Mass Concentration of Two-Spinless Fermi Systems with Attractive Interactions

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Abstract

We study the two-spinless mass-critical Fermi systems with attractive interactions and trapping potentials. We prove that ground states of the system exist, if and only if the strength a of attractive interactions satisfies $0 < a < a_2^*$, where $0 < a_2^* < +\infty$ is the best constant of a dual finite-rank Lieb-Thirring inequality. By the blow-up analysis of many-fermion systems, we show that ground states of the system concentrate at the flattest minimum points of the trapping potential $V(x)$ as $a \nearrow a_2^*$.

Keywords: Fermi systems; ground states; mass concentration

1 Introduction

Over the past few decades, experimental achievements of trapped atomic gases have revealed (cf. [2, 3, 7, 13]) the beautiful and subtle physics of the quantum world for ultracold atoms. These experiments were usually carried out in the presence of optical laser traps that confine the particles in a limited region of the space, see [2, 20]. In particular, spinless fermions in harmonic traps have played a crucial role of recent developments (cf. [4, 13, 28]), given that trapping potentials in many experiments can be safely approximated with the harmonic form. Moreover, when spinless Fermi gases are confined in inhomogeneous traps [22], the nonuniform density leads to the spatially varying energy and length scales. We also refer the reader to [21] for creating homogeneous Fermi gases of ultracold atoms in a uniform potential. These experiments have generated some interesting theoretical questions. Numerical simulations and mathematical theories of trapped fermions have therefore been a focus of research interests in physics and mathematics since the last decades (cf. [4, 9, 10, 13, 18, 26]).

Following the arguments of [11, 14, 18], ground states of two-spinless mass-critical Fermi systems with attractive interactions and trapping potentials can be described by

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the minimizers of the following constraint variational problem:

$$\begin{aligned} E_a(2) :&= \inf\Big\{\mathcal{E}_a(\Psi):\ \|\Psi\|_2^2=1,\ \Psi\in\wedge^2 L^2(\mathbb{R}^3,\mathbb{C})\cap H^1(\mathbb{R}^6,\mathbb{C}),\\ &\qquad \sum_{i=1}^{2}\int_{\mathbb{R}^6} V(x_i)|\Psi|^2dx_1dx_2<\infty\Big\},\quad a>0, \end{aligned} \tag{1.1}$$

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

$$\mathcal{E}_a(\Psi) := \sum_{i=1}^{2}\int_{\mathbb{R}^6}\Big(|\nabla_{x_i}\Psi|^2+V(x_i)|\Psi|^2\Big)dx_1dx_2 - a\int_{\mathbb{R}^3}\rho_\Psi^{\frac{5}{3}}(x)dx.$$

Here $\wedge^2 L^2(\mathbb{R}^3,\mathbb{C})$ is the subspace of $L^2(\mathbb{R}^6,\mathbb{C})$ consisting of all antisymmetric wave functions, $V(x)\geq 0$ denotes the trapping potential, $a>0$ represents the attractive strength of the quantum particles, and the one-particle density ρ_Ψ associated with Ψ is defined by

$$\rho_\Psi(x) := 2\int_{\mathbb{R}^3}|\Psi(x,x_2)|^2dx_2.$$

Applying the approach of [5, Appendix A and Lemma 2.3], the problem (1.1) can be reduced equivalently to the following form

$$\begin{aligned} E_a(2) &= \inf\Big\{\mathcal{E}_a(\gamma):\ \gamma=\sum_{i=1}^{2}|u_i\rangle\langle u_i|,\ u_i\in\mathcal{H},\\ &\qquad (u_i,u_j)=\delta_{ij},\ i,j=1,2\Big\},\quad a>0, \end{aligned} \tag{1.2}$$

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

$$\mathcal{E}_a(\gamma) := \mathrm{Tr}\big(-\Delta+V(x)\big)\gamma - a\int_{\mathbb{R}^3}\rho_\gamma^{\frac{5}{3}}(x)dx, \tag{1.3}$$

and the Hilbert space $\mathcal{H}$ is defined by

$$\mathcal{H} := \Big\{u\in H^1(\mathbb{R}^3,\mathbb{R}):\ \int_{\mathbb{R}^3}V(x)|u(x)|^2dx<\infty\Big\}.$$

Here the non-negative self-adjoint operator $\gamma=\sum_{i=1}^2|u_i\rangle\langle u_i|$ on $L^2(\mathbb{R}^3,\mathbb{R})$ satisfies

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

the kinetic energy of γ is denoted by

$$\mathrm{Tr}(-\Delta\gamma) := \sum_{j=1}^{3}\mathrm{Tr}(P_j\gamma P_j) = \sum_{j=1}^{3}\sum_{i=1}^{2}\|P_ju_i\|_{L^2}^2 = \sum_{i=1}^{2}\int_{\mathbb{R}^3}|\nabla u_i(x)|^2dx, \tag{1.4}$$

where $P_j := -i\partial_{x_j}$, and the corresponding density of γ is defined as

$$\rho_\gamma(x) := \sum_{i=1}^{2}|u_i(x)|^2. \tag{1.5}$$

If the trapping potential $V(x)$ in (1.3) is ignored, the existence of minimizers for $E_a(2)$ in the L^2-subcritical case was analyzed in [14]. Motivated by [14], the authors in [5] studied the existence and concentration behavior of minimizers for $E_a(2)$ in the L^2-subcritical case, where $V(x) < 0$ is the Coulomb potential. Further, the L^2-critical case of $E_a(2)$ with the Coulomb potential was recently considered in [6]. On the other hand, the physical experiments of Fermi gases were also performed in other types of trapping potentials over the past few years, such as harmonic potentials, double-well potentials, and so on (cf. [4, 13, 26, 28]). Moreover, once the problem $E_a(2)$ is analyzed with other types of traps, instead of the Coulomb form, some extra difficulties appear especially in the analysis of the Lagrange multipliers for $E_a(2)$. Inspired by above facts, the purpose of the present paper is to study the problem $E_a(2)$ with the trap $0 \leq V(x) \in L^\infty_{loc}(\mathbb{R}^3)$ satisfying $\lim_{|x|\to\infty} V(x) = \infty$.

The existing investigations (cf. [6]) show that the problem $E_a(2)$ is related to the following minimization problem

$$0 < a_2^* := \inf \Big\{ \frac{\|\gamma\|^{\frac{2}{3}} \operatorname{Tr}(-\Delta\gamma)}{\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x)dx} : \ 0 \leq \gamma = \gamma^*, \ \operatorname{Rank}(\gamma) \leq 2 \Big\}. \tag{1.6}$$

Here γ is of the form $\gamma = \sum_{i=1}^2 n_i |u_i\rangle\langle u_i|$, where $n_i \geq 0$ and $u_i \in H^1(\mathbb{R}^3)$ satisfies $(u_i, u_j) = \delta_{ij}$ for $i, j = 1, 2$, $\rho_\gamma(x)$ is defined as $\rho_\gamma(x) = \sum_{i=1}^2 n_i u_i^2(x)$, and $\|\gamma\|$ is the operator norm. Note from [11, Theorem 6] that the problem a_2^* defined in (1.6) admits at least one minimizer. Moreover, any minimizer $\gamma^{(2)}$ of the problem a_2^* has rank 2, and can be written in the form

$$\gamma^{(2)} = \|\gamma^{(2)}\| \sum_{i=1}^2 |Q_i\rangle\langle Q_i|, \quad Q_i \in H^1(\mathbb{R}^3), \quad (Q_i, Q_j) = \delta_{ij}, \quad i, j = 1, 2,$$

where the orthonormal system (Q_1, Q_2) satisfies the following nonlinear Schrödinger system

$$\Big[-\Delta - \frac{5a_2^*}{3} \Big(\sum_{j=1}^2 Q_j^2 \Big)^{\frac{2}{3}} \Big] Q_i = \hat{\mu}_i Q_i \ \text{ in } \ \mathbb{R}^3, \quad i = 1, 2, \tag{1.7}$$

and $\hat{\mu}_1 < \hat{\mu}_2 < 0$ are the 2-first negative eigenvalues of the operator $-\Delta - \frac{5a_2^*}{3} \Big(\sum_{j=1}^2 Q_j^2 \Big)^{\frac{2}{3}}$ in $\mathbb{R}^3$.

Associated to the problem $E_a(2)$, we now define ground states of a fermionic nonlinear Schrödinger system, in the following sense that

Definition 1.1. (*Ground states*). Suppose $0 \leq V(x) \in L^\infty_{loc}(\mathbb{R}^3)$ satisfies $\lim_{|x|\to\infty} V(x) = \infty$. A system $(u_1, u_2) \in \big(H^1(\mathbb{R}^3)\big)^2$, where $(u_i, u_j) = \delta_{ij}$ holds for $i, j = 1, 2$, is called a ground state of

$$H_V u_i := \Big[-\Delta + V(x) - \frac{5a}{3} \Big(\sum_{j=1}^2 u_j^2 \Big)^{\frac{2}{3}} \Big] u_i = \mu_i u_i \ \text{ in } \ \mathbb{R}^3, \quad i = 1, 2, \quad a > 0, \tag{1.8}$$

if it satisfies the system (1.8), where $\mu_1 < \mu_2$ are the 2-first eigenvalues of the operator H_V in $\mathbb{R}^3$.

The first result of the present paper is concerned with the following existence of minimizers for $E_a(2)$ defined in (1.2).

Theorem 1.1. *Let $a_2^* > 0$ be defined by* (1.6)*, and assume the potential $0 \le V(x) \in L^\infty_{loc}(\mathbb{R}^3)$ satisfies $\lim_{|x|\to\infty} V(x) = \infty$. Then we have*

1. *If $0 < a < a_2^*$, then there exists at least one minimizer $\gamma = \sum_{i=1}^2 |u_i\rangle\langle u_i|$ of $E_a(2)$, where (u_1, u_2) is a ground state of* (1.8).

2. *If $a \ge a_2^*$, then there is no minimizer of $E_a(2)$.*

When the Coulomb potential $V(x) < 0$ is considered, the non-existence of minimizers for $E_a(2)$ is proved in [6], which gives that $E_a(2) = -\infty$ for $a \ge a_2^*$, by applying the properties of the Coulomb potential and the monotonicity of the energy $E_a(2)$ with respect to the parameter $a > 0$. Different from [6], we shall however derive that $E_{a_2^*}(2) = 0$ and $E_a(2) = -\infty$ for $a > a_2^*$ by constructing suitable orthogonal test functions. The non-existence result of $E_{a_2^*}(2)$ is further proved by applying the properties of minimizers for the problem a_2^* defined in (1.6).

On the other hand, the existence of Theorem 1.1 is derived by analyzing the compactness of the minimizing sequences, which can actually be extended to the problem $E_a(N)$ with any $N \in \mathbb{N}^+$. Moreover, we shall prove, in a simplifier way than those of [5,6,14], that the minimizers of $E_a(2)$ are essentially ground states of (1.8). Further, assume $\gamma_a = \sum_{i=1}^2 |u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$ for $0 < a < a_2^*$, then the proof of Theorem 1.1 yields that $\int_{\mathbb{R}^3} V(x)\rho_{\gamma_a}(x)dx \to \inf_{x\in\mathbb{R}^3} V(x)$ as $a \nearrow a_2^*$, which implies roughly that the mass of the minimizers γ_a concentrates at the global minimum points of $V(x)$ as $a \nearrow a_2^*$. The main purpose of the present paper is to further analyze the mass concentration behavior of the minimizers γ_a as $a \nearrow a_2^*$.

Towards the above main purpose, we now assume that there exist positive constants $p_1, \cdots, p_l$ and C such that

$$V(x) = g(x) \prod_{m=1}^{l} |x - x_m|^{p_m} \quad \text{and} \quad C < g(x) < \frac{1}{C} \quad \text{in} \quad \mathbb{R}^3, \tag{1.9}$$

where $x_m \ne x_n$ for $m \ne n$, $g(x) \in C^\kappa_{loc}(\mathbb{R}^3)$ for some $\kappa \in (0,1)$, and the limits $\lim\limits_{x\to x_m} g(x)$ exist for all $1 \le m \le l$. Denote

$$p = \max\{p_1, \cdots, p_l\} > 0, \quad \Lambda := \{x \in \mathbb{R}^3 : V(x) = 0\} = \{x_1, \cdots, x_l\}, \tag{1.10}$$

and

$$\mathcal{Z} := \{x_m \in \Lambda : \ \alpha_m = \alpha\}, \tag{1.11}$$

where

$$\alpha := \min_{1\le m\le l} \{\alpha_m\} > 0, \quad \text{and} \quad \alpha_m = \lim_{x\to x_m} \frac{V(x)}{|x - x_m|^p} \in (0, +\infty]. \tag{1.12}$$

Note from (1.11) that the set $\mathcal{Z}$ denotes the locations of the flattest global minimum points for $V(x)$. We remark that (1.9) covers both the harmonic trap and double-well trap, which were achieved experimentally in [4,13,26,28].

Using above notations, the main result of the present paper can be stated as the following theorem:

Theorem 1.2. *Suppose $V(x)$ satisfies (1.9), and 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 u_i^a satisfies (1.8) for $i = 1, 2$. Then for any given sequence $\{a_n\}$ with $a_n \nearrow a_2^*$ as $n \to \infty$, there exists a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ such that for $i = 1, 2$,*

$$\begin{aligned} w_i^{a_n}(x) &:= (a_2^* - a_n)^{\frac{3}{2(p+2)}} u_i^{a_n}\Big((a_2^* - a_n)^{\frac{1}{p+2}} x + x_{a_n}\Big) \\ &\quad \to w_i(x) \quad \text{strongly in} \quad H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3) \quad \text{as} \quad n \to \infty, \end{aligned} \tag{1.13}$$

where $p > 0$ is as in (1.10), $\gamma := \sum_{i=1}^{2} |w_i\rangle\langle w_i|$ is a minimizer of a_2^*, and the global maximum point x_{a_n} of the density $\rho_{\gamma_{a_n}}(x) = \sum_{i=1}^{2} |u_i^{a_n}|^2$ satisfies

$$\lim_{n\to\infty} \frac{x_{a_n} - x_k}{(a_2^* - a_n)^{\frac{1}{p+2}}} = \bar{x} \tag{1.14}$$

for some points $x_k \in \mathcal{Z}$ and $\bar{x} \in \mathbb{R}^3$.

Remark 1.1. (1). It follows from Theorem 1.2 that the minimizers of $E_{a_n}(2)$ concentrate at the flattest minimum points of $V(x)$ as $a_n \nearrow a_2^*$.

(2). Under the assumption (1.9), Theorem 1.2 yields that the minimizer $\gamma_{a_n} = \sum_{i=1}^{2} |u_i^{a_n}\rangle\langle u_i^{a_n}|$, where $u_i^{a_n}$ satisfies (1.8) for $i = 1, 2$, of $E_{a_n}(2)$ behaves like

$$\gamma_{a_n}(x, y) \approx (a_2^* - a_n)^{-\frac{3}{p+2}} \gamma\Big(\frac{x - x_{a_n}}{(a_2^* - a_n)^{\frac{1}{p+2}}}, \frac{y - x_{a_n}}{(a_2^* - a_n)^{\frac{1}{p+2}}}\Big) \quad \text{as} \quad a_n \nearrow a_2^*,$$

where $\gamma(x, y) = \sum_{i=1}^{2} w_i(x) w_i(y)$ is the integral kernel of γ, and the energy $E_{a_n}(2)$ satisfies

$$\lim_{a_n \nearrow a_2^*} \frac{E_{a_n}(2)}{(a_2^* - a_n)^{\frac{p}{p+2}}} = \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x) dx + \alpha \int_{\mathbb{R}^3} |x + \bar{x}|^p \rho_\gamma(x) dx,$$

where $\alpha > 0$ is defined by (1.12).

There are several further comments on Theorem 1.2 which is proved by the blow-up analysis of many-body fermions. Firstly, comparing with the existing results of [6], Theorem 1.2 can provide additionally the refined information on the maximum point of the density $\rho_{\gamma_{a_n}}(x)$ as $a_n \nearrow a_2^*$. Secondly, the argument of [5, 6] is improved to obtain the H^1-convergence (1.13) of Theorem 1.2. Thirdly, the proof of Theorem 1.2 needs the following estimates:

$$\mu_1^{a_n} < \mu_2^{a_n} < 0 \quad \text{as} \quad a_n \nearrow a_2^*, \tag{1.15}$$

where $\mu_1^{a_n}$ and $\mu_2^{a_n}$ are the 2-first eigenvalues of the operator $-\Delta + V(x) - \frac{5a_n}{3} \rho_{\gamma_{a_n}}^{2/3}$ in $\mathbb{R}^3$. We shall derive (1.15) in Section 4 by the refined analysis of the energy $E_{a_n}(2)$.

This paper is organized as follows. Section 2 is devoted to the proof of Theorem 1.1 on the existence and non-existence of minimizers for $E_a(2)$. We analyze in Section 3 some refined estimates of minimizers for $E_a(2)$, based on which the proof of Theorem 1.2 is given in Section 4. The exponential decay of minimizers for a_2^* is finally addressed in Appendix A.

2 Existence and Non-existence of Minimizers

In this section, we shall establish Theorem 1.1 on the existence and non-existence of minimizers for $E_a(2)$ defined by (1.2). Towards this purpose, we first recall the following compactness result (see e.g. [24, Theorem XIII.67] or [1]):

Lemma 2.1. *Suppose $0 \le V(x) \in L^\infty_{loc}(\mathbb{R}^3)$ satisfies $\lim_{|x|\to\infty} V(x) = \infty$. Then for any $2 \le q < 6$, the embedding $\mathcal{H} \hookrightarrow L^q(\mathbb{R}^3)$ is compact.*

Employing Lemma 2.1, we next complete the proof of Theorem 1.1.

Proof of Theorem 1.1. Without loss of generality, we assume additionally that the potential $V(x) \ge 0$ satisfies $\inf_{x\in\mathbb{R}^3} V(x) = 0$.

1. We first prove the existence of minimizers for $E_a(2)$, where $0 < a < a_2^*$. Let $\gamma = \sum_{i=1}^2 |u_i\rangle\langle u_i|$ be an operator satisfying $u_i \in \mathcal{H}$ and $(u_i, u_j) = \delta_{ij}$ for $i, j = 1, 2$. Since $V(x) \ge 0$, we obtain from (1.6) that for any $0 < a < a_2^*$,

$$\begin{aligned}\mathcal{E}_a(\gamma) &= \mathrm{Tr}\big(-\Delta + V(x)\big)\gamma - a\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x)dx \\ &\ge \left(1 - \frac{a}{a_2^*}\right)\mathrm{Tr}(-\Delta\gamma) + \int_{\mathbb{R}^3} V(x)\rho_\gamma(x)dx \\ &\ge \left(1 - \frac{a}{a_2^*}\right)\mathrm{Tr}(-\Delta\gamma) \ge 0,\end{aligned} \tag{2.1}$$

due to the fact that $\|\gamma\| = 1$. This gives that $E_a(2)$ is bounded from below for $0 < a < a_2^*$.

Let $\{\gamma_n\}$ be a minimizing sequence of $E_a(2)$ satisfying $\gamma_n = \sum_{i=1}^2 |u_i^n\rangle\langle u_i^n|$, $u_i^n \in \mathcal{H}$, $(u_i^n, u_j^n) = \delta_{ij}$ for $i, j = 1, 2$, and $\lim_{n\to\infty} \mathcal{E}_a(\gamma_n) = E_a(2)$. We derive from (2.1) that $\{u_i^n\}$ is bounded uniformly in $\mathcal{H}$ for $i = 1, 2$. Following Lemma 2.1, we obtain that there exists a function $u_i(x) \in \mathcal{H}$ such that for $i = 1, 2$,

$$u_i^n \rightharpoonup u_i \ \text{ weakly in } \ \mathcal{H} \ \text{ and } \ u_i^n \to u_i \ \text{ strongly in } \ L^q(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \quad 2 \le q < 6.$$

Therefore, we have

$$(u_i, u_j) = \delta_{ij}, \quad i, j = 1, 2,$$

and

$$\rho_{\gamma_n} = \sum_{i=1}^2 |u_i^n|^2 \to \rho_\gamma = \sum_{i=1}^2 |u_i|^2 \ \text{ strongly in } \ L^r(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \quad 1 \le r < 3, \tag{2.2}$$

where $\gamma := \sum\limits_{i=1}^2 |u_i\rangle\langle u_i|$. Since $u_i \in \mathcal{H}$ satisfies $(u_i, u_j) = \delta_{ij}$ for $i, j = 1, 2$, we have

$$E_a(2) \le \mathcal{E}_a(\gamma).$$

Moreover, by the weak lower semi-continuity, we obtain from (2.2) that

$$E_a(2) = \lim_{n\to\infty} \mathcal{E}_a(\gamma_n) \ge \mathcal{E}_a(\gamma),$$

which implies that γ is a minimizer of $E_a(2)$ for $0 < a < a_2^*$. We then conclude that for any $0 < a < a_2^*$, there exists at least one minimizer of $E_a(2)$.

For any $0 < a < a_2^*$, assume γ is a minimizer of $E_a(2)$. Similar to the argument of [27, Appendix A], γ can be written in the form $\gamma = \sum_{i=1}^{2} |u_{k_i}\rangle\langle u_{k_i}|$, where u_{k_i} is an eigenfunction of the operator

$$H_V = -\Delta + V(x) - \frac{5a}{3}\rho_\gamma^{\frac{2}{3}}(x) \ \text{ in } \ \mathbb{R}^3,$$

and corresponds to the k_i-th eigenvalue μ_{k_i}. This gives that u_{k_i} satisfies

$$-\Delta u_{k_i} + V(x)u_{k_i} - \frac{5a}{3}\rho_\gamma^{\frac{2}{3}} u_{k_i} = \mu_{k_i} u_{k_i}, \quad i = 1, 2, \tag{2.3}$$

where $\rho_\gamma(x) = \sum_{j=1}^{2} |u_{k_j}|^2$. In the following, we prove that (u_{k_1}, u_{k_2}) is a ground state of (1.8). Noting from [17, Theorem 11.8] that $\mu_1 < \mu_2$, it suffices to show that μ_{k_1} and μ_{k_2} are the 2-first eigenvalues of the operator H_V, i.e., $\mu_{k_i} = \mu_i$ holds for $i = 1, 2$.

We first prove that $\mu_{k_1} = \mu_1$. On the contrary, suppose $\mu_{k_1} \neq \mu_1$, which then yields that $\mu_1 < \mu_{k_1} \leq \mu_{k_2}$. Hence, there is an eigenfunction $u_1 \in \mathcal{H}$ of H_V in $\mathbb{R}^3$, which corresponds to the first eigenvalue μ_1 and satisfies $(u_1, u_{k_2}) = \delta_{1k_2}$. Define the operator

$$\gamma' := \gamma - |u_{k_1}\rangle\langle u_{k_1}| + |u_1\rangle\langle u_1| = |u_1\rangle\langle u_1| + |u_{k_2}\rangle\langle u_{k_2}|.$$

We then calculate from (2.3) that

$$\begin{aligned}
\mathrm{Tr}(-\Delta\gamma') =& \mathrm{Tr}(-\Delta\gamma) - \int_{\mathbb{R}^3} |\nabla u_{k_1}|^2 dx + \int_{\mathbb{R}^3} |\nabla u_1|^2 dx \\
=& \mathrm{Tr}(-\Delta\gamma) + \int_{\mathbb{R}^3} V(x)\big(|u_{k_1}|^2 - |u_1|^2\big)dx + \frac{5a}{3}\int_{\mathbb{R}^3} \rho_\gamma^{\frac{2}{3}}\big(|u_1|^2 - |u_{k_1}|^2\big)dx \\
&+ \mu_1 - \mu_{k_1},
\end{aligned}$$

and

$$\mathrm{Tr}(V(x)\gamma') = \mathrm{Tr}(V(x)\gamma) + \int_{\mathbb{R}^3} V(x)\big(|u_1|^2 - |u_{k_1}|^2\big)dx.$$

Moreover, by the convexity of $t \mapsto t^{\frac{5}{3}}$ we get that

$$\int_{\mathbb{R}^3} (\rho'_\gamma)^{\frac{5}{3}} dx = \int_{\mathbb{R}^3} \big(\rho_\gamma + |u_1|^2 - |u_{k_1}|^2\big)^{\frac{5}{3}} dx \geq \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx + \frac{5}{3}\int_{\mathbb{R}^3} \rho_\gamma^{\frac{2}{3}}\big(|u_1|^2 - |u_{k_1}|^2\big)dx.$$

Since $\mu_1 < \mu_{k_1}$, we now conclude from above that

$$E_a(2) \leq \mathcal{E}_a(\gamma') \leq \mathcal{E}_a(\gamma) + \mu_1 - \mu_{k_1} < \mathcal{E}_a(\gamma) = E_a(2),$$

a contradiction. We hence obtain that $\mu_{k_1} = \mu_1$.

We next prove that $\mu_{k_2} = \mu_2$. On the contrary, suppose $\mu_{k_2} \neq \mu_2$. We then deduce from above that $\mu_{k_1} = \mu_1 < \mu_2 < \mu_{k_2}$. Hence, there exists an eigenfunction $u_2 \in \mathcal{H}$ of H_V in $\mathbb{R}^3$, which corresponds to the second eigenvalue μ_2 and satisfies $(u_{k_1}, u_2) = \delta_{k_1 2}$. By considering the following operator

$$\gamma' := \gamma - |u_{k_2}\rangle\langle u_{k_2}| + |u_2\rangle\langle u_2| = |u_{k_1}\rangle\langle u_{k_1}| + |u_2\rangle\langle u_2|,$$

the similar argument as above then yields again a contradiction. This proves that $\mu_{k_2} = \mu_2$. We therefore conclude that $\mu_{k_i} = \mu_i$ holds for $i = 1, 2$, which implies that (u_{k_1}, u_{k_2}) is a ground state of (1.8).

2. We next prove the non-existence of minimizers for $E_a(2)$ in the case $a \geq a_2^*$. Let $\gamma^{(2)} = \sum_{i=1}^{2} |Q_i\rangle\langle Q_i|$ be a minimizer of a_2^*, where $Q_i \in H^1(\mathbb{R}^3)$ satisfies $(Q_i, Q_j) = \delta_{ij}$ for $i, j = 1, 2$. Take a non-negative function $\varphi(x) \in C_0^\infty(\mathbb{R}^3, [0,1])$, such that $\varphi(x) \equiv 1$ for $|x| \leq 1$ and $\varphi(x) \equiv 0$ for $|x| \geq 2$. For any $x_0 \in \mathbb{R}^3$ and $\tau > 0$, define

$$Q_i^\tau(x) := A_i^\tau \tau^{\frac{3}{2}} \varphi(x - x_0) Q_i\big(\tau(x - x_0)\big), \quad i = 1, 2, \quad \text{and} \quad \gamma_\tau^{(2)} := \sum_{i=1}^{2} |Q_i^\tau\rangle\langle Q_i^\tau|, \tag{2.4}$$

where $A_i^\tau > 0$ is chosen such that $\int_{\mathbb{R}^3} |Q_i^\tau|^2 dx = 1$ for $i = 1, 2$. By the exponential decay of $|Q_i|$ in Lemma A.1, we then derive that

$$\frac{1}{(A_i^\tau)^2} = \tau^3 \int_{\mathbb{R}^3} \varphi^2(x - x_0) Q_i^2\big(\tau(x - x_0)\big) dx = 1 + O(\tau^{-\infty}) \ \text{ as } \ \tau \to \infty, \quad i = 1, 2.$$

Here and below we denote $f(t) = O(t^{-\infty})$, if the function $f(t)$ satisfies $\lim_{t\to\infty} |f(t)| t^s = 0$ for all $s > 0$. We therefore obtain that

$$A_i^\tau = 1 + O(\tau^{-\infty}), \quad i = 1, 2, \quad \text{and} \quad a_\tau := (Q_1^\tau, Q_2^\tau) = O(\tau^{-\infty}) \ \text{ as } \ \tau \to \infty, \tag{2.5}$$

where we have also used the fact $(Q_i, Q_j) = \delta_{ij}$ for $i, j = 1, 2$. It follows from (2.5) that the Gram matrix

$$G_\tau := \begin{pmatrix} Q_1^\tau \\ Q_2^\tau \end{pmatrix} \begin{pmatrix} Q_1^\tau & Q_2^\tau \end{pmatrix} = \begin{pmatrix} 1 & (Q_1^\tau, Q_2^\tau) \\ (Q_2^\tau, Q_1^\tau) & 1 \end{pmatrix} = \begin{pmatrix} 1 & a_\tau \\ a_\tau & 1 \end{pmatrix} \tag{2.6}$$

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

For $\tau > 0$ large enough, defining

$$\begin{pmatrix} \widetilde{Q}_1^\tau & \widetilde{Q}_2^\tau \end{pmatrix} := \begin{pmatrix} Q_1^\tau & Q_2^\tau \end{pmatrix} G_\tau^{-\frac{1}{2}}, \tag{2.7}$$

it then follows from (2.6) that

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

Moreover, using Taylor's expansion, one can obtain from (2.6) that

$$G_\tau^{-\frac{1}{2}} = I_2 - \frac{1}{2} a_\tau \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + O(a_\tau^2) \ \text{ as } \ \tau \to \infty,$$

where I_2 denotes the 2-order identity matrix. We hence deduce from (2.7) that

$$\begin{pmatrix} \widetilde{Q}_1^\tau & \widetilde{Q}_2^\tau \end{pmatrix} = \begin{pmatrix} Q_1^\tau & Q_2^\tau \end{pmatrix} - \frac{1}{2} a_\tau \begin{pmatrix} Q_2^\tau & Q_1^\tau \end{pmatrix} + O(a_\tau^2) \ \text{ as } \ \tau \to \infty. \tag{2.8}$$

Following Lemma A.1, one can derive from (2.4), (2.5) and (2.8) that for $\tau > 0$ large enough,

$$\begin{aligned} \int_{\mathbb{R}^3} V(x) |\widetilde{Q}_i^\tau|^2 dx &= \int_{\mathbb{R}^3} V(x) \Big[Q_i^\tau - \frac{1}{2} a_\tau Q_j^\tau + O(a_\tau^2) \Big]^2 dx \\ &= \int_{\mathbb{R}^3} V\Big(\frac{x}{\tau} + x_0\Big) \varphi^2\Big(\frac{x}{\tau}\Big) Q_i^2(x) dx + O(\tau^{-\infty}) \\ &\leq \int_{|x| \leq 2\tau} V\left(\frac{x}{\tau} + x_0\right) Q_i^2(x) dx + O(\tau^{-\infty}) \\ &\leq C \int_{\mathbb{R}^3} Q_i^2(x) dx + O(\tau^{-\infty}) < \infty, \quad i = 1, 2, \end{aligned}$$

and similarly,

$$\int_{\mathbb{R}^3} |\nabla \widetilde{Q}_i^\tau|^2 dx = \tau^2 \int_{\mathbb{R}^3} |\nabla Q_i|^2 dx + O(\tau^{-\infty}) < \infty, \quad i = 1, 2,$$

due to the fact that $Q_i \in H^1(\mathbb{R}^3)$ holds for $i = 1, 2$. This implies that for $\tau > 0$ large enough, $\widetilde{Q}_i^\tau \in \mathcal{H}$ holds for $i = 1, 2$.

For $\tau > 0$ large enough, denoting

$$\widetilde{\gamma}_\tau^{(2)} := \sum_{i=1}^{2} |\widetilde{Q}_i^\tau\rangle\langle\widetilde{Q}_i^\tau|, \tag{2.9}$$

where $\widetilde{Q}_1^\tau$ and $\widetilde{Q}_2^\tau$ are as in (2.7), we next estimate each term of $\mathcal{E}_a(\widetilde{\gamma}_\tau^{(2)})$. It follows from Lemma A.1, (2.4), (2.5) and (2.8) that

$$\begin{aligned}
&\mathrm{Tr}(-\Delta\widetilde{\gamma}_\tau^{(2)}) - a\int_{\mathbb{R}^3} \rho_{\widetilde{\gamma}_\tau^{(2)}}^{\frac{5}{3}} dx \\
=&\sum_{i=1}^{2} \int_{\mathbb{R}^3} |\nabla \widetilde{Q}_i^\tau|^2 dx - a\int_{\mathbb{R}^3} \Big(\sum_{j=1}^{2} |\widetilde{Q}_j^\tau|^2\Big)^{\frac{5}{3}} dx \\
=&\tau^2\Big[\mathrm{Tr}(-\Delta\gamma^{(2)}) - a\int_{\mathbb{R}^3} \rho_{\gamma^{(2)}}^{\frac{5}{3}} dx\Big] + O(\tau^{-\infty}) \\
=&(a_2^* - a)\tau^2 \int_{\mathbb{R}^3} \rho_{\gamma^{(2)}}^{\frac{5}{3}} dx + O(\tau^{-\infty}) \quad \text{as} \quad \tau \to \infty,
\end{aligned} \tag{2.10}$$

due to the fact that $\gamma^{(2)}$ is a minimizer of a_2^* with $\|\gamma^{(2)}\| = 1$. On the other hand, since the function $x \mapsto V(x)\varphi^2(x - x_0)$ is bounded and has compact support, we deduce from Lemma A.1, (2.4), (2.5) and (2.8) that

$$\begin{aligned}
\lim_{\tau\to\infty} \mathrm{Tr}\big(V(x)\widetilde{\gamma}_\tau^{(2)}\big) &= \lim_{\tau\to\infty} \sum_{i=1}^{2} \int_{\mathbb{R}^3} V(x)|\widetilde{Q}_i^\tau|^2 dx \\
&= \lim_{\tau\to\infty} \sum_{i=1}^{2} \int_{\mathbb{R}^3} V\left(\frac{x}{\tau} + x_0\right)\varphi^2\left(\frac{x}{\tau}\right) Q_i^2(x) dx \\
&= V(x_0)\int_{\mathbb{R}^3} \rho_{\gamma^{(2)}}(x) dx = 2V(x_0).
\end{aligned} \tag{2.11}$$

Combining (2.10) with (2.11) yields that for $a > a_2^*$,

$$\begin{aligned}
E_a(2) &\le \lim_{\tau\to\infty} \mathcal{E}_a(\widetilde{\gamma}_\tau^{(2)}) \\
&= \lim_{\tau\to\infty} \Big\{\mathrm{Tr}(-\Delta + V(x))\widetilde{\gamma}_\tau^{(2)} - a\int_{\mathbb{R}^3} \rho_{\widetilde{\gamma}_\tau^{(2)}}^{\frac{5}{3}} dx\Big\} = -\infty,
\end{aligned}$$

and hence there is no minimizer of $E_a(2)$ for $a > a_2^*$.

As for the case $a = a_2^*$, taking the infimum over $x_0 \in \mathbb{R}^3$, it then follows from (2.1), (2.10) and (2.11) that $E_{a_2^*}(2) = 0$. We next prove the non-existence of minimizers for $E_{a_2^*}(2)$. On the contrary, assume that $\gamma = \sum_{i=1}^{2} |u_i\rangle\langle u_i|$, where $u_i \in \mathcal{H}$ and $(u_i, u_j) = \delta_{ij}$ for $i, j = 1, 2$, is a minimizer of $E_{a_2^*}(2)$. We then obtain from (1.6) that for $V(x) \ge 0$,

$$\int_{\mathbb{R}^3} V(x)\rho_\gamma(x) dx = 0, \tag{2.12}$$

and

$$\mathrm{Tr}(-\Delta\gamma) = a_2^* \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x)dx. \tag{2.13}$$

Since $\lim_{|x|\to\infty} V(x) = \infty$, we derive from (2.12) that $\rho_\gamma(x)$ has compact support. Following (2.13), one can obtain that γ is a minimizer of a_2^*, which implies from [11, Theorem 6] that $u_1(x)$ and $u_2(x)$ are the 2-first eigenfunctions of the operator $-\Delta - \frac{5}{3}a_2^*\rho_\gamma^{2/3}(x)$ in $\mathbb{R}^3$. Hence $\rho_\gamma(x) = u_1^2(x) + u_2^2(x) > 0$ in $\mathbb{R}^3$, in view of the fact (cf. [17, Theorem 11.8]) that the first eigenfunction $u_1(x)$ satisfies $u_1^2(x) > 0$ in $\mathbb{R}^3$. This is however a contradiction, and therefore there is no minimizer for $E_{a_2^*}(2)$. This completes the proof of Theorem 1.1. $\square$

Note from the proof of Theorem 1.1 that $\lim_{a\nearrow a_2^*} E_a(2) = E_{a_2^*}(2) = \inf_{x\in\mathbb{R}^3} V(x) = 0$. Indeed, by taking $a \nearrow a_2^*$ and setting $\tau \to \infty$, we derive from (2.10) and (2.11) that $\limsup_{a\nearrow a_2^*} E_a(2) \le 2V(x_0)$. The above result can be then obtained by taking the infimum over $x_0 \in \mathbb{R}^3$.

3 Estimates of Minimizers as $a \nearrow a_2^*$

Assume $V(x)$ satisfies (1.9), it follows from Theorem 1.1 that $E_a(2)$ admits minimizers, if and only if $0 < a < a_2^*$. In this section, we shall establish some refined estimates of minimizers for $E_a(2)$ as $a \nearrow a_2^*$. We first address the following energy estimates of $E_a(2)$ as $a \nearrow a_2^*$.

Lemma 3.1. *Assume $V(x)$ satisfies* (1.9). *Then there exist two positive constants m and M, independent of $0 < a < a_2^*$, such that*

$$0 < m(a_2^* - a)^{\frac{p}{p+2}} \le E_a(2) \le M(a_2^* - a)^{\frac{p}{p+2}} \quad as \quad a \nearrow a_2^*, \tag{3.1}$$

where $p > 0$ is as in (1.10).

Proof. For any $0 < a < a_2^*$, $\beta > 0$, and $\gamma = \sum_{i=1}^2 |u_i\rangle\langle u_i|$, where $u_i \in \mathcal{H}$ and $(u_i, u_j) = \delta_{ij}$ for $i, j = 1, 2$, we obtain from Young's inequality and (1.6) that

$$\begin{aligned}
\mathcal{E}_a(\gamma) \ge& \int_{\mathbb{R}^3} V(x)\rho_\gamma(x)dx + (a_2^* - a)\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x)dx \\
=& 2\beta + \int_{\mathbb{R}^3} \left(V(x) - \beta\right)\rho_\gamma(x)dx + (a_2^* - a)\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x)dx \\
\ge& 2\beta - \int_{\mathbb{R}^3} \big[\beta - V(x)\big]_+\rho_\gamma(x)dx + (a_2^* - a)\int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}}(x)dx \\
\ge& 2\beta - \frac{2}{5}\left(\frac{3}{5}\right)^{\frac{3}{2}} \frac{1}{(a_2^* - a)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \big[\beta - V(x)\big]_+^{\frac{5}{2}} dx,
\end{aligned} \tag{3.2}$$

where $[\cdot]_+ = \max\{0, \cdot\}$ denotes the positive part.

For $\beta > 0$ small enough, since $V(x)$ satisfies (1.9), the set $\{x \in \mathbb{R}^3 : V(x) \le \beta\}$ is contained in the union of l disjoint balls, each of which has the center at the minimum point x_m $(m = 1, \cdots, l)$, together with the radius no more than $K\beta^{\frac{1}{p}}$ for some suitable constant $K > 0$. Moreover, $V(x) \geq (\frac{|x-x_m|}{K})^p$ holds in these disjoint balls. We therefore derive that

$$\begin{aligned}\int_{\mathbb{R}^3} \big[\beta - V(x)\big]_+^{\frac{5}{2}} dx &\leq l \int_{|x|\leq K\beta^{\frac{1}{p}}} \Big[\beta - \Big(\frac{|x|}{K}\Big)^p\Big]^{\frac{5}{2}} dx \\ &= lK^3\beta^{\frac{5p+6}{2p}} \int_{|x|\leq 1} (1-|x|^p)^{\frac{5}{2}} dx \leq \frac{4\pi l K^3}{3}\beta^{\frac{5p+6}{2p}}.\end{aligned} \tag{3.3}$$

Applying (3.2) and (3.3), there exists a constant $m > 0$ such that

$$\mathcal{E}_a(\gamma) \geq 2\beta - C_0 \frac{\beta^{\frac{5p+6}{2p}}}{(a_2^* - a)^{\frac{3}{2}}} \geq m(a_2^* - a)^{\frac{p}{p+2}} > 0,$$

where $C_0 := \frac{8\pi l K^3}{15}(\frac{3}{5})^{\frac{3}{2}} > 0$, and the second inequality is derived by taking $\beta = (a_2^* - a)^{\frac{p}{p+2}}\left[\frac{4p}{(5p+6)C_0}\right]^{\frac{2p}{3p+6}} > 0$. This gives the lower bound of (3.1) as $a \nearrow a_2^*$.

In order to derive the upper bound of (3.1), we take the test function $\widetilde{\gamma}_\tau^{(2)}$ of the form (2.9), where the point x_0 in (2.4) is chosen such that $x_0 \in \mathcal{Z}$ defined in (1.11). Choose sufficiently small $\mathcal{R} > 0$ so that

$$V(x) \leq C_1|x - x_0|^p \quad \text{for} \quad |x - x_0| \leq \mathcal{R}.$$

We therefore obtain from Lemma A.1, (2.4), (2.5) and (2.8) that

$$\begin{aligned}\mathrm{Tr}(V\widetilde{\gamma}_\tau^{(2)}) &= \sum_{i=1}^{2}\int_{\mathbb{R}^3} V(x)|\widetilde{Q}_i^\tau(x)|^2 dx \\ &= \sum_{i=1}^{2}\int_{\mathbb{R}^3} V\left(\frac{x}{\tau} + x_0\right)\varphi^2\left(\frac{x}{\tau}\right) Q_i^2(x)dx + O(\tau^{-\infty}) \\ &\leq C_1\tau^{-p}\int_{\mathbb{R}^3} |x|^p \rho_{\gamma^{(2)}}(x)dx + O(\tau^{-\infty}) \quad \text{as} \quad \tau \to \infty,\end{aligned}$$

which then yields from (2.10) that

$$\begin{aligned}E_a(2) \leq \mathcal{E}_a(\widetilde{\gamma}_\tau^{(2)}) \leq (a_2^* - a)\tau^2 &\int_{\mathbb{R}^3} \rho_{\gamma^{(2)}}^{\frac{5}{3}}(x)dx \\ &+ C_1\tau^{-p}\int_{\mathbb{R}^3} |x|^p\rho_{\gamma^{(2)}}(x)dx + O(\tau^{-\infty}) \quad \text{as} \quad \tau \to \infty.\end{aligned}$$

Setting $\tau = (a_2^* - a)^{-\frac{1}{p+2}} > 0$ into the above estimate thus gives the upper bound of (3.1) as $a \nearrow a_2^*$. This therefore completes the proof of Lemma 3.1. □

Applying the energy estimates of Lemma 3.1, we next address the following estimates of $\rho_{\gamma_a}(x)$ as $a \nearrow a_2^*$, where γ_a is a minimizer of $E_a(2)$.

Lemma 3.2. *Assume $V(x)$ satisfies (1.9), and suppose $\gamma_a = \sum_{i=1}^2 |u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$, where $u_i^a \in \mathcal{H}$ satisfies $(u_i^a, u_j^a) = \delta_{ij}$ for $i, j = 1, 2$. Then there exists a constant $L > 0$, independent of $0 < a < a_2^*$, such that*

$$0 < L(a_2^* - a)^{-\frac{2}{p+2}} \leq \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \leq \frac{1}{L}(a_2^* - a)^{-\frac{2}{p+2}} \quad \textit{as} \quad a \nearrow a_2^*, \tag{3.4}$$

where $p > 0$ is as in (1.10), and $\rho_{\gamma_a}(x) = \sum_{i=1}^2 |u_i^a(x)|^2$.

Proof. By Lemma 3.1, it follows from (1.6) and (1.9) that

$$M(a_2^* - a)^{\frac{p}{p+2}} \geq E_a(2) \geq (a_2^* - a) \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \quad \text{as} \quad a \nearrow a_2^*,$$

which yields the upper bound of (3.4).

We next prove the lower bound of (3.4). For any $0 < b < a < a_2^*$, we derive that

$$E_b(2) \leq \mathcal{E}_b(\gamma_a) = E_a(2) + (a-b) \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx.$$

Following Lemma 3.1, we have

$$\begin{aligned}\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \geq \frac{E_b(2) - E_a(2)}{a-b} &\geq \frac{m(a_2^* - b)^{\frac{p}{p+2}} - M(a_2^* - a)^{\frac{p}{p+2}}}{a-b} \\ &= (a_2^* - a)^{-\frac{2}{p+2}} \frac{m(1+\delta)^{\frac{p}{p+2}} - M}{\delta} \quad \text{as} \quad a \nearrow a_2^*,\end{aligned}$$

by taking $b = a - \delta(a_2^* - a) \in (0, a)$. When $a > 0$ is sufficiently close to a_2^*, one can choose sufficiently large $\delta > 0$, so that the last fraction of the above estimate is positive. This gives the lower bound of (3.4), and the proof of Lemma 3.2 is therefore complete. □

Under the assumption (1.9), we now define

$$\varepsilon_a := (a_2^* - a)^{\frac{1}{p+2}} > 0, \quad 0 < a < a_2^*, \tag{3.5}$$

where $p > 0$ is as in (1.10). The following lemma is then concerned with the analysis properties of minimizers for $E_a(2)$ in terms of $\varepsilon_a > 0$.

Lemma 3.3. *Assume $V(x)$ satisfies (1.9), and suppose $\gamma_a = \sum_{i=1}^2 |u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$, where $u_i^a \in \mathcal{H}$ satisfies (1.8) and $(u_i^a, u_j^a) = \delta_{ij}$ for $i, j = 1, 2$. Then we have*

1. *There exist a sequence $\{y_{\varepsilon_a}\} \subset \mathbb{R}^3$, positive constants R_0 and η such that the sequence*

$$\bar{w}_i^a(x) := \varepsilon_a^{\frac{3}{2}} u_i^a(\varepsilon_a x + \varepsilon_a y_{\varepsilon_a}), \quad i = 1, 2, \quad \bar{\gamma}_a := \sum_{i=1}^2 |\bar{w}_i^a\rangle\langle \bar{w}_i^a|, \tag{3.6}$$

satisfies

$$\liminf_{a \nearrow a_2^*} \int_{B_{R_0}(0)} \rho_{\bar{\gamma}_a}(x)dx \geq \eta > 0, \tag{3.7}$$

where $\rho_{\bar{\gamma}_a}(x) := \sum_{i=1}^2 |\bar{w}_i^a(x)|^2$, and $\varepsilon_a > 0$ is defined by (3.5).

2. *The point $\bar{x}_a := \varepsilon_a y_{\varepsilon_a}$ satisfies*

$$\lim_{a \nearrow a_2^*} \mathrm{dist}(\bar{x}_a, \Lambda) = 0, \tag{3.8}$$

where the set Λ is defined by (1.10). Moreover, 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 $x_k \in \Lambda$ such that

$$\bar{x}_{a_n} \xrightarrow{n} x_k \quad \text{and} \quad \bar{w}_i^{a_n}(x) := \varepsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}(\varepsilon_{a_n} x + \bar{x}_{a_n}) \xrightarrow{n} \bar{w}_i(x) \tag{3.9}$$

strongly in $H^1(\mathbb{R}^3)$, where $\bar{\gamma} := \sum_{i=1}^2 |\bar{w}_i\rangle\langle \bar{w}_i|$ is a minimizer of a_2^* defined by (1.6).

Proof. 1. Assume $\gamma_a = \sum_{i=1}^2 |u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$, where $u_i^a \in \mathcal{H}$ satisfies $(u_i^a, u_j^a) = \delta_{ij}$ for $i, j = 1, 2$. Applying Lemma 3.1, it then follows from (1.6) and (1.9) that

$$0 \le \mathrm{Tr}(-\Delta\gamma_a) - a\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \le E_a(2) \to 0 \ \text{ as } \ a \nearrow a_2^*.$$

Note from Lemma 3.2 that $\lim\limits_{a\nearrow a_2^*} \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \to \infty$, and hence

$$0 \le \frac{\mathrm{Tr}(-\Delta\gamma_a)}{\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx} - a \le \frac{E_a(2)}{\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx} \to 0 \ \text{ as } \ a \nearrow a_2^*,$$

which gives that

$$\frac{\mathrm{Tr}(-\Delta\gamma_a)}{\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx} \to a_2^* \ \text{ as } \ a \nearrow a_2^*.$$

Taking $m_1 = \max\{\frac{3a_2^*}{2}, \frac{2}{a_2^*}\}$, it yields that

$$0 < \frac{1}{m_1}\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \le \mathrm{Tr}\big(-\Delta\gamma_a\big) \le m_1\int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}}(x)dx \ \text{ as } \ a \nearrow a_2^*.$$

We then deduce from Lemma 3.2 that there exists $C_2 := \frac{m_1}{L} > 0$ such that

$$0 < \frac{1}{C_2}(a_2^* - a)^{-\frac{2}{p+2}} \le \mathrm{Tr}(-\Delta\gamma_a) \le C_2(a_2^* - a)^{-\frac{2}{p+2}} \ \text{ as } \ a \nearrow a_2^*. \tag{3.10}$$

Denote

$$\widetilde{w}_i^a(x) := \varepsilon_a^{\frac{3}{2}} u_i^a(\varepsilon_a x), \quad i = 1, 2, \quad \widetilde{\gamma}_a := \sum_{i=1}^2 |\widetilde{w}_i^a\rangle\langle\widetilde{w}_i^a|,$$

where $\varepsilon_a > 0$ is as in (3.5). It then follows from Lemma 3.2 and (3.10) that

$$0 < \frac{1}{C_2} \le \mathrm{Tr}(-\Delta\widetilde{\gamma}_a) \le C_2 \ \text{ and } \ 0 < L \le \int_{\mathbb{R}^3} \rho_{\widetilde{\gamma}_a}^{\frac{5}{3}}(x)dx \le \frac{1}{L} \ \text{ as } \ a \nearrow a_2^*. \tag{3.11}$$

On the other hand, the Hoffmann-Ostenhof inequality [16] gives that

$$\mathrm{Tr}(-\Delta\widetilde{\gamma}_a) \ge \int_{\mathbb{R}^3} |\nabla\sqrt{\rho_{\widetilde{\gamma}_a}}|^2 dx. \tag{3.12}$$

We therefore deduce from (3.11) and (3.12) that the sequence $\{\sqrt{\rho_{\widetilde{\gamma}_a}}\}$ is bounded uniformly in $H^1(\mathbb{R}^3)$ as $a \nearrow a_2^*$.

We next claim that there exist a sequence $\{y_{\varepsilon_a}\} \subset \mathbb{R}^3$, $R_0 > 0$ and $\eta > 0$ such that

$$\liminf_{a\nearrow a_2^*} \int_{B_{R_0}(y_{\varepsilon_a})} \rho_{\widetilde{\gamma}_a}(x)dx \ge \eta > 0. \tag{3.13}$$

Indeed, if (3.13) is not true, then for any $R > 0$, there exists a sequence $\{a_n\}$, where $a_n \nearrow a_2^*$ as $n \to \infty$, such that

$$\lim_{n\to\infty} \sup_{y\in\mathbb{R}^3} \int_{B_R(y)} \rho_{\widetilde{\gamma}_{a_n}}(x)dx = 0.$$

Since the sequence $\{\sqrt{\rho_{\bar{\gamma}_{a_n}}}\}$ is bounded uniformly in $H^1(\mathbb{R}^3)$ as $n \to \infty$, we derive from [29, Theorem 1.21] that $\rho_{\bar{\gamma}_{a_n}}(x) \to 0$ strongly in $L^q(\mathbb{R}^3)$ as $n \to \infty$ for $1 < q < 3$. This is however a contradiction in view of (3.11). We therefore obtain that the claim (3.13) holds true, which further yields that (3.7) holds true.

2. We first prove that (3.8) holds true. On the contrary, assume that (3.8) is not true. Then there exist a sequence $\{a_n\}$, where $a_n \nearrow a_2^*$ as $n \to \infty$, and a constant $\delta > 0$ such that

$$\mathrm{dist}(\bar{x}_{a_n}, \Lambda) \geq \delta > 0 \quad \text{as} \quad n \to \infty,$$

which yields that there exists a constant $C(\delta) > 0$ such that

$$V(\bar{x}_{a_n}) \geq C(\delta) > 0 \quad \text{as} \quad n \to \infty.$$

By Fatou's lemma, we therefore derive from (3.7) that

$$\begin{aligned} \liminf_{n\to\infty} \int_{\mathbb{R}^3} V(\varepsilon_{a_n} x + \bar{x}_{a_n}) \rho_{\bar{\gamma}_{a_n}}(x) dx &\geq \int_{B_{R_0}(0)} \liminf_{n\to\infty} V(\varepsilon_{a_n} x + \bar{x}_{a_n}) \rho_{\bar{\gamma}_{a_n}}(x) dx \\ &\geq \frac{C(\delta)}{2} \eta > 0. \end{aligned} \tag{3.14}$$

On the other hand, one can deduce from (1.6) and Lemma 3.1 that

$$0 \leq \int_{\mathbb{R}^3} V(\varepsilon_{a_n} x + \bar{x}_{a_n}) \rho_{\bar{\gamma}_{a_n}}(x) dx = \int_{\mathbb{R}^3} V(x) \rho_{\gamma_{a_n}}(x) dx \leq E_{a_n}(2) \to 0 \text{ as } n \to \infty, \tag{3.15}$$

which however contradicts with (3.14), and hence (3.8) holds true.

We now focus on the proof of (3.9). Towards this purpose, we first claim that

$$\mathrm{Tr}(-\Delta \bar{\gamma}_a) = a_2^* \int_{\mathbb{R}^3} \rho_{\bar{\gamma}_a}^{\frac{5}{3}}(x) dx + o(1) \quad \text{as} \quad a \nearrow a_2^*, \tag{3.16}$$

where $\bar{\gamma}_a$ is defined by (3.6). Indeed, note that $\gamma_a = \sum_{i=1}^2 |u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$, where (u_1^a, u_2^a) satisfies the following system

$$-\Delta u_i^a + V(x) u_i^a - \frac{5a}{3} \rho_{\gamma_a}^{\frac{2}{3}} u_i^a = \mu_i^a u_i^a \quad \text{in} \quad \mathbb{R}^3, \quad i = 1, 2. \tag{3.17}$$

Here $\rho_{\gamma_a}(x) = \sum_{i=1}^2 |u_i^a(x)|^2$, and $\mu_1^a < \mu_2^a$ are the 2-first eigenvalues of the operator $-\Delta + V(x) - \frac{5a}{3} \rho_{\gamma_a}^{\frac{2}{3}}$ in $\mathbb{R}^3$. We hence deduce from Lemma 3.1 and (3.17) that

$$\sum_{i=1}^2 \mu_i^a \varepsilon_a^2 = \varepsilon_a^2 E_a(2) - \frac{2a}{3} \varepsilon_a^2 \int_{\mathbb{R}^3} \rho_{\gamma_a}^{\frac{5}{3}} dx = -\frac{2a}{3} \int_{\mathbb{R}^3} \rho_{\bar{\gamma}_a}^{\frac{5}{3}}(x) dx + o(1) \quad \text{as} \quad a \nearrow a_2^*. \tag{3.18}$$

On the other hand, we obtain from (3.6) and (3.17) that

$$-\Delta \bar{w}_i^a + \varepsilon_a^2 V(\varepsilon_a x + \bar{x}_a) \bar{w}_i^a - \frac{5a}{3} \rho_{\bar{\gamma}_a}^{\frac{2}{3}} \bar{w}_i^a = \mu_i^a \varepsilon_a^2 \bar{w}_i^a \quad \text{in} \quad \mathbb{R}^3, \quad i = 1, 2, \tag{3.19}$$

which implies that

$$\mathrm{Tr}(-\Delta \bar{\gamma}_a) + \varepsilon_a^2 \int_{\mathbb{R}^3} V(\varepsilon_a x + \bar{x}_a) \rho_{\bar{\gamma}_a}(x) dx - \frac{5a}{3} \int_{\mathbb{R}^3} \rho_{\bar{\gamma}_a}^{\frac{5}{3}}(x) dx = \sum_{i=1}^2 \mu_i^a \varepsilon_a^2. \tag{3.20}$$

It follows from (3.15) that

$$\varepsilon_a^2 \int_{\mathbb{R}^3} V(\varepsilon_a x + \bar{x}_a)\rho_{\bar{\gamma}_a}(x)dx \to 0 \ \text{ as } \ a \nearrow a_2^*,$$

which and (3.20) give that

$$\mathrm{Tr}(-\Delta\bar{\gamma}_a) - \frac{5a}{3}\int_{\mathbb{R}^3} \rho_{\bar{\gamma}_a}^{\frac{5}{3}}(x)dx = \sum_{i=1}^{2} \mu_i^a \varepsilon_a^2 + o(1) \ \text{ as } \ a \nearrow a_2^*. \tag{3.21}$$

Combining (3.18) with (3.21) yields that

$$\mathrm{Tr}(-\Delta\bar{\gamma}_a) = a_2^* \int_{\mathbb{R}^3} \rho_{\bar{\gamma}_a}^{\frac{5}{3}}(x)dx + o(1) \ \text{ as } \ a \nearrow a_2^*,$$

and hence the claim (3.16) holds true.

Let $\{a_n\}$ be any sequence satisfying $a_n \nearrow a_2^*$ as $n \to \infty$. It follows from (3.8) that there exist a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ and a point $x_k \in \Lambda$ such that

$$\bar{x}_{a_n} \to x_k \ \text{ as } \ n \to \infty. \tag{3.22}$$

Similar to (3.11), we obtain that $\{\bar{w}_i^{a_n}\}$ is bounded uniformly in $H^1(\mathbb{R}^3)$ as $n \to \infty$ for $i = 1, 2$. Hence, up to a subsequence if necessary, there exists a function $\bar{w}_i \in H^1(\mathbb{R}^3)$ such that

$$\bar{w}_i^{a_n} \rightharpoonup \bar{w}_i \ \text{ weakly in } \ H^1(\mathbb{R}^3) \quad \text{ as } \ n \to \infty, \ \ i = 1, 2, \tag{3.23}$$

and

$$\bar{w}_i^{a_n} \to \bar{w}_i \ \text{ strongly in } \ L^q_{loc}(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \ \ 2 \le q < 6, \ \ i = 1, 2.$$

This gives that

$$\bar{w}_i^{a_n} \to \bar{w}_i \ \text{ a.e. in } \ \mathbb{R}^3 \ \text{ as } \ n \to \infty, \ \ i = 1, 2,$$

and

$$\rho_{\bar{\gamma}_n} \to \rho_{\bar{\gamma}} := \bar{w}_1^2 + \bar{w}_2^2 \ \text{ strongly in } \ L^r_{loc}(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \ \ 1 \le r < 3,$$

where we denote $\bar{\gamma}_n := \bar{\gamma}_{a_n}$ and $\bar{\gamma} := \sum_{i=1}^2 |\bar{w}_i\rangle\langle\bar{w}_i|$.

By an adaptation of the classical dichotomy result (cf. [19, Section 3.3]), one can deduce from (3.7) that up to a subsequence of $\{a_n\}$ if necessary, there exists a sequence $\{R_n\}$ with $R_n \to \infty$ as $n \to \infty$ such that

$$0 < \lim_{n\to\infty} \int_{|x|\le R_n} \rho_{\bar{\gamma}_n} dx = \int_{\mathbb{R}^3} \rho_{\bar{\gamma}} dx \ \text{ and } \ \lim_{n\to\infty} \int_{R_n \le |x| \le 2R_n} \rho_{\bar{\gamma}_n} dx = 0. \tag{3.24}$$

Let $\chi(x) \in C_0^\infty(\mathbb{R}^3, [0,1])$ be a cut-off function satisfying $\chi(x) \equiv 1$ for $|x| \le 1$ and $\chi(x) \equiv 0$ for $|x| \ge 2$. Taking $\chi_n(x) := \chi(\frac{x}{R_n})$ and $\eta_n(x) = \sqrt{1 - \chi_n^2(x)}$, we then obtain from (3.24) that

$$\chi_n^2 \rho_{\bar{\gamma}_n} \to \rho_{\bar{\gamma}} \ \text{ strongly in } \ L^r(\mathbb{R}^3) \ \text{ as } \ n \to \infty, \ \ 1 \le r < 3. \tag{3.25}$$

Following the IMS formula [8, Theorem 3.2] and Fatou's lemma [25, Theorem 2.7], we derive that

$$\begin{aligned}
\mathrm{Tr}(-\Delta\bar{\gamma}_n) &= \mathrm{Tr}(-\Delta\chi_n\bar{\gamma}_n\chi_n) + \mathrm{Tr}(-\Delta\eta_n\bar{\gamma}_n\eta_n) - \int_{\mathbb{R}^3} (|\nabla\chi_n|^2 + |\nabla\eta_n|^2)\rho_{\bar{\gamma}_n} dx \\
&\ge \mathrm{Tr}(-\Delta\chi_n\bar{\gamma}_n\chi_n) + \mathrm{Tr}(-\Delta\eta_n\bar{\gamma}_n\eta_n) - 2CR_n^{-2} \\
&= \mathrm{Tr}(-\Delta\chi_n\bar{\gamma}_n\chi_n) + \mathrm{Tr}(-\Delta\eta_n\bar{\gamma}_n\eta_n) + o(1) \\
&\ge \mathrm{Tr}(-\Delta\bar{\gamma}) + \mathrm{Tr}(-\Delta\eta_n\bar{\gamma}_n\eta_n) + o(1) \ \text{ as } \ n \to \infty.
\end{aligned} \tag{3.26}$$

Moreover, we deduce from (3.25) that

$$\begin{aligned}\int_{\mathbb{R}^3}\rho_{\bar\gamma_n}^{\frac53}dx&=\int_{\mathbb{R}^3}\chi_n^2\rho_{\bar\gamma_n}^{\frac53}dx+\int_{\mathbb{R}^3}(\eta_n^2\rho_{\bar\gamma_n})^{\frac53}dx+\int_{\mathbb{R}^3}(\eta_n^2-\eta_n^{\frac{10}{3}})\rho_{\bar\gamma_n}^{\frac53}dx\\&=\int_{\mathbb{R}^3}\rho_{\bar\gamma}^{\frac53}dx+\int_{\mathbb{R}^3}(\eta_n^2\rho_{\bar\gamma_n})^{\frac53}dx+o(1)\ \text{ as }\ n\to\infty.\end{aligned}\tag{3.27}$$

Since $\|\bar\gamma\|\le\liminf_{n\to\infty}\|\bar\gamma_n\|=1$ and $\|\eta_n\bar\gamma_n\eta_n\|\le\|\bar\gamma_n\|=1$, we obtain from (1.6), (3.16), (3.26) and (3.27) that

$$\begin{aligned}0=&\lim_{n\to\infty}\Big\{\mathrm{Tr}(-\Delta\bar\gamma_n)-a_2^*\int_{\mathbb{R}^3}\rho_{\bar\gamma_n}^{\frac53}dx\Big\}\\\ge&\mathrm{Tr}(-\Delta\bar\gamma)-a_2^*\int_{\mathbb{R}^3}\rho_{\bar\gamma}^{\frac53}dx+\lim_{n\to\infty}\Big\{\mathrm{Tr}(-\Delta\eta_n\bar\gamma_n\eta_n)-a_2^*\int_{\mathbb{R}^3}(\eta_n^2\rho_{\bar\gamma_n})^{\frac53}dx\Big\}\\\ge&\|\bar\gamma\|^{\frac23}\mathrm{Tr}(-\Delta\bar\gamma)-a_2^*\int_{\mathbb{R}^3}\rho_{\bar\gamma}^{\frac53}dx\\&+\lim_{n\to\infty}\Big\{\|\eta_n\bar\gamma_n\eta_n\|^{\frac23}\mathrm{Tr}(-\Delta\eta_n\bar\gamma_n\eta_n)-a_2^*\int_{\mathbb{R}^3}(\eta_n^2\rho_{\bar\gamma_n})^{\frac53}dx\Big\}\\\ge&\|\bar\gamma\|^{\frac23}\mathrm{Tr}(-\Delta\bar\gamma)-a_2^*\int_{\mathbb{R}^3}\rho_{\bar\gamma}^{\frac53}dx\ge0,\end{aligned}\tag{3.28}$$

which implies that $\bar\gamma$ is a minimizer of a_2^* and $\|\bar\gamma\|=1$. It also follows from [11, Theorem 6] that any minimizer $\gamma^{(2)}$ of a_2^* is of the form

$$\gamma^{(2)}=\|\gamma^{(2)}\|\sum_{i=1}^2|Q_i\rangle\langle Q_i|,\quad(Q_i,Q_j)=\delta_{ij},\quad i,j=1,2.$$

We therefore obtain that $\bar\gamma=\|\bar\gamma\|\sum\limits_{i=1}^2|Q_i\rangle\langle Q_i|=\sum\limits_{i=1}^2|Q_i\rangle\langle Q_i|$, and hence

$$2=\lim_{n\to\infty}\int_{\mathbb{R}^3}\rho_{\bar\gamma_n}dx=\int_{\mathbb{R}^3}\rho_{\bar\gamma}dx.\tag{3.29}$$

Moreover, one can also derive from (3.28) and (3.29) that

$$\lim_{n\to\infty}\mathrm{Tr}(-\Delta\bar\gamma_n)=\mathrm{Tr}(-\Delta\bar\gamma)\ \text{ and }\ \lim_{n\to\infty}\int_{\mathbb{R}^3}\rho_{\bar\gamma_n}^{\frac53}dx=\int_{\mathbb{R}^3}\rho_{\bar\gamma}^{\frac53}dx.\tag{3.30}$$

We then derive from (3.29) and (3.30) that up to a subsequence if necessary,

$$\bar w_i^{a_n}(x):=\varepsilon_{a_n}^{\frac32}u_i^{a_n}(\varepsilon_{a_n}x+\bar x_{a_n})\to\bar w_i(x)\ \text{ strongly in }\ H^1(\mathbb{R}^3)\ \text{ as }\ n\to\infty,\tag{3.31}$$

where $\bar\gamma=\sum_{i=1}^2|\bar w_i\rangle\langle\bar w_i|$ is a minimizer of a_2^*. We therefore conclude from (3.22) and (3.31) that (3.9) holds true. This completes the proof of Lemma 3.3. □

4 Mass Concentration of Minimizers as $a\nearrow a_2^*$

Applying the refined estimates of the previous section, in this section we shall complete the proof of Theorem 1.2 on the concentration behavior of minimizers $\gamma_a=\sum_{i=1}^2|u_i^a\rangle\langle u_i^a|$ for $E_a(2)$ as $a\nearrow a_2^*$, where $u_i^a\in\mathcal{H}$ satisfies (1.8) and $(u_i^a,u_j^a)=\delta_{ij}$ for $i,j=1,2$. We start with the exponential decay of $\bar w_i^a(x)$ defined in (3.6) for $i=1,2$.

Lemma 4.1. *Under the assumption (1.9), suppose $\{\bar{w}_i^{a_n}(x)\}$ is the convergent subsequence obtained in Lemma 3.3 (2), where $\gamma_{a_n}=\sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ is a minimizer of $E_{a_n}(2)$ satisfying $a_n \nearrow a_2^*$ as $n\to\infty$. Then there exists a constant $C>0$, independent of a_n, such that for $i=1,2$,*

$$|\bar{w}_i^{a_n}(x)| \leq Ce^{-\frac{\sqrt{|\lambda_i|}}{2}|x|} \ \ \text{and} \ \ \rho_{\bar{\gamma}_{a_n}}(x) \leq Ce^{-\sqrt{|\lambda_2|}|x|} \ \ \text{uniformly in} \ \ \mathbb{R}^3 \tag{4.1}$$

as $n\to\infty$, where $\lambda_i<0$ is the i-th eigenvalue of the operator $H_{\bar{\gamma}}:=-\Delta-\frac{5a_2^*}{3}\rho_{\bar{\gamma}}^{\frac{2}{3}}$ in $\mathbb{R}^3$, and $\bar{\gamma}=\sum_{i=1}^2|\bar{w}_i\rangle\langle\bar{w}_i|$ is as in Lemma 3.3 (2).

Proof. Since $\gamma_{a_n}=\sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ is a minimizer of $E_{a_n}(2)$, where $u_i^{a_n}\in\mathcal{H}$ satisfies (1.8) and $(u_i^{a_n},u_j^{a_n})=\delta_{ij}$ for $i,j=1,2$, we first claim that

$$\mu_1^{a_n}<\mu_2^{a_n}<0 \ \text{ as } \ n\to\infty, \tag{4.2}$$

where $\mu_1^{a_n}<\mu_2^{a_n}$ are the 2-first eigenvalues of the operator $-\Delta+V(x)-\frac{5a_n}{3}\rho_{\gamma_{a_n}}^{\frac{2}{3}}$ in $\mathbb{R}^3$, and $\rho_{\gamma_{a_n}}=\sum_{i=1}^2|u_i^{a_n}|^2$. To prove the above claim, we define

$$E_a(1)=\inf\Big\{\mathrm{Tr}\big(-\Delta+V(x)\big)\gamma-a\int_{\mathbb{R}^3}\rho_\gamma^{\frac{5}{3}}dx: \ \gamma=|u\rangle\langle u|, \ \|u\|_{L^2}^2=1, \ u\in\mathcal{H}\Big\}, \quad a>0.$$

Denote

$$a_1^*=\inf\Big\{\frac{\|\gamma\|^{\frac{2}{3}}\mathrm{Tr}(-\Delta\gamma)}{\int_{\mathbb{R}^3}\rho_\gamma^{\frac{5}{3}}dx}: \ 0\leq\gamma=\gamma^*, \ \mathrm{Rank}(\gamma)\leq 1\Big\},$$

where $\rho_\gamma=\beta_1|u|^2$, and $\gamma=\beta_1|u\rangle\langle u|$ holds for $\beta_1\geq 0$ and $u\in H^1(\mathbb{R}^3)$. It follows from [11, Theorem 6] that $0<a_2^*<a_1^*$. The similar argument of (2.1) yields that $E_{a_n}(1)\geq 0$ holds for $0<a_n<a_2^*<a_1^*$, and hence

$$\begin{aligned}
0\leq E_{a_n}(1)&\leq\int_{\mathbb{R}^3}\Big(|\nabla u_1^{a_n}|^2+V(x)|u_1^{a_n}|^2\Big)dx-a_n\int_{\mathbb{R}^3}|u_1^{a_n}|^{\frac{10}{3}}dx\\
&=\mathrm{Tr}(-\Delta\gamma_{a_n})+\int_{\mathbb{R}^3}V(x)\rho_{\gamma_{a_n}}dx-a_n\int_{\mathbb{R}^3}\rho_{\gamma_{a_n}}^{\frac{5}{3}}dx+a_n\int_{\mathbb{R}^3}\rho_{\gamma_{a_n}}^{\frac{5}{3}}dx\\
&\quad-\int_{\mathbb{R}^3}|\nabla u_2^{a_n}|^2dx-\int_{\mathbb{R}^3}V(x)|u_2^{a_n}|^2dx-a_n\int_{\mathbb{R}^3}\big(\rho_{\gamma_{a_n}}-|u_2^{a_n}|^2\big)^{\frac{5}{3}}dx\\
&=E_{a_n}(2)-\mu_2^{a_n}+a_n\int_{\mathbb{R}^3}\rho_{\gamma_{a_n}}^{\frac{5}{3}}dx\\
&\quad-\frac{5a_n}{3}\int_{\mathbb{R}^3}\rho_{\gamma_{a_n}}^{\frac{2}{3}}|u_2^{a_n}|^2dx-a_n\int_{\mathbb{R}^3}\big(\rho_{\gamma_{a_n}}-|u_2^{a_n}|^2\big)^{\frac{5}{3}}dx
\end{aligned}$$

in view of (3.17). Applying Lemmas 3.1 and 3.3, we then deduce that

$$\begin{aligned}
\mu_2^{a_n}\varepsilon_{a_n}^2&\leq\varepsilon_{a_n}^2E_{a_n}(2)+a_n\int_{\mathbb{R}^3}\rho_{\bar{\gamma}_{a_n}}^{\frac{5}{3}}dx\\
&\quad-\frac{5a_n}{3}\int_{\mathbb{R}^3}\rho_{\bar{\gamma}_{a_n}}^{\frac{2}{3}}|\bar{w}_2^{a_n}|^2dx-a_n\int_{\mathbb{R}^3}(\rho_{\bar{\gamma}_{a_n}}-|\bar{w}_2^{a_n}|^2)^{\frac{5}{3}}dx\\
&=a_2^*\int_{\mathbb{R}^3}\rho_{\bar{\gamma}}^{\frac{5}{3}}dx-\frac{5a_2^*}{3}\int_{\mathbb{R}^3}\rho_{\bar{\gamma}}^{\frac{2}{3}}|\bar{w}_2|^2dx-a_2^*\int_{\mathbb{R}^3}\big(\rho_{\bar{\gamma}}-|\bar{w}_2|^2\big)^{\frac{5}{3}}dx+o(1)\\
&<0 \ \text{ as } \ n\to\infty,
\end{aligned}$$

where the strict convexity of $t \mapsto t^{\frac{5}{3}}$ is used in the last inequality. We therefore obtain that the claim (4.2) holds true.

Following Lemma 3.2, we obtain from (3.18) that there exist constants $C_3 > 0$ and $C_4 > 0$ such that

$$-C_3 \le \sum_{i=1}^{2} \mu_i^{a_n} \varepsilon_{a_n}^2 \le -C_4 \quad \text{as} \quad n \to \infty. \tag{4.3}$$

Since $\mu_1^{a_n} < \mu_2^{a_n} < 0$ as $n \to \infty$, we derive from (4.3) that $\{\mu_i^{a_n} \varepsilon_{a_n}^2\}$ is bounded uniformly as $n \to \infty$ for $i = 1, 2$. We thus assume that up to a subsequence if necessary,

$$\lim_{n\to\infty} \mu_i^{a_n} \varepsilon_{a_n}^2 = \lambda_i \le 0, \quad i = 1, 2. \tag{4.4}$$

Taking the weak limit of (3.19), we then deduce from Lemma 3.3 (2) that

$$-\Delta \bar{w}_i - \frac{5a_2^*}{3} \rho_{\bar{\gamma}}^{\frac{2}{3}} \bar{w}_i = \lambda_i \bar{w}_i \quad \text{in} \quad \mathbb{R}^3, \quad i = 1, 2,$$

where $\bar{w}_i$ is as in (3.9) and $\rho_{\bar{\gamma}} = \sum_{j=1}^2 |\bar{w}_j|^2$. Since $\bar{\gamma} = \sum_{i=1}^2 |\bar{w}_i\rangle\langle\bar{w}_i|$ is a minimizer of a_2^*, where $\bar{w}_i \in H^1(\mathbb{R}^3)$ satisfies $(\bar{w}_i, \bar{w}_j) = \delta_{ij}$ for $i, j = 1, 2$, one can obtain from (1.7) (or [11, Theorem 6]) that λ_1 and λ_2 are the 2-first negative eigenvalues of the operator $H_{\bar{\gamma}} := -\Delta - \frac{5a_2^*}{3} \rho_{\bar{\gamma}}^{\frac{2}{3}}$ in $\mathbb{R}^3$, and hence $\lambda_1 < \lambda_2 < 0$.

To prove (4.1), we now establish the exponential decay of $|\bar{w}_i^{a_n}|$ as $n \to \infty$ for $i = 1, 2$. By Kato's inequality [23, Theorem X.27], we derive from (3.19) that

$$-\Delta |\bar{w}_i^{a_n}| + \Big(- \frac{5a_n}{3} \rho_{\bar{\gamma}_{a_n}}^{\frac{2}{3}} - \mu_i^{a_n} \varepsilon_{a_n}^2 \Big) |\bar{w}_i^{a_n}| \le 0 \quad \text{in} \quad \mathbb{R}^3, \quad i = 1, 2. \tag{4.5}$$

Because $\{\sqrt{\rho_{\bar{\gamma}_{a_n}}}\}$ is bounded uniformly in $H^1(\mathbb{R}^3)$ as $n \to \infty$, by Sobolev embedding theorem, it yields that $\{\rho_{\bar{\gamma}_{a_n}}\}$ is bounded uniformly in $L^q(\mathbb{R}^3)$ as $n \to \infty$, where $1 \le q \le 3$. We therefore obtain that $\big\{\rho_{\bar{\gamma}_{a_n}}^{\frac{2}{3}}\big\}$ is bounded uniformly in $L^r(\mathbb{R}^3)$ as $n \to \infty$, where $\frac{3}{2} \le r \le \frac{9}{2}$. Applying De Giorgi-Nash-Moser theory (cf. [15, Theorem 4.1]), we then deduce from (4.4) and (4.5) that for any $y \in \mathbb{R}^3$,

$$\sup_{B_1(y)} |\bar{w}_i^{a_n}| \le C \|\bar{w}_i^{a_n}\|_{L^2(B_2(y))} \quad \text{as} \quad n \to \infty, \quad i = 1, 2,$$

which thus yields that for $i = 1, 2$,

$$|\bar{w}_i^{a_n}| \le C \quad \text{and} \quad \lim_{|x|\to\infty} |\bar{w}_i^{a_n}| = 0 \quad \text{uniformly} \quad \text{as} \quad n \to \infty$$

in view of (3.9). This also gives that

$$\rho_{\bar{\gamma}_{a_n}} \le C \quad \text{and} \quad \lim_{|x|\to\infty} \rho_{\bar{\gamma}_{a_n}} = 0 \quad \text{uniformly} \quad \text{as} \quad n \to \infty. \tag{4.6}$$

Using the comparison principle, we then derive from (4.5) that

$$|\bar{w}_i^{a_n}| \le C e^{-\frac{\sqrt{|\lambda_i|}}{2}|x|} \quad \text{uniformly in} \quad \mathbb{R}^3 \quad \text{as} \quad n \to \infty, \quad i = 1, 2,$$

where $\lambda_1 < \lambda_2 < 0$ are the 2-first eigenvalues of the operator $H_{\bar{\gamma}} := -\Delta - \frac{5a_2^*}{3} \rho_{\bar{\gamma}}^{\frac{2}{3}}$ in $\mathbb{R}^3$.

To obtain the exponential decay of $\rho_{\bar{\gamma}_{a_n}}$ as $n \to \infty$, we note from (3.19) that for $i = 1, 2$,

$$-\frac{1}{2}\Delta|\bar{w}_i^{a_n}|^2 + |\nabla \bar{w}_i^{a_n}|^2 + \varepsilon_{a_n}^2 V(\varepsilon_{a_n}x + \bar{x}_{a_n})|\bar{w}_i^{a_n}|^2 - \frac{5a_n}{3}\rho_{\bar{\gamma}_{a_n}}^{\frac{2}{3}}|\bar{w}_i^{a_n}|^2 = \mu_i^{a_n}\varepsilon_{a_n}^2|\bar{w}_i^{a_n}|^2 \ \text{ in } \mathbb{R}^3,$$

which implies that

$$-\frac{1}{2}\Delta\rho_{\bar{\gamma}_{a_n}} + \Big(- \mu_2^{a_n}\varepsilon_{a_n}^2 - \frac{5a_n}{3}\rho_{\bar{\gamma}_{a_n}}^{\frac{2}{3}}\Big)\rho_{\bar{\gamma}_{a_n}} \leq 0 \ \text{ in } \ \mathbb{R}^3 \ \text{ as } \ n \to \infty. \tag{4.7}$$

Applying the comparison principle to (4.7), we thus obtain from (4.4) and (4.6) that

$$\rho_{\bar{\gamma}_{a_n}}(x) \leq Ce^{-\sqrt{|\lambda_2|}|x|} \ \text{ uniformly in } \ \mathbb{R}^3 \ \text{ as } \ n \to \infty,$$

where $\lambda_2 < 0$ is the second eigenvalue of the operator $H_{\bar{\gamma}}$ in $\mathbb{R}^3$. This completes the proof of Lemma 4.1. □

In order to prove Theorem 1.2, we next address the existence of global maximum points for $\rho_{\gamma_a}(x)$, where $\gamma_a = \sum_{i=1}^2 |u_i^a\rangle\langle u_i^a|$ is a minimizer of $E_a(2)$, and $u_i^a \in \mathcal{H}$ satisfies (1.8) and $(u_i^a, u_j^a) = \delta_{ij}$ for $i, j = 1, 2$. Note from (3.17) that u_i^a satisfies

$$-\frac{1}{2}\Delta|u_i^a|^2 + |\nabla u_i^a|^2 + V(x)|u_i^a|^2 - \frac{5a}{3}\rho_{\gamma_a}^{\frac{2}{3}}|u_i^a|^2 = \mu_i^a|u_i^a|^2 \ \text{ in } \ \mathbb{R}^3, \quad i = 1, 2.$$

We therefore obtain that

$$-\frac{1}{2}\Delta\rho_{\gamma_a} + \Big(- \frac{5a}{3}\rho_{\gamma_a}^{\frac{2}{3}} - \mu_2^a\Big)\rho_{\gamma_a} \leq 0 \ \text{ in } \ \mathbb{R}^3, \tag{4.8}$$

due to the fact that $\mu_1^a < \mu_2^a$. Since $u_i^a \in H^1(\mathbb{R}^3)$ for $i = 1, 2$, it yields from (3.12) that $\sqrt{\rho_{\gamma_a}} \in H^1(\mathbb{R}^3)$. By Sobolev's embedding theorem, it then gives that $\rho_{\gamma_a} \in L^q(\mathbb{R}^3)$ for $1 \leq q \leq 3$, and hence $\rho_{\gamma_a}^{\frac{2}{3}} \in L^r(\mathbb{R}^3)$ for $\frac{3}{2} \leq r \leq \frac{9}{2}$. Following De Giorgi-Nash-Moser theory (cf. [15, Theorem 4.1]), we then obtain from (4.8) that for any $y \in \mathbb{R}^3$,

$$\sup_{B_1(y)} \rho_{\gamma_a}(x) \leq C\|\rho_{\gamma_a}\|_{L^1(B_2(y))},$$

which yields that $\lim_{|x|\to\infty} \rho_{\gamma_a}(x) = 0$. Because $\int_{\mathbb{R}^3} \rho_{\gamma_a}(x)dx = 2$, this further gives that global maximum points of $\rho_{\gamma_a}(x)$ exist in a bounded ball $B_R(0)$, where $R > 0$ is large enough.

Applying the above existence of global maximum points for $\rho_{\gamma_a}(x)$, we next analyze the following convergence.

Lemma 4.2. *Under the assumption* (1.9)*, assume the constant $p > 0$ and the set Λ are defined by* (1.10)*. Suppose $\{\bar{w}_i^{a_n}(x)\}$ is the convergent subsequence obtained in Lemma 3.3 (2), where $\gamma_{a_n} = \sum_{i=1}^2 |u_i^{a_n}\rangle\langle u_i^{a_n}|$ is a minimizer of $E_{a_n}(2)$ satisfying $a_n \nearrow a_2^*$ as $n \to \infty$. Then up to a subsequence if necessary,*

$$w_i^{a_n}(x) := \varepsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}(\varepsilon_{a_n}x + x_{a_n}) \xrightarrow{n} w_i(x), \quad \varepsilon_{a_n} := (a_2^* - a_n)^{\frac{1}{p+2}} > 0 \tag{4.9}$$

strongly in $H^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ for $i = 1, 2$, where $\gamma := \sum_{i=1}^2 |w_i\rangle\langle w_i|$ is a minimizer of a_2^* defined by (1.6)*, and there exists a point $x_k \in \Lambda$ such that the global maximum point $x_{a_n} \in \mathbb{R}^3$ of $\rho_{\gamma_{a_n}}(x) = \sum_{i=1}^2 |u_i^{a_n}|^2$ satisfies*

$$x_{a_n} \longrightarrow x_k \ \ as \ \ n \to \infty. \tag{4.10}$$

Proof. Define for $i = 1, 2$,

$$w_i^{a_n}(x) := \varepsilon_{a_n}^{\frac{3}{2}} u_i^{a_n}(\varepsilon_{a_n} x + x_{a_n}) = \bar{w}_i^{a_n}\Big(x + \frac{x_{a_n} - \bar{x}_{a_n}}{\varepsilon_{a_n}}\Big), \quad \varepsilon_{a_n} := (a_2^* - a_n)^{\frac{1}{p+2}} > 0, \tag{4.11}$$

and

$$\hat{\gamma}_{a_n} := \sum_{i=1}^{2} |w_i^{a_n}\rangle\langle w_i^{a_n}|, \tag{4.12}$$

where $\bar{w}_i^{a_n}(x)$ and $\bar{x}_{a_n} \in \mathbb{R}^3$ are as in (3.9), and $x_{a_n} \in \mathbb{R}^3$ is a global maximum point of $\rho_{\gamma_{a_n}}(x) = \sum_{i=1}^{2} |u_i^{a_n}|^2$. It then follows from (3.17) and (4.11) that $w_i^{a_n}(x)$ satisfies the following system

$$-\Delta w_i^{a_n} + \varepsilon_{a_n}^2 V(\varepsilon_{a_n} x + x_{a_n}) w_i^{a_n} - \frac{5a_n}{3} \rho_{\hat{\gamma}_{a_n}}^{\frac{2}{3}} w_i^{a_n} = \mu_i^{a_n} \varepsilon_{a_n}^2 w_i^{a_n} \ \text{ in } \ \mathbb{R}^3, \quad i = 1, 2, \tag{4.13}$$

where $\rho_{\hat{\gamma}_{a_n}} = \sum_{j=1}^{2} |w_j^{a_n}|^2$, and $\mu_1^{a_n} < \mu_2^{a_n}$ are the 2-first eigenvalues of the operator $-\Delta + V(x) - \frac{5a_n}{3} \rho_{\gamma_{a_n}}^{\frac{2}{3}}$ in $\mathbb{R}^3$.

We first claim that there exists a constant $C > 0$, independent of $a_n > 0$, such that

$$\frac{|x_{a_n} - \bar{x}_{a_n}|}{\varepsilon_{a_n}} \leq C \ \text{ uniformly as } \ n \to \infty. \tag{4.14}$$

In fact, if (4.14) is false, then there exists a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ such that $\frac{|x_{a_n} - \bar{x}_{a_n}|}{\varepsilon_{a_n}} \to \infty$ as $n \to \infty$. It thus follows from (4.1) that

$$\rho_{\gamma_{a_n}}(x_{a_n}) = \varepsilon_{a_n}^{-3} \rho_{\bar{\gamma}_{a_n}}\Big(\frac{x_{a_n} - \bar{x}_{a_n}}{\varepsilon_{a_n}}\Big) \leq C \varepsilon_{a_n}^{-3} e^{-\frac{\sqrt{|\lambda_2|}|x_{a_n} - \bar{x}_{a_n}|}{\varepsilon_{a_n}}} = o(\varepsilon_{a_n}^{-3}) \ \text{ as } \ n \to \infty, \tag{4.15}$$

where $\bar{\gamma}_{a_n}$ is as in (3.6). On the other hand, it follows from (4.8) that $\rho_{\gamma_{a_n}}(x) = \sum_{i=1}^{2} |u_i^{a_n}|^2$ satisfies

$$-\frac{1}{2} \Delta \rho_{\gamma_{a_n}}(x) - \frac{5a_n}{3} \rho_{\gamma_{a_n}}^{\frac{5}{3}}(x) \leq \mu_2^{a_n} \rho_{\gamma_{a_n}}(x) \ \text{ in } \ \mathbb{R}^3.$$

Since $x_{a_n} \in \mathbb{R}^3$ is a maximum point of $\rho_{\gamma_{a_n}}(x)$, we have $-\frac{1}{2}\Delta \rho_{\gamma_{a_n}}(x_{a_n}) \geq 0$, and hence

$$\rho_{\gamma_{a_n}}(x_{a_n}) \geq \Big(\frac{-3\mu_2^{a_n}}{5a_n}\Big)^{\frac{3}{2}} \geq C \varepsilon_{a_n}^{-3} \ \text{ as } \ n \to \infty,$$

due to the fact that $\lim_{n\to\infty} \mu_2^{a_n} \varepsilon_{a_n}^2 = \lambda_2 < 0$. This however contradicts with (4.15). We therefore derive that the claim (4.14) holds true.

Applying (4.14), then there exists a constant $R_1 > 0$, independent of a_n, such that $\frac{|x_{a_n} - \bar{x}_{a_n}|}{\varepsilon_{a_n}} < \frac{R_1}{2}$ as $n \to \infty$. Moreover, it then yields from (3.9) that there exists a point $x_k \in \Lambda$ such that the maximum point x_{a_n} of $\rho_{\gamma_{a_n}}(x)$ satisfies

$$\lim_{n\to\infty} x_{a_n} = \lim_{n\to\infty} \bar{x}_{a_n} = x_k \in \Lambda, \tag{4.16}$$

which thus proves (4.10). Following (4.11), we have

$$\rho_{\hat{\gamma}_{a_n}}(x) = \rho_{\bar{\gamma}_{a_n}}\Big(x + \frac{x_{a_n} - \bar{x}_{a_n}}{\varepsilon_{a_n}}\Big),$$

where $\rho_{\hat{\gamma}_{a_n}}(x)=\sum_{i=1}^2|w_i^{a_n}|^2$ and $\rho_{\bar{\gamma}_{a_n}}(x)=\sum_{i=1}^2|\bar{w}_i^{a_n}|^2$. It then follows from (3.7) that

$$\begin{aligned}\lim_{n\to\infty}\int_{B_{R_0+R_1}(0)}\rho_{\hat{\gamma}_{a_n}}(x)dx&=\lim_{n\to\infty}\int_{B_{R_0+R_1}(\frac{x_{a_n}-\bar{x}_{a_n}}{\varepsilon_{a_n}})}\rho_{\bar{\gamma}_{a_n}}(x)dx\\&\geq\lim_{n\to\infty}\int_{B_{R_0}(0)}\rho_{\bar{\gamma}_{a_n}}(x)dx\geq\eta>0.\end{aligned}$$

The similar argument of proving (3.9) thus yields that there exist a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ and $w_i\in H^1(\mathbb{R}^3)$ such that for $i=1,2$,

$$w_i^{a_n}(x):=\varepsilon_{a_n}^{\frac{3}{2}}u_i^{a_n}(\varepsilon_{a_n}x+x_{a_n})\to w_i(x)\ \text{ strongly in }\ H^1(\mathbb{R}^3)\ \text{ as }\ n\to\infty,\tag{4.17}$$

where $\gamma:=\sum_{i=1}^2|w_i\rangle\langle w_i|$ is a minimizer of a_2^* defined by (1.6).

We next prove (4.9) on the L^∞-uniform convergence of $w_i^{a_n}(x)$ as $n\to\infty$. Similar to Lemmas A.1 and 4.1, one can derive that

$$|w_i(x)|,\ |w_i^{a_n}(x)|\leq Ce^{-\frac{\sqrt{|\mu_i|}}{2}|x|}\ \text{ uniformly in }\ \mathbb{R}^3\ \text{ as }\ n\to\infty,\quad i=1,2,\tag{4.18}$$

where $\mu_1<\mu_2<0$ are the 2-first eigenvalues of the operator $H_\gamma:=-\Delta-\frac{5a_2^*}{3}\rho_\gamma^{\frac{2}{3}}$ in $\mathbb{R}^3$. On the other hand, define

$$G_i^{a_n}(x):=-\varepsilon_{a_n}^2V(\varepsilon_{a_n}x+x_{a_n})w_i^{a_n}(x)+\frac{5a_n}{3}\rho_{\hat{\gamma}_{a_n}}^{\frac{2}{3}}w_i^{a_n}(x)+\mu_i^{a_n}\varepsilon_{a_n}^2w_i^{a_n}(x),\quad i=1,2,$$

so that the system (4.13) can be rewritten as

$$-\Delta w_i^{a_n}(x)=G_i^{a_n}(x)\ \text{ in }\ \mathbb{R}^3,\quad i=1,2.\tag{4.19}$$

Since it follows from (4.18) that $\{w_i^{a_n}\}$ and $\{\rho_{\hat{\gamma}_{a_n}}\}$ are bounded uniformly in $L^\infty(\mathbb{R}^3)$ as $n\to\infty$, we deduce from (1.9), (4.4) and (4.16) that $\{G_i^{a_n}\}$ is bounded uniformly in $L^p_{loc}(\mathbb{R}^3)$ for $p>2$ as $n\to\infty$. Applying the L^p theory to (4.19), it further yields that $\{w_i^{a_n}\}$ is bounded uniformly in $W^{2,p}_{loc}(\mathbb{R}^3)$ as $n\to\infty$. We therefore obtain from [12, Theorem 7.26] that there exist a subsequence, still denoted by $\{w_i^{a_n}\}$, of $\{w_i^{a_n}\}$ and $\hat{w}_i(x)$ such that

$$w_i^{a_n}(x)\to\hat{w}_i(x)\ \text{ uniformly in }\ L^\infty_{loc}(\mathbb{R}^3)\ \text{ as }\ n\to\infty,\quad i=1,2.$$

Note from (4.17) that $\hat{w}_i(x)=w_i(x)$, and hence

$$w_i^{a_n}(x):=\varepsilon_{a_n}^{\frac{3}{2}}u_i^{a_n}(\varepsilon_{a_n}x+x_{a_n})\to w_i(x)\ \text{ uniformly in }\ L^\infty_{loc}(\mathbb{R}^3)\ \text{ as }\ n\to\infty,\quad i=1,2.\tag{4.20}$$

We thus conclude from (4.16)–(4.18) and (4.20) that the L^∞-uniform convergence (4.9) holds true, which therefore completes the proof of Lemma 4.2. □

Applying Lemma 4.2, we are now ready to establish Theorem 1.2.

Proof of Theorem 1.2. In view of Lemma 4.2, to complete the proof of Theorem 1.2, it suffices to prove that the point x_k of (4.10) satisfies

$$x_k\in\mathcal{Z}\ \text{ and }\ \lim_{n\to\infty}\frac{x_{a_n}-x_k}{\varepsilon_{a_n}}=\bar{x},\quad\varepsilon_{a_n}=(a_2^*-a_n)^{\frac{1}{p+2}}>0,\tag{4.21}$$

where the set $\mathcal{Z}$ is defined by (1.11), $\bar{x}$ is some point in $\mathbb{R}^3$, and $x_{a_n} \in \mathbb{R}^3$ is a maximum point of $\rho_{\gamma_{a_n}}(x) = \sum_{i=1}^2 |u_i^{a_n}|^2$. By direct calculations, we deduce from (1.6) and (4.9) that

$$\begin{aligned} E_{a_n}(2) &= \mathrm{Tr}\big(-\Delta + V(x)\big)\gamma_{a_n} - a_n \int_{\mathbb{R}^3} \rho_{\gamma_{a_n}}^{\frac{5}{3}} dx \\ &= \varepsilon_{a_n}^{-2}\Big(\mathrm{Tr}(-\Delta\hat{\gamma}_{a_n}) - a_2^* \int_{\mathbb{R}^3} \rho_{\hat{\gamma}_{a_n}}^{\frac{5}{3}} dx\Big) \\ &\quad + \int_{\mathbb{R}^3} V(\varepsilon_{a_n}x + x_{a_n})\rho_{\hat{\gamma}_{a_n}} dx + \varepsilon_{a_n}^p \int_{\mathbb{R}^3} \rho_{\hat{\gamma}_{a_n}}^{\frac{5}{3}} dx \\ &\geq \int_{\mathbb{R}^3} V(\varepsilon_{a_n}x + x_{a_n})\rho_{\hat{\gamma}_{a_n}} dx + \varepsilon_{a_n}^p \int_{\mathbb{R}^3} \rho_{\hat{\gamma}_{a_n}}^{\frac{5}{3}} dx, \end{aligned} \tag{4.22}$$

where $\rho_{\hat{\gamma}_{a_n}} = \sum_{i=1}^2 |w_i^{a_n}|^2$, and $\hat{\gamma}_{a_n} = \sum_{i=1}^2 |w_i^{a_n}\rangle\langle w_i^{a_n}|$ is defined by (4.12).

We now claim that

$$\Big\{\frac{|x_{a_n} - x_k|}{\varepsilon_{a_n}}\Big\} \text{ is bounded uniformly as } n \to \infty. \tag{4.23}$$

On the contrary, assume that (4.23) is false. We then obtain that there exists a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ such that

$$\lim_{n\to\infty} \frac{|x_{a_n} - x_k|}{\varepsilon_{a_n}} = \infty.$$

It thus follows from Fatou's lemma that for any sufficiently large $M' > 0$,

$$\begin{aligned} &\liminf_{n\to\infty} \varepsilon_{a_n}^{-p_k} \int_{\mathbb{R}^3} V(\varepsilon_{a_n}x + x_{a_n})\rho_{\hat{\gamma}_{a_n}} dx \\ =&\liminf_{n\to\infty} \int_{\mathbb{R}^3} \frac{V(\varepsilon_{a_n}x + x_{a_n})}{|\varepsilon_{a_n}x + x_{a_n} - x_k|^{p_k}} \Big|x + \frac{x_{a_n} - x_k}{\varepsilon_{a_n}}\Big|^{p_k} \rho_{\hat{\gamma}_{a_n}} dx \\ \geq& \int_{\mathbb{R}^3} \liminf_{n\to\infty} \frac{V(\varepsilon_{a_n}x + x_{a_n})}{|\varepsilon_{a_n}x + x_{a_n} - x_k|^{p_k}} \Big|x + \frac{x_{a_n} - x_k}{\varepsilon_{a_n}}\Big|^{p_k} \rho_{\hat{\gamma}_{a_n}} dx \geq M', \end{aligned} \tag{4.24}$$

where $p_k > 0$ is as in (1.9). We further derive from (3.5), (4.22) and (4.24) that

$$E_{a_n}(2) \geq \frac{M'}{2}\varepsilon_{a_n}^{p_k} = \frac{M'}{2}(a_2^* - a_n)^{\frac{p_k}{p+2}} \quad \text{as} \quad n \to \infty \tag{4.25}$$

holds for above any constant $M' > 0$, which however contradicts with Lemma 3.1. We therefore conclude that the claim (4.23) holds true. The same argument of (4.24) and (4.25) also yields that $p_k = p$.

It follows from the claim (4.23) that there exist a subsequence, still denoted by $\{a_n\}$, of $\{a_n\}$ and a point $\bar{x} \in \mathbb{R}^3$ such that

$$\lim_{n\to\infty} \frac{x_{a_n} - x_k}{\varepsilon_{a_n}} = \bar{x}. \tag{4.26}$$

We then obtain from Lemma 4.2 and (1.12) that

$$\begin{aligned} &\liminf_{n\to\infty} \varepsilon_{a_n}^{-p} \int_{\mathbb{R}^3} V(\varepsilon_{a_n}x + x_{a_n})\rho_{\hat{\gamma}_{a_n}} dx \\ =&\liminf_{n\to\infty} \int_{\mathbb{R}^3} \frac{V(\varepsilon_{a_n}x + x_{a_n})}{|\varepsilon_{a_n}x + x_{a_n} - x_k|^p} \Big|x + \frac{x_{a_n} - x_k}{\varepsilon_{a_n}}\Big|^p \rho_{\hat{\gamma}_{a_n}} dx \\ \geq&\alpha_k \int_{\mathbb{R}^3} |x + \bar{x}|^p \rho_\gamma dx \geq \alpha \int_{\mathbb{R}^3} |x + \bar{x}|^p \rho_\gamma dx, \end{aligned} \tag{4.27}$$

where $\gamma = \sum_{i=1}^2 |w_i\rangle\langle w_i|$ is as in Lemma 4.2, and all above identities hold, if and only if $\alpha_k = \alpha$ is as in (1.12). We thus deduce from (4.22) and (4.27) that

$$\liminf_{n\to\infty} \frac{E_{a_n}(2)}{\varepsilon_{a_n}^p} \geq \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx + \alpha \int_{\mathbb{R}^3} |x+\bar{x}|^p \rho_\gamma dx. \tag{4.28}$$

On the other hand, defining

$$u_i(x) = \varepsilon_{a_n}^{-\frac{3}{2}} w_i\Big(\frac{x-x_m}{\varepsilon_{a_n}} - \bar{x}\Big), \quad i = 1, 2,$$

where $x_m \in \mathcal{Z}$ is as in (1.11), choose $\gamma_1 = \sum_{i=1}^2 |u_i\rangle\langle u_i|$ as a trail operator of $E_{a_n}(2)$, and assume $\gamma = \sum_{i=1}^2 |w_i\rangle\langle w_i|$ defined in Lemma 4.2 is a minimizer of a_2^* and $\|\gamma\| = 1$. We then deduce from (3.5) that

$$\begin{aligned}
E_{a_n}(2) &\leq \mathrm{Tr}\big(-\Delta + V(x)\big)\gamma_1 - a_n \int_{\mathbb{R}^3} \rho_{\gamma_1}^{\frac{5}{3}} dx \\
&= \varepsilon_{a_n}^{-2}\Big(\mathrm{Tr}(-\Delta\gamma) - a_n \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx\Big) + \int_{\mathbb{R}^3} V\big(\varepsilon_{a_n}(x+\bar{x}) + x_m\big)\rho_\gamma dx \\
&= \varepsilon_{a_n}^p \Big\{ \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx + \int_{\mathbb{R}^3} \frac{V\big(\varepsilon_{a_n}(x+\bar{x}) + x_m\big)}{|\varepsilon_{a_n}(x+\bar{x}) + x_m - x_m|^p} |x+\bar{x}|^p \rho_\gamma dx \Big\},
\end{aligned}$$

which yields that

$$\limsup_{n\to\infty} \frac{E_{a_n}(2)}{\varepsilon_{a_n}^p} \leq \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx + \alpha \int_{\mathbb{R}^3} |x+\bar{x}|^p \rho_\gamma dx. \tag{4.29}$$

We thus conclude from (4.28) and (4.29) that

$$\lim_{n\to\infty} \frac{E_{a_n}(2)}{\varepsilon_{a_n}^p} = \int_{\mathbb{R}^3} \rho_\gamma^{\frac{5}{3}} dx + \alpha \int_{\mathbb{R}^3} |x+\bar{x}|^p \rho_\gamma dx.$$

Together with (4.27), this further implies that $\alpha_k = \alpha$, and hence (4.21) holds true. This completes the proof of Theorem 1.2. □

A Appendix

For the reader's convenience, the purpose of this appendix is to establish the following exponential decay of minimizers for a_2^*.

Lemma A.1. *Assume*

$$\gamma^{(2)} = \|\gamma^{(2)}\| \sum_{i=1}^2 |Q_i\rangle\langle Q_i|, \quad Q_i \in H^1(\mathbb{R}^3), \quad (Q_i, Q_j) = \delta_{ij}, \quad i, j = 1, 2, \tag{A.1}$$

is a minimizer of a_2^* defined by (1.6)*. Then we have*

$$Q_i \in C^2(\mathbb{R}^3), \quad |Q_i| \leq Ce^{-\frac{\sqrt{|\hat{\mu}_i|}}{2}|x|} \quad \text{and} \quad |\nabla Q_i| \leq Ce^{-\frac{\sqrt{|\hat{\mu}_i|}}{4}|x|} \quad \text{in} \ \ \mathbb{R}^3, \quad i = 1, 2,$$

where $\hat{\mu}_1 < \hat{\mu}_2 < 0$ are the 2-first negative eigenvalues of the operator

$$\hat{H}_\gamma := -\Delta - \frac{5}{3} a_2^* \rho_\gamma^{\frac{2}{3}} \quad \text{in} \ \ \mathbb{R}^3, \quad \rho_\gamma = \sum_{j=1}^2 |Q_j|^2 \quad \text{and} \quad \gamma := \sum_{i=1}^2 |Q_i\rangle\langle Q_i|. \tag{A.2}$$

Proof. Since $\gamma^{(2)}$ is a minimizer of a_2^*, $Q_i(x)$ satisfies the following system

$$-\Delta Q_i(x) - \frac{5}{3}a_2^*\rho_\gamma^{\frac{2}{3}}Q_i(x) = \hat{\mu}_i Q_i(x) \ \text{ in } \ \mathbb{R}^3, \quad i = 1,2, \tag{A.3}$$

where $\hat{\mu}_1 < \hat{\mu}_2 < 0$ are the 2-first negative eigenvalues of the operator $\hat{H}_\gamma$ defined in (A.2). We first claim that

$$Q_i(x) \in C^2(\mathbb{R}^3) \ \text{ and } \ \lim_{|x|\to\infty} |Q_i(x)| = 0, \quad i = 1,2. \tag{A.4}$$

In fact, by Kato's inequality (cf. [23, Theorem X.27]), we derive from (A.3) that

$$-\Delta|Q_i| + \Big(-\frac{5}{3}a_2^*\rho_\gamma^{\frac{2}{3}} - \hat{\mu}_i\Big)|Q_i| \le 0 \ \text{ in } \ \mathbb{R}^3, \quad i = 1,2. \tag{A.5}$$

Since $Q_i(x) \in H^1(\mathbb{R}^3)$ for $i = 1,2$, we have $\rho_\gamma(x) \in L^q(\mathbb{R}^3)$ for $1 \le q \le 3$, and hence $\rho_\gamma^{\frac{2}{3}}(x) \in L^r(\mathbb{R}^3)$ for $\frac{3}{2} \le r \le \frac{9}{2}$. Applying De Giorgi-Nash-Moser theory (cf. [15, Theorem 4.1]), it then yields from (A.5) that for any $y \in \mathbb{R}^3$,

$$\sup_{B_1(y)} |Q_i| \le C\|Q_i\|_{L^2(B_2(y))}, \quad i = 1,2,$$

which implies that $Q_i(x) \in L^\infty(\mathbb{R}^3)$ and $\lim\limits_{|x|\to\infty} |Q_i| = 0$ for $i = 1,2$. This also gives that $\rho_\gamma(x) \in L^\infty(\mathbb{R}^3)$ and $\lim\limits_{|x|\to\infty} \rho_\gamma(x) = 0$.

We next prove the continuity of $Q_i(x)$ for $i = 1,2$. Denoting

$$G_i(x) := \Big(\frac{5}{3}a_2^*\rho_\gamma^{\frac{2}{3}} + \hat{\mu}_i\Big)Q_i(x),$$

we obtain from (A.3) that

$$-\Delta Q_i(x) = G_i(x) \ \text{ in } \ \mathbb{R}^3, \quad i = 1,2. \tag{A.6}$$

Since $Q_i(x) \in L^\infty(\mathbb{R}^3)$, we derive that $G_i(x) \in L^q_{loc}(\mathbb{R}^3)$ holds for $q > 2$. Applying the L^p theory (cf. [12, Theorem 9.11]), we then deduce from (A.6) that $Q_i(x) \in W^{2,q}_{loc}(\mathbb{R}^3)$ for $i = 1,2$. The standard Sobolev embedding theorem thus gives that $Q_i(x) \in C^\theta_{loc}(\mathbb{R}^3)$ holds for some $\theta \in (0,1)$. By the Schauder estimate (cf. [12, Theorem 6.2]), we further obtain that $Q_i \in C^{2,\theta}_{loc}(\mathbb{R}^3)$, and hence $Q_i(x) \in C^2(\mathbb{R}^3)$ for $i = 1,2$. This gives the proof of (A.4).

We finally prove the exponential decay of $|Q_i|$ for $i = 1,2$. Since $\lim_{|x|\to\infty} \rho_\gamma(x) = 0$, applying the comparison principle, it gives from (A.5) that there exists a constant $C > 0$ such that

$$|Q_i| \le Ce^{-\frac{\sqrt{|\hat{\mu}_i|}}{2}|x|} \ \text{ in } \ \mathbb{R}^3, \quad i = 1,2. \tag{A.7}$$

By gradient estimates of (3.15) in [12], we further derive from (A.3) and (A.7) that

$$|\nabla Q_i| \le Ce^{-\frac{\sqrt{|\hat{\mu}_i|}}{4}|x|} \ \text{ in } \ \mathbb{R}^3, \quad i = 1,2,$$

which therefore completes the proof of Lemma A.1. $\square$

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