\equiv 0$ in $\mathbb{R}^3$, applying (4.6) and (4.7), one can further derive from (4.32) and (4.33) that

$$\sum_{i=1}^{3}\hat{\mu}_i=\sum_{i\neq 2}^{3}\int_{\mathbb{R}^3}|\nabla w_i|^2dx-\frac{5}{3}a_3^*\int_{\mathbb{R}^3}\Big(\sum_{i\neq 2}^{3}w_i^2\Big)^{\frac{5}{3}}dx,\tag{4.34}$$

and

$$\begin{aligned}\sum_{i\neq 2}^{3}\hat{\mu}_i =&\sum_{i\neq 2}^{3}\int_{\mathbb{R}^3}|\nabla w_i|^2dx-\frac{5}{3}a_3^*\int_{\mathbb{R}^3}\Big(\sum_{i\neq 2}^{3}w_i^2\Big)^{\frac{5}{3}}dx\\ &+\frac{5}{3}\lim_{n\to\infty}a_n\int_{\mathbb{R}^3}\Big(\sum_{i=1}^{3}|w_i^{a_n}|^2\Big)^{\frac{2}{3}}|w_2^{a_n}|^2dx\\ :=&\sum_{i\neq 2}^{3}\int_{\mathbb{R}^3}|\nabla w_i|^2dx-\frac{5}{3}a_3^*\int_{\mathbb{R}^3}\Big(\sum_{i\neq 2}^{3}w_i^2\Big)^{\frac{5}{3}}dx+\frac{5}{3}A.\end{aligned}\tag{4.35}$$

Note from (4.10) that

$$w_2^{a_n}\to w_2\equiv 0 \quad \text{strongly in } \ L^\infty(\mathbb{R}^3) \ \text{ as } \ n\to\infty,$$

which yields that

$$\begin{aligned}0\leq A:=&\lim_{n\to\infty}a_n\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{\frac{2}{3}}|w_2^{a_n}|^2dx\\ \leq& a_3^*\lim_{n\to\infty}\|w_2^{a_n}\|_\infty\int_{\mathbb{R}^3}\rho_{\tilde{\gamma}_{a_n}}^{\frac{2}{3}}|w_2^{a_n}|dx\\ \leq& a_3^*\lim_{n\to\infty}\|w_2^{a_n}\|_\infty\ \|\rho_{\tilde{\gamma}_{a_n}}\|_{4/3}^{2/3}\ \|w_2^{a_n}\|_2\\ =&0,\end{aligned}\tag{4.36}$$

i.e., $A = 0$, where the last identity follows from the uniform boundedness of the sequence $\{\rho_{\tilde{\gamma}_{a_n}}\} = \big\{\sum_{i=1}^{3}|w_i^{a_n}|^2\big\}$ in $L^1(\mathbb{R}^3)\cap L^3(\mathbb{R}^3)$. We thus conclude from (4.34)–(4.36) that

$$\sum_{i=1}^{3}\hat{\mu}_i = \sum_{i\neq 2}^{3}\hat{\mu}_i,$$

which however contradicts with (4.31). This proves that $i_* \neq 2$.

Repeating the above argument, one can obtain that $i_* \neq 1$ holds for (4.30), too. Hence, it necessarily has $i_* = 3$, and Step 2 is proved in view of Step 1. This completes the proof of Theorem 1.3 (2), and we are done. □

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