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ABSTRACT

We consider minimization problems of the Thomas–Fermi–Dirac–von Weizsäcker (TFDW) type in which the Newtonian potential is perturbed by a background potential satisfying mild conditions, which ensures the existence of minimizers. We describe the structure of minimizing sequences for those variants and obtain a more precise characterization of patterns in minimizing sequences for the TFDW functionals regularized by long-range perturbations.

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I. INTRODUCTION

In this paper, we are concerned with energy functionals that include the Thomas–Fermi–Dirac–von Weizsäcker (TFDW) model, a physical model describing ground state electron configurations of many-body systems. More precisely, we consider the following variational problem:

$$I_V(M) := \inf\{\mathcal{E}_V(u) : u \in \mathcal{H}^1(\mathbb{R}^3), \|u\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = M\}, \quad (1.1)$$

where the energy \mathcal{E}_V is defined as

$$\begin{aligned} \mathcal{E}_V(u) := & \int_{\mathbb{R}^3} \left[|\nabla u(x)|^2 + c_1 |u(x)|^{\frac{10}{3}} - c_2 |u(x)|^{\frac{8}{3}} - V(x)u^2(x) \right] dx \\ & + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy, \end{aligned}$$

with $c_1, c_2 > 0$,

$$V \geq 0, \quad V \in \mathcal{L}^{\frac{3}{2}}(\mathbb{R}^3) + \mathcal{L}^{\infty}(\mathbb{R}^3), \text{ and } \lim_{|x| \rightarrow \infty} V(x) = 0. \quad (1.2)$$

The conditions above ensure that I_V is finite, \mathcal{E}_V is coercive in $\mathcal{H}^1(\mathbb{R}^3)$ on the constraint set, and

$$u \in \mathcal{H}^1(\mathbb{R}^3) \mapsto \int_{\mathbb{R}^3} V(x)u^2(x)dx$$

is weakly continuous.

The TFDW model corresponds to the choice

$$V_{TF}(x) = \sum_{k=1}^K \frac{\alpha_k}{|x - r_k|}, \quad (1.3)$$

with $K \in \mathbb{N}$, $\{\alpha_k\}_{k=1}^K \subset \mathbb{R}^+$ and $\{r_k\}_{k=1}^K \subset \mathbb{R}^3$ all fixed. In this case, $\mathcal{E}_V(M)$ is to be thought of as the energy of a system of M electrons interacting with K nuclei. Each nucleus has charge $\alpha_k > 0$, and it is fixed at a position r_k . The total nuclear charge is denoted as

$$\mathcal{L} = \sum_{k=1}^K \alpha_k > 0$$

and plays a key role in existence results (see the works of Frank, Nam, and Van Den Bosch¹ and Lieb² for a survey).

In this paper, we explore the structure of minimizing sequences for I_V , with V chosen to be a perturbation of the molecular potential V_{TF} . Despite the coercivity of the problem, the existence of a minimizer for I_V is a highly nontrivial problem due to the lack of compactness at infinity. For the unperturbed TFDW problem, $V = V_{TF}$, Lions³ proved that there exists a minimizer if $M \leq \mathcal{L}$ and Le Bris⁴ extended this result to $M \leq \mathcal{L} + \epsilon$ for some $\epsilon = \epsilon(\mathcal{L}) > 0$. With regard to non-existence, Nam and Van Den Bosch proved that there are no minimizers if both M is sufficiently large and \mathcal{L} is sufficiently small, and Frank, Nam, and Van Den Bosch⁵ proved the nonexistence of a minimizer for $M > \mathcal{L} + C$, for some universal $C > 0$, in the case there is only one nucleus [i.e., $K = 1$ in (1.3)].

There is a special class of potentials V for which the existence problem for I_V is completely understood. We say that V is a long-range potential if it satisfies (1.2) and

$$\liminf_{t \rightarrow \infty} t \left(\inf_{|x|=t} V(x) \right) = \infty. \quad (1.4)$$

For example, the homogeneous potentials $V^\nu(x) = |x|^{-\nu}$ are of long-range for $0 < \nu < 1$. For long-range potentials (1.4), Alama *et al.*⁶ showed that $I_V(M)$ is attained for every $M > 0$. Thus, we may perturb the TFDW potential via a long-range potential of the form V^ν and think of this as a regularized version of TFDW. We, thus, define a family of long-range potentials,

$$V_Z(x) = V_{TF}(x) + \frac{Z}{|x|^\nu}, \quad 0 < \nu < 1, \quad (1.5)$$

with parameter $Z > 0$. By taking a sequence $Z_n \rightarrow 0$, we recover the TFDW model, but via a special minimizing sequence u_n composed of minimizers of the long-range problem, $\mathcal{E}_{V_n}(u_n) = I_{V_n}$. A special role is played by the minimization problem I_0 , that is with potential $V \equiv 0$, which is the “energy at infinity” obtained by translating $u(\cdot + x_n)$ with $|x_n| \rightarrow \infty$. The existence properties for $I_0(M)$ are analogous to those of $I_{V_{TF}}$: the minimizer exists for sufficiently small $M > 0$ [see Ref. 5, Lemma 9 (iii)], and there is no minimizer for all large M (see Ref. 7).

It will be convenient to introduce the following set of values of the constrained mass M in $I_V(M)$,

$$\mathcal{M}_V := \left\{ M > 0 \mid I_V(M) \text{ has a minimizer } u \in \mathcal{H}^1(\mathbb{R}^3), \int_{\mathbb{R}^3} u^2 = M \right\}.$$

It is an open question to determine whether \mathcal{M}_V is an interval, for any choice of potential V .

In case $u \in \mathcal{H}^1(\mathbb{R}^3)$ attains the minimum in I_V [respectively, $u_0 \in \mathcal{H}^1(\mathbb{R}^3)$ attains the minimum in I_0], the minimizers will satisfy the partial differential equations (PDEs),

$$-\Delta u + \frac{5}{3} c_1 u |u|^{\frac{4}{3}} - \frac{4}{3} c_2 u |u|^{\frac{2}{3}} - Vu + (|u|^2 * |\cdot|^{-1})u = \mu u, \quad (1.6)$$

$$-\Delta u_0 + \frac{5}{3} c_1 u_0 |u_0|^{\frac{4}{3}} - \frac{4}{3} c_2 u_0 |u_0|^{\frac{2}{3}} + (|u_0|^2 * |\cdot|^{-1})u_0 = \mu u_0, \quad (1.7)$$

with Lagrange multiplier μ induced by the mass constraint.

As mentioned above, the existence question is complicated by noncompactness due to translations of mass to infinity. However, minimizing sequences may be characterized using a general concentration–compactness structure (see Refs. 8 and 3).

Concentration Theorem I.1. *Let $\{u_n\}_{n \in \mathbb{N}}$ be a minimizing sequence for $I_V(M)$, where V satisfies (1.2). Then, there exist a number $N \in \mathbb{N} \cup \{0\}$, masses $\{m^i\}_{i=0}^N \subset \mathbb{R}^+$, translations $\{x_n^0\}_{n \in \mathbb{N}}, \dots, \{x_n^N\}_{n \in \mathbb{N}} \subset \mathbb{R}^3$, and functions $\{u^i\}_{i=0}^N \subset \mathcal{H}^1(\mathbb{R}^3)$ such that, up to a subsequence,*

$$u_n(\cdot) - \sum_{i=0}^N u^i(\cdot - x_n^i) \rightarrow 0 \text{ in } \mathcal{H}^1(\mathbb{R}^3), \quad (1.8)$$

$$I_V(m^0) = \mathcal{E}_V(u^0), \quad I_0(m^i) = \mathcal{E}_0(u^i), i > 0, \quad (1.9)$$

where $\|u^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = m^i,$

$$\sum_{i=0}^N m^i = M, \quad I_V(m^0) + \sum_{i=0}^N I_0(m^i) = I_V(M), \quad (1.10)$$

$$|x_n^i - x_n^j| \rightarrow \infty, \quad i \neq j. \quad (1.11)$$

The functions u^i satisfy (1.6) for $i = 1, \dots, N$ and u^0 satisfies (1.7), each with the same Lagrange multiplier $\mu \leq 0$.

Moreover, if $V \not\equiv 0$, then we can take $x_n^0 = 0$.

If a minimizer exists, then no splitting is necessary, and there exist minimizing sequences with $N = 0$. This occurs for V_{TF} when the mass is not much larger than the total charge, $M \leq \mathcal{Z} + \epsilon$ (by Ref. 4), for instance, or for any $M > 0$ in the class of long-range potentials (1.4). However, for TFDW with large mass M we expect splitting, but the pieces resulting from noncompactness must each minimize I_V or I_0 for its given mass, that is,

$$m^0 \in \mathcal{M}_V, \quad m^i \in \mathcal{M}_0, i > 0.$$

The basic idea behind the result is very elegant and intuitive. Minimizing sequences u_n for $I_V(M)$ may lose compactness due to splitting into widely spaced components, each of which tends to a minimizer of I_V or (for those components which translate off to infinity) I_0 . Asymptotically, all of the mass M is accounted for by this splitting. Although the pieces eventually move infinitely far away, they retain some information on the original minimization problem in that they share the same Lagrange multiplier.

Concentration results of this type have appeared in many papers. For TFDW, a very similar result is outlined (although with possibly infinitely many components u^i) in Ref. 3 and a proof of the exact decomposition of energy (1.10) for the case $V \equiv 0$ is given in Ref. 5, Lemma 9. Since this concentration theorem is central to the statements and proof of our results, we provide a proof in Appendix A. The finiteness of the components is a result of the concavity of the energy \mathcal{E}_V for small masses, which we prove in Appendix B.

For perturbations of TFDW, we obtain more precise information on the splitting structure. In particular, when mass splits off to infinity, the piece which remains localized must have mass $m^0 \geq \mathcal{Z}$, the total nuclear charge.

Theorem I.2. Assume V satisfies (1.2) and

$$V(x) \geq V_{TF}(x) = \sum_{k=1}^K \frac{\alpha_k}{|x - r_k|}, \quad a.e. \text{ in } \mathbb{R}^3,$$

for some $K \in \mathbb{N}$, $\{\alpha_k\}_{k=1}^K \subset \mathbb{R}^+$ and $\{r_k\}_{k=1}^K \subset \mathbb{R}^3$.

Then, with the notation of Theorem I.1, for any minimizing sequence $\{u_n\}_{n \in \mathbb{N}}$ of $I_V(M)$, either $M \in \mathcal{M}_V$ or splitting occurs with $m^0 \geq \mathcal{Z} = \sum_{k=1}^K \alpha_k$.

Heuristically, this is a satisfying result: after splitting, the nuclei should still capture as many electrons as the total nuclear charge \mathcal{Z} . One might expect that it should be able to retain more electrons to form a negatively charged ion.

Finally, we consider in greater detail the loss of compactness which may occur for the long-range regularized families V_n satisfying (1.12) with $0 < v < 1$. First, minimizers of $I_{V_n}(M)$ form a minimizing sequence for $I_{TF}(M)$, so when M is large compared to \mathcal{Z} , compactness is lost and mass splits off to infinity as described in Theorem I.1.

Proposition I.3. Let $Z_n \rightarrow 0$ and

$$V_n(x) = V_{TF}(x) + \frac{Z_n}{|x|^v}, \quad (1.12)$$

with $0 < v < 1$, and $\mathcal{Z} = \sum_{k=0}^K \alpha_k$. Let u_n minimize $I_{V_n}(M)$, $n \in \mathbb{N}$. Then,

- (i) $\{u_n\}_{n \in \mathbb{N}}$ is a minimizing sequence for I_{V_n} .
- (ii) Either $M \in \mathcal{M}_{V_n}$ or splitting occurs with $m^0 \geq \mathcal{Z}$.

The nonlocal term in \mathcal{E}_{V_n} exerts a repulsive effect on the components u^i , while the vanishing long-range potential provides some degree of containment. The combination of attractive and repulsive terms generally leads to pattern formation, at a scale determined by the relative strengths of the competitors. This phenomenon has been identified in nonlocal isoperimetric problems (such as the Gamow liquid drop model, see Refs. 9 and 10).

However, for potentials V_n of the form (1.12), the interactions between the fleeing components u^i appear in the energy at order $Z_n^{\frac{1}{1-v}}$. Thus, we require some information about the spatial decay of the minimizers of \mathcal{E}_{V_n} away from the centers of the support in order to control the errors in an expansion of the energy in terms of $Z_n \rightarrow 0$. In the liquid drop problems, the splitting is into characteristic functions of disjoint bounded domains and this issue does not arise. In order to calculate interactions, we require exponential decay of the solutions, which is connected to the delicate question of the Lagrange multiplier μ . In particular, we obtain exponential decay when $\mu < 0$,

$$|u(x)| \leq Ce^{-\lambda|x|},$$

for any $0 < \lambda < \sqrt{-\mu}$. As the energy value $I_V(M)$ is strictly decreasing in M , we have $\mu \leq 0$ and in fact we would expect that $\mu < 0$ should hold, if not always, at least for all but a residual set of M . It is an open question whether $\mu < 0$ holds whenever $M \in \mathcal{M}$. The strict negativity is known for the cases $V \equiv 0$ with sufficiently small mass or with $V = V_{TF}$ with $M < \mathcal{Z} + \kappa$ with $\kappa = \kappa(V_{TF}) > 0$ (see Proposition II.2).

We may now state our result on the distribution of masses in the case of splitting. First, we define

$$\mathcal{M}_V^* = \{M \in \mathcal{M}_V : \text{every minimizer } u \text{ of } I_V(M) \text{ satisfies (1.6) with } \mu < 0\}. \quad (1.13)$$

Theorem I.4. Let u_n be minimizers of $I_{V_n}(M)$ with V_n satisfying (1.12) with $0 < v < 1$ and $Z_n \rightarrow 0$. Let N , $\{m^i\}_{i=0}^N$ and $\{x_n^0\}_{n \in \mathbb{N}}, \dots, \{x_n^N\}_{n \in \mathbb{N}}$ be as in Theorem I.1. Assume $N \geq 1$ and $m^0 \in \mathcal{M}_{V_{TF}}^*$. Then, up to a subsequence and relabeling, either

- (i) $m^0 > Z$ and

$$Z_n^{\frac{1}{1-v}} x_n^i \rightarrow y^i, \quad i = 1, \dots, N,$$

where (y^1, \dots, y^N) minimizes the interaction energy

$$F_{N, (m^0, m^1, \dots, m^N)}(w^1, \dots, w^N) := \sum_{1 \leq i < j} \frac{m^i m^j}{|w^i - w^j|} + (m^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m^i}{|w^i|} - \sum_{i=1}^N \frac{m^i}{|w^i|^v}$$

over

$$\Sigma_N := \{(w^1, \dots, w^N) \in (\mathbb{R}^3 \setminus \{0\})^N : w^i \neq w^j\}$$

or

- (ii) $m^0 = Z$, $Z_n^{\frac{1}{1-v}} x_n^1 \rightarrow 0$ and if $N \geq 2$ we have

$$Z_n^{\frac{1}{1-v}} x_n^i \rightarrow y^i, \quad i = 2, \dots, N,$$

where (y^2, \dots, y^N) minimizes the interaction energy

$$\bar{F}_{N, (m^1, m^2, \dots, m^N)}(w^2, \dots, w^N) := \sum_{2 \leq i < j} \frac{m^i m^j}{|w^i - w^j|} + m^1 \sum_{i=2}^N \frac{m^i}{|w^i|} - \sum_{i=2}^N \frac{m^i}{|w^i|^v}$$

over

$$\bar{\Sigma}_N := \{(w^2, \dots, w^N) \in (\mathbb{R}^3 \setminus \{0\})^{N-1} : w^i \neq w^j\}.$$

Remark I.5. 1. The degenerate case $m^0 = \mathcal{Z}$ is very delicate, as the term measuring the repulsion between the weakly convergent component supported near zero and the diverging pieces is nearly exactly canceled by the attractive effect of the nuclear potential V_{TF} . Thus, the error terms in the expansion of the energy may exceed the principal term creating a net repulsion (or attraction) to the nuclei which is difficult to estimate. For instance, if $N = 1$ and only one component splits to infinity, then all we can say when $m^0 = \mathcal{Z}$ is that it diverges at a rate much slower than $Z^{-\frac{1}{1-v}}$. In some sense, there is no natural scale for its interaction distance to the nuclei. For this reason, we believe that in fact $m^0 > \mathcal{Z}$ but have no proof of this conjecture.

2. If $m^0 = \mathcal{Z}$, then $m^0 \in \mathcal{M}_{V_{TF}}^*$ automatically [see Proposition II.2 (ii)].
3. The proof of the compactness of all minimizing sequences of $\inf F_{N, (m^0, m^1, \dots, m^N)}$ and $\inf \bar{F}_{N, (m^1, m^2, \dots, m^N)}$ follows with little modification from the proof of Ref. 9, Proposition 8.
4. By Theorem I.1, each of the components u^i shares the same Lagrange multiplier μ , and hence it suffices that any one of the components satisfies (1.6) with $\mu < 0$.
5. We do not know whether the condition $\mu < 0$ could be improved. We use $\mu < 0$ for uniform exponential decay of the functions u_n away from x_n^i , but some weaker uniform decay away from the mass centers may be sufficient. However, it is unclear how rapidly minimizers of (1.1) decay when $\mu = 0$.

Finally, we note that the specific choice of powers $p = \frac{10}{3}$ and $q = \frac{8}{3}$ in the nonlinear potential well $W(u) = c_1|u|^p - c_2|u|^q$ are physically appropriate for the TFDW model, but from the point of view of analysis, other choices are possible. Indeed, most of the results of this paper may be extended to the case $2 < q < 3$ and $q < p < 6$. However, for $q > 3$, the behavior of minimizers may be substantially different: in such case $I_V(M) = I_V^{p,q}(M)$ may vanish identically and minimizers may never exist for any $M > 0$ (see Lions³ for various examples). Thus, it is not sufficient to have potentials W with a “double well” structure to observe the properties of TFDW minimizers; the relationship between the powers appearing in the functional is of importance, as well.

II. BOUNDEDNESS AND DECAY OF MINIMIZERS

In this section, we prove various basic properties of $I_V(M)$ and its minimizers and we discuss the role of the Lagrange multiplier in the decay of solutions.

The following properties are well-known for variational problems of the form (1.1):

Proposition II.1. *Let V satisfy (1.2).*

- (i) *For any $M > 0$, $I_V(M) < 0$, and is strictly decreasing in M .*
- (ii) *The following “binding inequality” holds for any $0 < m < M$:*

$$I_V(M) \leq I_V(m) + I_0(M - m). \quad (2.1)$$

- (iii) *If $I_V(M)$ is attained at $u \in \mathcal{H}^1(\mathbb{R}^3)$, then u solves (1.6) with Lagrange multiplier $\mu \leq 0$ and we may take $u \geq 0$ in \mathbb{R}^3 . It is possible to choose $u > 0$ if $V = V_{TF}$ or $V = V_Z$ as defined in (1.5).*

Proof. Statements (i) and (ii) can be proven as Lemma 5 of Nam and Van Den Bosch.⁵ With regard to (iii), (1.6) corresponds to the Euler–Lagrange equation associated with $I_V(M)$, while $\mu \leq 0$ due to $I_V(M)$ being decreasing in M . We may take $u \geq 0$ in \mathbb{R}^3 as $I_V(M) = \mathcal{E}_V(u) = \mathcal{E}(|u|)$. Finally, for potentials of the form V_{TF} or as perturbed in (1.5), the positivity of minimizers follows from the Harnack inequality. \square

When the Lagrange multiplier $\mu < 0$, we obtain exponential decay [see (66) in Ref. 3]: for all $0 < \lambda < \sqrt{-\mu}$, there exists a constant C with

$$|u(x)| + |\nabla u(x)| \leq Ce^{-\lambda x}, \quad \text{a.e. in } \mathbb{R}^3. \quad (2.2)$$

A categorization of the potentials V and masses M for which $\mu < 0$ remains an important open question. The following proposition gives various criteria under which the Lagrange multiplier $\mu < 0$. We recall the definition of \mathcal{M}_V^* in (1.13).

Proposition II.2. (i) *For $V \equiv 0$, $\exists M_0 > 0$ so that if $M < M_0$, then $M \in \mathcal{M}_V^*$.*

(ii) *For $V \geq V_{TF}$ satisfying (1.2), $\exists \kappa = \kappa(\mathcal{L}) > 0$ so that if $M < \mathcal{L} + \kappa$, then $M \in \mathcal{M}_{V_{TF}}^*$.*

(iii) *For V with long-range decay (1.4), every $M \in \mathcal{M}_V^*$.*

(iv) *For V satisfying (1.2) such that*

$$E := \inf \left\{ \int_{\mathbb{R}^3} (|\nabla u|^2 - Vu^2) dx : u \in \mathcal{H}^1(\mathbb{R}^3), \|u\|_{\mathcal{L}^2(\mathbb{R}^3)} = 1 \right\} < 0, \quad (2.3)$$

- (v) *there exists $M_V > 0$ so that if $M < M_V$, then $M \in \mathcal{M}_V^*$.*
- (v) *For*

$$V(x) = \sum_{k=1}^K \frac{\alpha_k}{|x - r_k|^\tau}, \quad \text{a.e. in } \mathbb{R}^3,$$

with $\{\alpha_k\}_{k=1}^K \subset \mathbb{R}^+$, $\{r_k\}_{k=1}^K \subset \mathbb{R}^3$, and $0 < \tau < 2$, there exists $M_V > 0$ so that if $M < M_V$, then $M \in \mathcal{M}_V^$.*

Proof. To verify (i), suppose that u is a minimizer. Equation (1.7) corresponds to the Euler–Lagrange equation associated with $I_0(M)$. Regarding the strict negativity of μ , note that from (1.7),

$$\begin{aligned} \mu M &= \int_{\mathbb{R}^3} |\nabla u(x)|^2 dx + \frac{5}{3} c_1 \int_{\mathbb{R}^3} |u(x)|^{\frac{10}{3}} dx - \frac{4}{3} c_2 \int_{\mathbb{R}^3} |u(x)|^{\frac{8}{3}} dx \\ &\quad + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy. \end{aligned} \quad (2.4)$$

Moreover, since $I_0(M) = \mathcal{E}_0(u)$ and $\|\sigma^{\frac{3}{2}}u(\sigma\cdot)\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = M$ for all $\sigma > 0$,

$$\begin{aligned} 0 &= \frac{d}{d\sigma} [\mathcal{E}_0(\sigma^{\frac{3}{2}}u(\sigma\cdot))] \Big|_{\sigma=1} \\ &= 2 \int_{\mathbb{R}^3} |\nabla u(x)|^2 dx + 2c_1 \int_{\mathbb{R}^3} |u(x)|^{\frac{10}{3}} dx - c_2 \int_{\mathbb{R}^3} |u(x)|^{\frac{8}{3}} dx + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy \end{aligned}$$

or, equivalently,

$$\begin{aligned} \frac{5}{3} c_1 \int_{\mathbb{R}^3} |u(x)|^{\frac{10}{3}} dx &= -\frac{5}{3} \int_{\mathbb{R}^3} |\nabla u(x)|^2 dx + \frac{5}{6} c_2 \int_{\mathbb{R}^3} |u(x)|^{\frac{8}{3}} dx \\ &\quad - \frac{5}{12} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy. \end{aligned} \quad (2.5)$$

Then, inserting (2.5) into (2.4) gives

$$\mu M = -\frac{2}{3} \int_{\mathbb{R}^3} |\nabla u(x)|^2 dx - \frac{1}{2} c_2 \int_{\mathbb{R}^3} |u(x)|^{\frac{8}{3}} dx + \frac{7}{12} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy.$$

We conclude by noting that, by Hardy–Littlewood’s inequality and the interpolation inequality in Lebesgue spaces,

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy \leq CM^{\frac{2}{3}} \int_{\mathbb{R}^3} |u(x)|^{\frac{8}{3}} dx.$$

We observe that the Pohozaev identity associated with (1.7) does not bring new information about μ .

Statement (ii) is Theorem 1 by Le Bris,⁴ and (iii) is Theorem 2 of Alama–Bronsard–Choksi–Topaloglu.⁶

Statement (iv) follows by the same reasoning as in the proof of Lions (Ref. 3, Corollary II.2). Finally, (v) is a consequence of part (iv). Indeed, note that the \mathcal{L}^2 -norm in \mathbb{R}^3 is invariant under the transformation $u \mapsto u_\sigma := \sigma^{\frac{3}{2}}u(\sigma\cdot)$. Therefore, we can prove Eq. (2.3) holds by first fixing any $u \in \mathcal{H}^1(\mathbb{R}^3)$ with $\|u\|_{\mathcal{L}^2(\mathbb{R}^3)} = 1$, and then taking σ sufficiently small so that

$$\int_{\mathbb{R}^3} (|\nabla u_\sigma|^2 - Vu_\sigma^2) dx = \int_{\mathbb{R}^3} \left[\sigma^2 |\nabla u(x)|^2 - \sigma^\tau \sum_{k=1}^K \frac{\alpha_k}{|x-\sigma r_k|^\tau} u^2(x) \right] dx < 0.$$

□

We will require the following basic energy bound in many of our proofs. This result is proven in Lemma 6 of Alama–Bronsard–Choksi–Topaloglu,⁶ although there it is stated for minimizing sequences, it is clear from the proof that in fact it applies to any function with negative energy.

Lemma II.3. Assume V satisfies (1.2), and $u \in \mathcal{H}^1(\mathbb{R}^3)$ with $\|u\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = M$ and $\mathcal{E}_V(u) < 0$. Then, there exists a constant $C_0 = C_0(V) > 0$ such that

$$\|u\|_{\mathcal{H}^1(\mathbb{R}^3)}^2 + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x)u^2(y)}{|x-y|} dx dy + \int_{\mathbb{R}^3} V(x)u^2(x) dx \leq C_0 M. \quad (2.6)$$

Remark II.4. Note that boundedness of a sequence $\{u_n\}_{n \in \mathbb{N}}$ in $\mathcal{H}^1(\mathbb{R}^3)$ implies boundedness of the same sequence in $\mathcal{L}^r(\mathbb{R}^3)$ for $2 \leq r \leq 6$.

The following is stated as part of Proposition I.3, but its proof only depends on the bounds stated in Lemma II.3, and the result will be needed below.

Proposition II.5. Let u_n minimize $I_{V_n}(M)$, where V_n is as in (1.12). Then, $\{u_n\}_{n \in \mathbb{N}}$ is a minimizing sequence for $I_{V_{TF}}(M)$.

Proof. Let $\{u_n\}$ be minimizers for I_{V_n} , $n \in \mathbb{N}$. First, note that $V_1 \geq V_n(x) \geq V_{TF}(x)$ for all x , and hence

$$\mathcal{E}_{V_1}(u_n) \leq \mathcal{E}_{V_n}(u_n) = I_{V_n} \leq I_{TF} < 0$$

for all n . Applying Lemma II.3 with $V = V_1$, the sequence $\{u_n\}_{n \in \mathbb{N}}$ satisfies the bounds (2.6) uniformly in $n \in \mathbb{N}$. Next, we observe that $|x|^{-v} \in \mathscr{L}_{loc}^{\frac{3}{2}}(\mathbb{R}^3)$ for $0 < v < 1$, and thus

$$\begin{aligned} Z_n \int_{\mathbb{R}^3} \frac{u_n^2(x)}{|x|^v} dx &\leq Z_n \int_{B_1(0)} \frac{u_n^2(x)}{|x|^v} dx + Z_n \int_{\mathbb{R}^3 \setminus B_1(0)} u_n^2(x) dx \\ &\leq Z_n \|u_n\|_{\mathscr{L}^6(\mathbb{R}^3)}^2 \| |x|^{-v} \|_{\mathscr{L}^{\frac{3}{2}}(B_1(0))} + Z_n M \\ &\leq c Z_n \|\nabla u_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 + Z_n M \rightarrow 0. \end{aligned}$$

In particular, $\mathcal{E}_{V_n}(u_n) = \mathcal{E}_{V_{TF}}(u_n) + o(1)$, and therefore we may conclude

$$I_{V_{TF}} \leq \liminf_{n \rightarrow \infty} \mathcal{E}_{V_{TF}}(u_n) = \liminf_{n \rightarrow \infty} \mathcal{E}_{V_n}(u_n) = \liminf_{n \rightarrow \infty} I_{V_n} \leq \limsup_{n \rightarrow \infty} I_{V_n} \leq I_{V_{TF}}.$$

□

Lemma II.6. Under all hypotheses of Theorem I.4, we have that, up to a subsequence, for all $0 < t < \sqrt{-\mu}$, there exists a constant C independent of n with

$$0 < |u_n(x)| + |\nabla u_n(x)| \leq C e^{-t\sigma_n(x)}, \text{ a.e. in } \mathbb{R}^3, \quad (2.7)$$

where

$$\sigma_n(x) := \min_{0 \leq i \leq N} |x - x_n^i|,$$

and x_n^i are as in the Concentration Theorem I.1.

Proof. By Proposition II.1 (iii), we may take $u_n(x) > 0$ in \mathbb{R}^3 . Alama *et al.*⁶ proved that

$$-\Delta u_n = \left(\mu_n - \frac{5}{3} c_1 u_n^{\frac{4}{3}} + \frac{4}{3} c_2 u_n^{\frac{2}{3}} + V_n - u_n^2 \star |\cdot|^{-1} \right) u_n \quad (2.8)$$

for some $\mu_n < 0$. In addition to this, by the final step in the Proof of the Concentration Theorem I.1, the Lagrange multipliers $\mu_n \rightarrow \mu$ converge. Fix $t \in (0, \sqrt{-\mu})$, then for all n sufficiently large,

$$-\Delta u_n + t^2 u_n < \left[\frac{1}{2} (t^2 + \mu) + \frac{4}{3} c_2 u_n^{\frac{2}{3}} \right] u_n.$$

Moreover, by Lemma II.3 and Eq. (2.8), we have that $\{u_n\}_{n \in \mathbb{N}}$ is bounded in $\mathscr{H}^2(\mathbb{R}^3)$ and hence in $\mathscr{L}^\infty(\mathbb{R}^3)$. Therefore, we can make use of Theorem 8.17 by Gilbarg and Trudinger¹¹ to obtain

$$\|u_n\|_{\mathscr{L}^\infty(B_1(y))} \leq C \|u_n\|_{\mathscr{L}^2(B_2(y))} \leq C \|u_n\|_{\mathscr{L}^2(\mathbb{R}^3 \setminus \cup B_{R/2}(x_n^i))}, \quad y \in \mathbb{R}^3 \setminus \cup B_R(x_n^i), R \gg 1,$$

where C is a constant independent of n, R , and y . By covering $\mathbb{R}^3 \setminus \cup B_R(x_n^i)$ with balls of radius one centered at points in the same set, we obtain

$$\|u_n\|_{\mathscr{L}^\infty(\mathbb{R}^3 \setminus \cup B_R(x_n^i))} \leq C \|u_n\|_{\mathscr{L}^2(\mathbb{R}^3 \setminus \cup B_{R/2}(x_n^i))}.$$

On the other hand, by Proposition II.5, $\{u_n\}_{n \in \mathbb{N}}$ is a minimizing sequence for $I_{V_{TF}}(M)$, and hence the conclusions of Concentration Theorem I.1 hold. In particular, this implies that given $\epsilon > 0$, there exists $R_0 = R_0(\epsilon) \geq 1$ such that

$$\|u^i\|_{\mathscr{L}^2(\mathbb{R}^3 \setminus B_{R/2}(0))}^2 < \frac{\epsilon}{N+1}, \quad i = 0, \dots, N, R \geq R_0,$$

and (1.8), (1.11), Rellich–Kondrakov theorem, and the decay of all u^i (2.2) ensure that, up to a subsequence,

$$u_n(\cdot + x_n^i) \rightarrow u^i \text{ in } \mathcal{L}^2(B_{R/2}(0)), \quad i = 0, \dots, N, R \geq R_0.$$

As a result,

$$\begin{aligned} \lim_{n \rightarrow \infty} \|u_n\|_{\mathcal{L}^2(\mathbb{R}^3 \setminus B_{R/2}(x_n^i))}^2 &= M - \lim_{n \rightarrow \infty} \|u_n\|_{\mathcal{L}^2(\cup B_{R/2}(x_n^i))}^2 \\ &= M - \lim_{n \rightarrow \infty} \sum_{i=0}^N \|u_n(x + x_n^i)\|_{\mathcal{L}^2(B_{R/2}(0))}^2 \\ &= M - \sum_{i=0}^N \|u^i\|_{\mathcal{L}^2(B_{R/2}(0))}^2 \\ &= \sum_{i=0}^N \|u^i\|_{\mathcal{L}^2(\mathbb{R}^3 \setminus B_{R/2}(0))}^2 < \epsilon. \end{aligned}$$

Then, given any $\epsilon > 0$, by choosing $R_0 = R_0(\epsilon)$ larger if necessary, we have

$$\limsup_{n \rightarrow \infty} \|u_n\|_{\mathcal{L}^\infty(\mathbb{R}^3 \setminus \cup B_R(x_n^i))} \leq \epsilon, R \geq R_0,$$

and hence for large enough n and R ,

$$-\Delta u_n + t^2 u_n < 0, \text{ a.e. in } \mathbb{R}^3 \setminus \cup B_R(x_n^i).$$

Next, it is not hard to check that

$$-\Delta e^{-t\sigma_n} + t^2 e^{-t\sigma_n} > 0, \text{ a.e. in } \mathbb{R}^3 \setminus \cup B_R(x_n^i)$$

and that there exists $C > 0$ so that

$$u_n|_{\partial \cup B_R(x_n^i)} \leq C e^{-tR} = C e^{-t\sigma_n(x)}|_{\partial \cup B_R(x_n^i)}.$$

Thus,

$$-\Delta [u_n(x) - C e^{-t\sigma_n(x)}] + t^2 [u_n(x) - C e^{-t\sigma_n(x)}] < 0, \text{ a.e. in } \mathbb{R}^3 \setminus \cup B_R(x_n^i).$$

At this point, we would like to invoke the maximum principle to assert that $u_n(x)$ is dominated by the supersolution $v(x) = C e^{-t\sigma_n}$ in the domain $\Omega_n := \mathbb{R}^3 \setminus \cup B_R(x_n^i)$. As the domain is unbounded, this requires some care, but applying Stampacchia's method as that of Benguria, Brezis, and Lieb (Ref. 12, Lemma 8), we obtain the desired bound,

$$0 < u_n(x) \leq v(x) = C e^{-t\sigma_n(x)}, \quad x \in \Omega_n.$$

The estimate on $|\nabla u_n|$ then follows from standard elliptic estimates (see, for instance, Theorems 8.22 and 8.32 of Ref. 11). \square

At this point, we would like to note that the functions u^i decay to zero at infinity, even if $m^0 \notin \mathcal{M}_{V_{TF}}^*$. This follows from Proposition II.1 (iii) and Theorem 8.17 uniformly by Gilbarg and Trudinger,¹¹ again.

III. PROOF OF THEOREM I.2

The Proof of Theorems I.2 and I.4 rely both on the splitting structure given in the Concentration Theorem I.1 and on the idea that, when calculating the interaction energy between very widely separated components $u^i(x + x_n^i)$, only the mass m^i and centers x_n^i enter into the computation at the first order. The following simple lemma makes this precise, at least for compactly supported components:

Lemma III.1.

(a) Let $v^1, v^2 \in \mathcal{H}^1(\mathbb{R}^3)$ with compact support, $\text{supp } v^i \subset B_\rho(\zeta^i)$, $i = 1, 2$, with $1 < \rho < \frac{1}{4}R$, $R = |\zeta^1 - \zeta^2| > 0$. Then,

$$\left| \int_{B_\rho(\zeta^1)} \int_{B_\rho(\zeta^2)} \frac{|v^1(x)|^2 |v^2(y)|^2}{|x - y|} dx dy - \frac{\|v^1\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \|v^2\|_{\mathcal{L}^2(\mathbb{R}^3)}^2}{|\zeta^1 - \zeta^2|} \right| \leq \frac{4\rho}{R^2} \|v^1\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \|v^2\|_{\mathcal{L}^2(\mathbb{R}^3)}^2.$$

(b) Let $v \in \mathcal{H}^1(\mathbb{R}^3)$ with compact support, $\text{supp } v \subset B_\rho(\zeta)$, with $1 < \rho < \frac{1}{4}R = |\zeta|$. For any $v > 0$ and fixed vector $r \in \mathbb{R}^3$ with $0 < |r| < \frac{1}{4}R$,

$$\left| \int_{B_\rho(\zeta)} \frac{|v(x)|^2}{|x - r|^v} dx - \frac{\|v\|_{\mathcal{L}^2(\mathbb{R}^3)}^2}{|\zeta|^v} \right| \leq C_v \frac{\rho}{R^{v+1}} \|v\|_{\mathcal{L}^2(\mathbb{R}^3)}^2.$$

Proof. These follow from the pointwise estimates,

$$\begin{aligned} \left| \frac{1}{|\zeta^1 - \zeta^2|} - \frac{1}{|x - y|} \right| &\leq \frac{2\rho}{(R - \rho)^2} \leq \frac{4\rho}{R^2}, \\ \left| \frac{1}{|\zeta|^\theta} - \frac{1}{|x - r|^\theta} \right| &\leq \frac{\theta\rho}{(|\zeta| - \rho - |r|)^{\theta+1}} \leq C_\theta \frac{\rho}{R^{1+\theta}}, \end{aligned}$$

for all $x \in B_\rho(\zeta^1)$, $y \in B_\rho(\zeta^2)$, and $1 < \rho < \frac{1}{4}R$. \square

Unlike the case of the Gamow liquid drop problem, our components u^i are not of compact support, so we need to resort to truncation. This will prove effective provided we are in a situation where the minimizers u^i have exponential decay. To generate localization functions, fix any smooth $\phi : \mathbb{R} \rightarrow [0, 1]$ for which

$$\phi \mathbb{1}_{(-\infty, 0]} \equiv 1, \quad \phi \mathbb{1}_{[1, \infty)} \equiv 0, \quad \|\phi'\|_{L^\infty(\mathbb{R})} \leq 2. \quad (3.1)$$

We are now ready to prove Theorem I.2 and Proposition I.3 on the size of the compact part of minimizing sequences. The argument for the first theorem is similar to Lions' proof of existence of minimizers³ for TDFW with $M \leq \mathcal{Z}$.

Proof of Theorem I.2. We write the potential $V = V_{TF} + W$, where $W(x) \geq 0$ and W satisfies (1.2). To obtain a contradiction, assume $\{u_n\}_{n \in \mathbb{N}}$ is a minimizing sequence for $I_V(M)$ for which there is splitting (i.e., $N \geq 1$ in Theorem I.1), but $0 < m^0 < \mathcal{Z}$. We let u^i , $m^i = \|u^i\|_{L^2(\mathbb{R}^3)}^2$, $i = 0, \dots, N$ be as given by Theorem I.1. Fix N distinct unit vectors $e^i \in \mathbb{R}^3$, and for $\rho > 1$, define q^i by

$$q^0 = 0, \quad q^1 = \rho^2 e^1, \quad q^i = \rho^3 e^i, \quad i = 2, \dots, N.$$

Then, we define the truncated components,

$$U_\rho^i(x) := \phi(|x - q^i| - \rho + 1) u^i(x - q^i), \quad i = 0, \dots, N.$$

That is, each U^i has been truncated to have support in the ball $B_\rho(q^i)$.

As $m^0 < \mathcal{Z}$, by Proposition II.2 (ii), $\mu < 0$ for all Lagrange multipliers corresponding to u^i , $i = 0, \dots, N$, and hence the exponential decay estimate (2.2) holds for all of them. Let $\lambda = \frac{1}{2}\sqrt{-\mu}$ for simplicity. Then,

$$m_\rho^i := \|U_\rho^i\|_{L^2(\mathbb{R}^3)}^2 \leq \int_{B_\rho(q^i)} |U_\rho^i(x)|^2 dx = m^i - O(e^{-\lambda\rho})$$

and

$$\mathcal{E}_V(U_\rho^0) = \mathcal{E}_V(u^0) + O(e^{-\lambda\rho}), \quad \mathcal{E}_0(U_\rho^i) = \mathcal{E}_0(u^i) + O(e^{-\lambda\rho}), \quad i = 1, \dots, N.$$

Let $w_\rho := U_\rho^0 + \sum_{i=1}^N U_\rho^i$. As $\|w_\rho\|_{L^2(\mathbb{R}^3)}^2 < M$; by monotonicity of $I_V(M)$, we have

$$\begin{aligned} I_V(M) &\leq I_V(\|w_\rho\|_{L^2(\mathbb{R}^3)}^2) \leq \mathcal{E}_V(w_\rho) \\ &\leq \mathcal{E}_V(U_\rho^0) + \sum_{i=1}^N \mathcal{E}_0(U_\rho^i) + \sum_{\substack{i,j=0 \\ i \neq j}}^N \int_{B_\rho(q^i)} \int_{B_\rho(q^j)} \frac{|U_\rho^i(x)|^2 |U_\rho^j(y)|^2}{|x - y|} dx dy \\ &\quad - \sum_{i=1}^N \int_{B_\rho(q^i)} [V_{TF}(x) + W(x)] |U_\rho^i(x)|^2 dx + O(e^{-\lambda\rho}) \\ &= I_V(m^0) + \sum_{i=1}^N I_0(m^i) + \sum_{\substack{i,j=0 \\ i \neq j}}^N \int_{B_\rho(q^i)} \int_{B_\rho(q^j)} \frac{|U_\rho^i(x)|^2 |U_\rho^j(y)|^2}{|x - y|} dx dy \\ &\quad - \sum_{i=1}^N \int_{B_\rho(q^i)} [V_{TF}(x) + W(x)] |U_\rho^i(x)|^2 dx + O(e^{-\lambda\rho}). \end{aligned} \quad (3.2)$$

Next, we use Lemma III.1 to evaluate the interaction terms. Note that $R^{ij} = |q^i - q^j|$ is of order ρ^2 when $i = 0, j = 1$, and of order ρ^3 otherwise, and $0 < m^i - m_\rho^i < O(e^{-\lambda\rho})$. Thus, we have

$$\int_{B_\rho(q^i)} \int_{B_\rho(q^j)} \frac{|U_\rho^i(x)|^2 |U_\rho^j(y)|^2}{|x - y|} dx dy = \begin{cases} \frac{m^0 m^1}{\rho^2} + O(\rho^{-3}), & \text{if } i + j = 1 \\ O(\rho^{-3}), & \text{otherwise,} \end{cases}$$

and for $i = 1, \dots, N, k = 1, \dots, K$, we evaluate the interaction with V_{TF} by

$$\int_{B_\rho(q^i)} \frac{|U_\rho^i(x)|^2}{|x - r^k|} dx = \begin{cases} \frac{m^1}{\rho^2} + O(\rho^{-3}), & \text{if } i = 1 \\ O(\rho^{-3}), & \text{if } i \geq 2. \end{cases}$$

Substituting into (3.2), and using $W \geq 0$, we obtain the strict subadditivity of $I_V(M)$,

$$I_V(M) - \left[I_V(m^0) + \sum_{i=1}^N I_0(m^i) \right] \leq \frac{m^0 m^1 - \mathcal{Z} m^1}{\rho^2} + O(\rho^{-3}) < 0,$$

for all ρ sufficiently large, since we are assuming $m^0 < \mathcal{Z}$. However, this contradicts (1.10) in the concentration theorem, and thus $m^0 \geq \mathcal{Z}$, and the theorem is proven. \square

Proof of Proposition I.3. In Proposition II.5, we have already shown that any sequence of minimizers u_n of I_{V_n} forms a minimizing sequence for $I_{V_{TF}}$. Part (ii) then follows from Theorem I.2. \square

IV. PROOF OF THEOREM I.4

The Proof of Theorem I.4 is more intricate than that of Theorem I.2, as it requires us to make a finer estimate of the smaller order terms in the expansion of the energy.

By (i) of Proposition I.3, $\{u_n\}_{n \in \mathbb{N}}$ is a minimizing sequence for $I_{V_{TF}}(M)$, and hence the conclusions of Concentration Theorem I.1 hold. We assume that there is splitting, that is $N \geq 1$, and let $u^i, m^i = \|u^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2$, and x_n^i (with $x_n^0 = 0$) be as in the concentration theorem. By hypothesis, the common value of the Lagrange multipliers of the limit components u^i is negative, $\mu < 0$.

As in the Proof of Theorem I.2, we construct comparison functions by localization to balls with centers q^i spreading to infinity. However, we have little control on the errors introduced by the passage of $u_n(\cdot - x_n^i) \rightarrow u^i$, and thus we use truncations of the minimizers u_n themselves to make these constructions.

Set

$$R_n := \min_{0 \leq i < j} |x_n^i - x_n^j|. \quad (4.1)$$

Consider also a sequence $\rho_n \rightarrow \infty$ and translations $\{q_n^0 = 0\}_{n \in \mathbb{N}}, \dots, \{q_n^N\}_{n \in \mathbb{N}} \subset \mathbb{R}^3$ (all to be chosen later) with

$$1 \leq \rho_n \leq \frac{1}{4} \min\{R_n, Q_n\}, \quad \text{where } Q_n := \min_{i < j} |q_n^i - q_n^j|. \quad (4.2)$$

Using the same cutoff functions ϕ defined in (3.1), we then set

$$\begin{aligned} \chi_{\rho_n}(\cdot) &:= \phi(|\cdot| - \rho_n + 1), \\ G_n^i(\cdot) &:= \chi_{\rho_n}(\cdot - x_n^i) u_n(\cdot), \quad \text{and} \quad H_n^i(\cdot) := G_n^i(\cdot + x_n^i - q_n^i). \end{aligned} \quad (4.3)$$

Thus, G_n^i are compactly supported in balls $B_{\rho_n}(x_n^i)$ centered at the x_n^i , chosen by the concentration theorem, while H_n^i are the same functions but translated to have centers at q_n^i , which we will choose to create appropriate comparison functions. Set

$$m_n^i := \|G_n^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = \|H_n^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2.$$

We first confirm that these truncations provide a good approximation to the limit profiles u^i in the \mathcal{L}^2 sense.

Lemma IV.1. For any ρ_n satisfying (4.2),

$$\lim_{n \rightarrow \infty} m_n^i = m^i = \|u^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2.$$

Proof. First, it is easy to show that $G_n^i(\cdot + x_n^i) \rightharpoonup u^i$, $i = 0, \dots, N$ weakly in $\mathcal{H}^1(\mathbb{R}^3)$, and in the norm on $\mathcal{L}_{loc}^2(\mathbb{R}^3)$. As a consequence,

$$m^i = \|u^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \leq \liminf_{n \rightarrow \infty} m_n^i. \quad (4.4)$$

To obtain the complementary bound, we note that $\sum_{i=0}^N G_n^i(x) \leq u_n(x)$ pointwise on \mathbb{R}^3 , and since the supports of the G_n^i are disjoint, we have

$$\limsup_{n \rightarrow \infty} \sum_{i=0}^N m_n^i < \|u_n\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = M = \sum_{i=0}^N m^i \leq \sum_{i=0}^N \liminf_{n \rightarrow \infty} m_n^i \leq \liminf_{n \rightarrow \infty} \sum_{i=0}^N m_n^i.$$

In particular, the limit $M = \lim_{n \rightarrow \infty} \sum_{i=0}^N m_n^i$ exists. Since individually the terms are bounded below via (4.4), we claim that each of the terms $m_n^i \rightarrow m^i$, $i = 0, \dots, N$. Indeed, for any $\epsilon > 0$, there exists $K > 0$ for which $\sum_{i=0}^N m_n^i < M + \epsilon$ and for any i , $m_n^i \geq m^i - \epsilon/N$, whenever $n \geq K$. Thus, for each j , we have

$$m_n^j + \sum_{i \neq j} m^i - \epsilon \leq \sum_{i=0}^N m_n^i < \sum_{i=0}^N m^i + \epsilon,$$

and so $m_n^j < m^j + 2\epsilon$, for all $n \geq K$, that is, $\limsup_{n \rightarrow \infty} m_n^j \leq m^j$, for each i , and the claim is proven. \square

Since we are assuming $\mu < 0$, the exponential decay of u_n away from balls $B_{\rho_n}(x_n^i)$ allows us to localize the energy $\mathcal{E}_{V_n}(u_n)$ with an exponentially small error.

Lemma IV.2. Let $\rho_n \rightarrow \infty$ with $\rho_n \leq \frac{1}{4}R_n$. Then,

$$\begin{aligned} \mathcal{E}_{V_n}(u_n) &\geq \mathcal{E}_{V_{TF}}(G_n^0) + \sum_{i=1}^N \mathcal{E}_0(G_n^i) - Z_n \int_{\mathbb{R}^3} \frac{|G_n^0(x)|^2}{|x|^v} dx \\ &\quad + \sum_{1 \leq i < j} \frac{m_n^i m_n^j}{|x_n^i - x_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|x_n^i|} - Z_n \sum_{i=1}^N \frac{m_n^i}{|x_n^i|^v} - \epsilon_{1,n}, \end{aligned}$$

where

$$|\epsilon_{1,n}| \leq C \left(\frac{\rho_n}{R_n^2} + \frac{Z_n \rho_n}{R_n^{1+v}} + e^{-\frac{\sqrt{-\mu}}{2} \rho_n} \right), \quad (4.5)$$

as $n \rightarrow \infty$, with C depending on $\{m^i\}$ and \mathcal{Z} , but independent of $\{x_n^i\}$.

Proof. By Lemma II.6, for sufficiently large n ,

$$\left| u_n(x) - \sum_{i=0}^N G_n^i(x) \right| \leq C e^{-\frac{\sqrt{-\mu}}{2} \sigma_n(x)}, \quad x \in \Omega_n := \mathbb{R}^3 \setminus \bigcup_{i=0}^N B_{\rho_n}(x_n^i),$$

where $\sigma_n(x)$ is as in Lemma II.6. This together with (2.7), (2.8), $\mu_n \rightarrow \mu$, Lemma II.3, $\|\nabla \chi_{n,\rho_n}\|_{\mathcal{L}^\infty(\mathbb{R}^3)} \leq 2$, and Hölder estimates for first derivatives imply

$$\left| \nabla \left(u_n(x) - \sum_{i=0}^N G_n^i(x) \right) \right| \leq C e^{-\frac{\sqrt{-\mu}}{2} \sigma_n(x)}.$$

As $G_n^i(x) = u_n(x)$ in $B_{\rho_n}(x_n^i)$ and has support in $B_{\rho_n+1}(x_n^i)$, the contribution to the energy is unchanged in $\bigcup_i B_{\rho_n}(x_n^i)$ and is exponentially small in the complementary region, Ω_n . Moreover, the energy density is integrable over Ω_n , and of order $\epsilon_{1,n} = O(e^{-\frac{\sqrt{-\mu}}{2}\rho_n})$. Hence, we calculate

$$\begin{aligned}
 \mathcal{E}_{V_n}(u_n) &= \sum_{i=0}^N \mathcal{E}_{V_n}(G_n^i) + \sum_{i < j} \int_{B_{\rho_n}(x_n^i)} \int_{B_{\rho_n}(x_n^j)} \frac{|G_n^i(x)|^2 |G_n^j(y)|^2}{|x-y|} dx dy + \epsilon_{1,n} \\
 &= \mathcal{E}_{V_{TF}}(G_n^0) - Z_n \int_{B_{\rho_n}(0)} \frac{|G_n^0(x)|^2}{|x|^v} dx \\
 &\quad + \sum_{i=1}^N \left[\mathcal{E}_0(G_n^i) - \int_{\mathbb{R}^3} V(x) |G_n^i(x)|^2 dx - Z_n \int_{B_{\rho_n}(x_n^i)} \frac{|G_n^i(x)|^2}{|x|^v} dx \right] \\
 &\quad + \sum_{i < j} \int_{B_{\rho_n}(x_n^i)} \int_{B_{\rho_n}(x_n^j)} \frac{|G_n^i(x)|^2 |G_n^j(y)|^2}{|x-y|} dx dy + \epsilon_{1,n} \\
 &= \mathcal{E}_{V_{TF}}(G_n^0) + \sum_{i=1}^N \mathcal{E}_0(G_n^i) - Z_n \int_{B_{\rho_n}(0)} \frac{|G_n^0(x)|^2}{|x|^v} dx \\
 &\quad + \sum_{i < j} \int_{B_{\rho_n}(x_n^i)} \int_{B_{\rho_n}(x_n^j)} \frac{|G_n^i(x)|^2 |G_n^j(y)|^2}{|x-y|} dx dy \\
 &\quad - \sum_{i=1}^N \sum_{k=1}^K \alpha_k \int_{\mathbb{R}^3} \frac{|G_n^i(x)|^2}{|x-r_k|} dx - Z_n \sum_{i=1}^N \int_{B_{\rho_n}(x_n^i)} \frac{|G_n^i(x)|^2}{|x|^v} dx + \epsilon_{1,n}.
 \end{aligned} \tag{4.6}$$

Now, we apply Lemma III.1 to evaluate the interaction terms. In this way, we have

$$\begin{aligned}
 \int_{B_{\rho_n}(x_n^i)} \int_{B_{\rho_n}(x_n^j)} \frac{|G_n^i(x)|^2 |G_n^j(y)|^2}{|x-y|} dx dy &\geq \frac{m_n^i m_n^j}{|x_n^i - x_n^j|} - 4m_n^i m_n^j \frac{\rho_n}{R_n^2}, \\
 \int_{\mathbb{R}^3} \frac{|G_n^i(x)|^2}{|x-r_k|} dx &\leq \frac{m_n^i}{|x_n^i|} + C_1 m_n^i \frac{\rho_n}{R_n^2}, \\
 \int_{B_{\rho_n}(x_n^i)} \frac{|G_n^i(x)|^2}{|x|^v} dx &\leq \frac{m_n^i}{|x_n^i|^v} + C_v m_n^i \frac{\rho_n}{R_n^{v+1}}.
 \end{aligned}$$

By substituting these estimates into (4.6), we arrive at the desired lower bound. \square

Next, we create an upper bound estimate on the minimum energy by moving the localized components H_n^i (which are simply translates of G_n^i) to study the role of the x_n^i . That is, we consider a trial function $w_n = \sum_{i=0}^N H_n^i$, which has the same localized components as u_n , but with centers q_n^i . The advantage of this over the upper bound constructed for the Proof of Theorem I.2 is that the terms of order $O(1)$ will exactly match those in the lower bound given by Lemma IV.2.

Lemma IV.3. Let $\{\rho_n\}_{n \in \mathbb{N}} \subset (1, \infty)$ and $\{q_n^0 = 0\}_{n \in \mathbb{N}}, \dots, \{q_n^N\}_{n \in \mathbb{N}} \subset \mathbb{R}^3$ satisfy (4.2). Then,

$$\begin{aligned}
 \mathcal{E}_{V_n}(u_n) &< \mathcal{E}_{V_{TF}}(G_n^0) + \sum_{i=1}^N \mathcal{E}_0(G_n^i) - Z_n \int_{\mathbb{R}^3} \frac{|G_n^0(x)|^2}{|x|^v} dx \\
 &\quad + \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|q_n^i - q_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|q_n^i|} - Z_n \sum_{i=1}^N \frac{m_n^i}{|q_n^i|^v} + \epsilon_{2,n},
 \end{aligned}$$

where

$$|\epsilon_{2,n}| \leq C \left(\frac{\rho_n}{Q_n^2} + \frac{Z_n \rho_n}{Q_n^{1+v}} + e^{-\frac{\sqrt{-\mu}}{2}\rho_n} \right), \tag{4.7}$$

as $n \rightarrow \infty$, with C depending on $\{m_n^i\}$ and \mathcal{Z} , but independent of $\{q_n^i\}$.

Proof. Set

$$w_n := \sum_{i=0}^N H_n^i.$$

As $0 \leq w_n(x) \leq u_n(x)$ for all $x \in \mathbb{R}^3$, $\|w_n\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 < \|u_n\|_{\mathcal{L}^2(\mathbb{R}^3)}^2$. By the monotonicity of $I_{V_n}(M)$ [Proposition II.1 (i)],

$$\mathcal{E}_{V_n}(u_n) = I_{V_n}(M) < I_{V_n}(\|w_n\|_{\mathcal{L}^2(\mathbb{R}^3)}^2) \leq \mathcal{E}_{V_n}(w_n).$$

Using the support properties of H_n^i and recognizing $\mathcal{E}_{V_T}(H_n^0) = \mathcal{E}_{V_T}(G_n^0)$, $\mathcal{E}_0(H_n^i) = \mathcal{E}_0(G_n^i)$, we expand as in the Proof of Lemma IV.2 to obtain the desired upper bound. \square

By matching the lower bound from Lemma IV.2 with the upper bound from Lemma IV.3, we conclude for any choice of ρ_n , $\{q_n^i\}$ satisfying (4.2), we have the following bound satisfied by the translations $\{x_n^i\}$,

$$\begin{aligned} & \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|x_n^i - x_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|x_n^i|} - Z_n \sum_{i=1}^N \frac{m_n^i}{|x_n^i|^v} \\ & \leq \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|q_n^i - q_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|q_n^i|} - Z_n \sum_{i=1}^N \frac{m_n^i}{|q_n^i|^v} + \epsilon_{1,n} + \epsilon_{2,n}, \end{aligned} \quad (4.8)$$

where $\epsilon_{1,n}, \epsilon_{2,n}$ are defined in the statements of Lemmas IV.2 and IV.3.

In what follows, we exploit the freedom we have of choosing vectors q_n^i and radii ρ_n to prove Theorem I.4. First, we must find the correct scale for the diverging centers $\{x_n^i\}$. We define

$$R_n^0 := \min_{1 \leq i \leq N} |x_n^i|,$$

and for $N \geq 2$,

$$\bar{R}_n := \min_{1 \leq i < j \leq N} |x_n^i - x_n^j|.$$

By Concentration Theorem I.1, each \bar{R}_n diverges to infinity, and moreover $R_n = \min\{\bar{R}_n, R_n^0\}$ [see (4.1)]. By passing to a subsequence and reordering the components if necessary, we may assume that the first diverging center is the closest,

$$|x_n^1| = R_n^0, \quad \forall n \in \mathbb{N}.$$

Lemma IV.4.

(a) If $m^0 > \mathcal{Z}$, then

$$\liminf_{n \rightarrow \infty} R_n Z_n^{\frac{1}{1-v}} > 0. \quad (4.9)$$

(b) If $N \geq 2$ and $\limsup_{n \rightarrow \infty} \frac{R_n^0}{\bar{R}_n} > 0$, then there exists a subsequence for which (4.9) holds.

(c) If $N \geq 2$ and $\frac{R_n^0}{\bar{R}_n} \rightarrow 0$, then

$$\liminf_{n \rightarrow \infty} \bar{R}_n Z_n^{\frac{1}{1-v}} > 0.$$

Proof. First assume $m^0 > \mathcal{Z}$. To derive a contradiction, assume that (along some subsequence) $R_n Z_n^{\frac{1}{1-v}} \rightarrow 0$. Choose $q_n^i = R_n p^i$, for distinct fixed vectors p^i , $i = 1, \dots, N$, and $p^0 = 0$. We also denote by $y_n^i = R_n^{-1} x_n^i$. By the definition of R_n , we have $|y_n^i| \geq 1$ for all $i = 1, \dots, N$, and $|y_n^i - y_n^j| \geq 1$ for all $0 \leq i < j \leq N$. Extracting a further subsequence if necessary, we may assume that either

$$|y_n^1| = 1 \text{ or there exists } i_0, j_0 \neq 0 \text{ for which } |y_n^{i_0} - y_n^{j_0}| = 1, \forall n \in \mathbb{N}. \quad (4.10)$$

Set $\rho_n = \sqrt{R_n}$, and so (4.2) is satisfied for these choices, and in fact $R_n \epsilon_{1,n}, R_n \epsilon_{2,n} \rightarrow 0$, where $\epsilon_{1,n}, \epsilon_{2,n}$ are the remainder terms defined in Lemmas IV.2 and IV.3.

We multiply (4.8) by R_n to obtain

$$\begin{aligned} & \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|y_n^i - y_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|y_n^i|} \\ & \leq \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|p^i|} \\ & \quad - Z_n R_n^{1-v} \sum_{i=1}^N \frac{m_n^i}{|p^i|^v} + Z_n R_n^{1-v} \sum_{i=1}^N \frac{m_n^i}{|y_n^i|^v} + R_n \epsilon_{1,n} + R_n \epsilon_{2,n} \\ & \leq \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|p^i|} + o(1), \end{aligned} \quad (4.11)$$

as $Z_n R_n^{1-\nu} \rightarrow 0$ by the contradiction hypothesis. Assuming that $|y_n^{i_0} - y_n^{j_0}| = 1$ is chosen in (4.10), we then obtain

$$m_n^{i_0} m_n^{j_0} \leq \sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|p^i|} + o(1),$$

which holds for all n and any choice of vectors p^i . Since $m_n^i \rightarrow m^i > 0$, we obtain a contradiction by choosing $|p^i - p^j|$ (with $0 \leq i < j \leq N$) sufficiently large. If the choice in (4.10) yields $|y_n^1| = 1$, we instead have

$$(m_n^0 - \mathcal{Z}) m_n^1 \leq \sum_{1 \leq i < j} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|p^i|} + o(1).$$

As we are assuming $m^0 = \lim_{n \rightarrow \infty} m_n^0 > \mathcal{Z}$, we arrive at the same contradiction as above, choosing $|p^i - p^j|$ (with $1 \leq i < j \leq N$) sufficiently large. This completes the proof of (a).

For (b), we assume $N \geq 2$ and there exists a subsequence and $r > 0$ for which $R_n^0 \geq r \bar{R}_n$, but $R_n Z_n^{1-\nu} \rightarrow 0$. Recall that $R_n = \min\{R_n^0, \bar{R}_n\}$, and so

$$\min\{r, 1\} \bar{R}_n \leq R_n \leq \bar{R}_n,$$

and so each of R_n^0, \bar{R}_n, R_n is of the same order of magnitude. As in part (a), let $y_n^i = R_n^{-1} x_n^i, q_n^i = R_n p^i$, and choose i_0, j_0 for which $|x_n^{i_0} - x_n^{j_0}| = \bar{R}_n$. Note that

$$|y_n^{i_0} - y_n^{j_0}|^{-1} = \frac{R_n}{\bar{R}_n} \geq \min\{1, r\}.$$

Again, multiply (4.8) by R_n , and pass to the limit as in (4.11) to obtain

$$\min\{1, r\} m_n^{i_0} m_n^{j_0} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|y_n^i|} \leq \sum_{0 < i < j} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|p^i|} + o(1),$$

for all n and any choice of vectors p^i . Since $m_n^i \rightarrow m^i > 0$ and $m^0 \geq \mathcal{Z}$ by Theorem I.2, we obtain a contradiction by choosing vectors p^i with $|p^i - p^j|$ sufficiently large.

To prove (c), assume $\frac{R_n^0}{\bar{R}_n} \rightarrow 0$, and suppose (for a contradiction) that $\bar{R}_n Z_n^{1-\nu} \rightarrow 0$. First, we note that

$$|x_n^i| = |x_n^i - x_n^1 + x_n^1| \geq |x_n^i - x_n^1| - |x_n^1| \geq \bar{R}_n - R_n^0 \geq \frac{1}{2} \bar{R}_n \gg |x_n^1|, \quad i \geq 2, n \gg 1,$$

and so only one of the centers is much closer to the origin than the others, $|x_n^i| \ll \bar{R}_n \leq |x_n^1|$, for all $i = 2, \dots, N$.

Choose cutoff radii ρ_n in Lemmas IV.2 and IV.3 with $R_n^0 \ll \rho_n \ll \bar{R}_n$, for instance, $\bar{\rho}_n = \sqrt{R_n^0 \bar{R}_n}$. Note that the ball $B_{\rho_n}(0)$ now includes both $x_n^0 = 0$ and x_n^1 . In particular, when defining the disjoint components G_n^i, H_n^i with \bar{R}_n and $\bar{\rho}_n$, we no longer have a component with $i = 1$, but the $i = 0$ piece accounts for the mass concentrating both at the origin and at x_n^1 . In particular, we will have

$$\|G_n^0\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = \|H_n^0\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = m^0 + m^1 + o(1) > \mathcal{Z}. \quad (4.12)$$

In this way, we return to the same situation as in part (a), but where \bar{R}_n replaces R_n as the decisive length scale. As in (a), we choose distinct vectors $q^0 = 0$ and $q^i, i = 2, \dots, N$, and set $p_n^i := \bar{R}_n q^i$, and (as before) $y_n^i = x_n^i / \bar{R}_n$. Modulo a subsequence, either there is a pair with $|y_n^{i_0} - y_n^{j_0}| = 1$, ($i_0, j_0 \geq 2$) or $i_0 \geq 2$ with $|y_n^{i_0}| = 1, \forall n$. Then, we multiply (4.8) by \bar{R}_n , to obtain

$$\begin{aligned} & \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{|y_n^i - y_n^j|} + (m^0 + m^1 - \mathcal{Z} + o(1)) \sum_{i=2}^N \frac{m_n^i}{|y_n^i|} - Z_n \bar{R}_n^{1-\nu} \sum_{i=2}^N \frac{m_n^i}{|y_n^i|^{\nu}} \\ & \leq \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m^0 + m^1 - \mathcal{Z} + o(1)) \sum_{i=2}^N \frac{m_n^i}{|p^i|} - Z_n \bar{R}_n^{1-\nu} \sum_{i=2}^N \frac{m_n^i}{|p^i|^{\nu}} + \bar{R}_n \bar{\epsilon}_{1,n} + \bar{R}_n \bar{\epsilon}_{2,n}, \end{aligned}$$

where $\bar{\epsilon}_{1,n}$ and $\bar{\epsilon}_{2,n}$ satisfy (4.5) and (4.7) for $\bar{R}_n, \bar{\rho}_n$ replacing R_n, ρ_n . In particular, $\bar{R}_n \bar{\epsilon}_{1,n}, \bar{R}_n \bar{\epsilon}_{2,n} \rightarrow 0$. Employing the contradiction hypothesis $\bar{R}_n Z_n^{1-\nu} \rightarrow 0$ and the choice of $\bar{R}_n, \bar{\rho}_n$, we deduce that (in the case $|y_n^{i_0} - y_n^{j_0}| = 1$)

$$m_n^{i_0} m_n^{j_0} \leq \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m^0 + m^1 - \mathcal{Z} + o(1)) \sum_{i=2}^N \frac{m_n^i}{|p^i|} + o(1)$$

or (in the case $|y_n^{j_0}| = 1$)

$$(m^0 + m^1 - \mathcal{Z}) m^{i_0} \leq \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{|p^i - p^j|} + (m^0 + m^1 - \mathcal{Z} + o(1)) \sum_{i=2}^N \frac{m_n^i}{|p^i|} + o(1).$$

In either case, we then arrive at the same contradiction as in (a), by choosing $|p^i - p^j|$ large enough, $i \neq j$. \square

We now prove the main theorem on the convergence of concentration points at the scale $R_n = O(Z_n^{-\frac{1}{1-v}})$.

Proof of Theorem I.4. Let u_n attain the minimum in I_{V_n} for each $n \rightarrow \infty$. Applying the Concentration Theorem I.1, we obtain values of N , masses m^0, \dots, m^N , and translations $\{x_n^i\}$.

For part (i), we assume $m^0 \in \mathcal{M}_{V_{TF}}^*$ and $m^0 > \mathcal{Z}$. For any choice of N and masses m^0, \dots, m^N with $m^0 > \mathcal{Z}$, all minimizing sequences for $F_{N, (m^0, \dots, m^N)}(w^1, \dots, w^N)$ on Σ_N are convergent. This follows by exactly the same argument as in the Proof of Proposition 8 of Alama et al.⁹ Let $(a^1, \dots, a^N) \in \Sigma_N$ be such a minimizer,

$$F_{N, (m^0, \dots, m^N)}(a^1, \dots, a^N) = \min_{(w^1, \dots, w^N) \in \Sigma_N} F_{N, (m^0, \dots, m^N)}(w^1, \dots, w^N) < 0.$$

Define $\xi_n^i := Z_n^{\frac{1}{1-v}} x_n^i$. By Lemma IV.4, $|\xi_n^i|, |\xi_n^i - \xi_n^j| \geq c > 0$ are bounded below for each $i = 1, \dots, N$ and $j \neq i$.

Set

$$\rho_n := Z_n^{-\frac{1}{2(1-v)}} \text{ and } q_n^i := Z_n^{-\frac{1}{1-v}} a^i.$$

Then, by the Lemma IV.4, up to a subsequence,

$$1 \leq \rho_n \leq \frac{1}{4} \min_{i < j} \{ |q_n^i - q_n^j|, R_n \},$$

so that Eq. (4.8) holds, and

$$\begin{aligned} & \sum_{1 \leq i < j} \frac{m_n^i m_n^j}{|\xi_n^i - \xi_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|\xi_n^i|} - \sum_{i=1}^N \frac{m_n^i}{|\xi_n^i|^v} \\ & \leq \sum_{1 \leq i < j} \frac{m_n^i m_n^j}{|a^i - a^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|a^i|} - \sum_{i=1}^N \frac{m_n^i}{|a^i|^v} + Z_n^{-\frac{1}{1-v}} (\epsilon_n + \hat{\epsilon}_n), \end{aligned} \quad (4.13)$$

where ϵ_n and $\hat{\epsilon}_n$ satisfy (4.5) and (4.7), respectively. In particular, $Z_n^{-\frac{1}{1-v}} \epsilon_n, Z_n^{-\frac{1}{1-v}} \hat{\epsilon}_n \rightarrow 0$.

In addition to this, by Lemma IV.4,

$$\liminf_{n \rightarrow \infty} |\xi_n^i - \xi_n^j| \geq \liminf_{n \rightarrow \infty} Z_n^{\frac{1}{1-v}} R_n > 0. \quad (4.14)$$

By Lemma IV.1, $\lim_{n \rightarrow \infty} m_n^i = m^i$ and hence applying (4.13) and (4.14), we obtain

$$\begin{aligned} & \limsup_{n \rightarrow \infty} F_{N, (m^0, \dots, m^N)}(\xi_n^1, \dots, \xi_n^N) \\ & = \limsup_{n \rightarrow \infty} \left[\sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|\xi_n^i - \xi_n^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|\xi_n^i|} - \sum_{i=1}^N \frac{m_n^i}{|\xi_n^i|^v} \right] \\ & \leq \limsup_{n \rightarrow \infty} \left[\sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{|a^i - a^j|} + (m_n^0 - \mathcal{Z}) \sum_{i=1}^N \frac{m_n^i}{|a^i|} - \sum_{i=1}^N \frac{m_n^i}{|a^i|^v} \right] \\ & = F_{N, (m^0, \dots, m^N)}(a^1, \dots, a^N) \\ & = \min_{(w^1, \dots, w^N) \in \Sigma_N} F_{N, (m^0, \dots, m^N)}(w^1, \dots, w^N). \end{aligned} \quad (4.15)$$

Therefore, $\{(\xi_n^1, \dots, \xi_n^N)\}_{n \in \mathbb{N}}$ is a minimizing sequence for $F_{N, (m^0, \dots, m^N)}$ in Σ_N , and by Ref. 9, Proposition 8, $\xi_n^i = x_n^i Z_n^{\frac{1}{1-v}} \rightarrow y^i$, $i = 0, \dots, N$, with (y^1, \dots, y^N) a minimizing configuration for $F_{N, (m^0, \dots, m^N)}$. This completes the proof in case $m^0 > \mathcal{L}$.

Now consider (ii), for which $m^0 = \mathcal{L}$. We first show that $|x_n^1| \ll Z_n^{\frac{1}{v-1}}$. Indeed, assume the contrary that, up to a subsequence, $|x_n^1| Z_n^{\frac{1}{v-1}} \geq c > 0$ for all n . In case $N \geq 2$, by part (b) of Lemma IV.4, then $R_n Z_n^{\frac{1}{v-1}} \geq c' > 0$. As in the proof of (i), define $\xi_n^i := x_n^i Z_n^{\frac{1}{v-1}}$, then $|\xi_n^i| \geq c$, $i = 1, \dots, N$, is bounded below. We also fix any distinct points $p^1, \dots, p^N \in \mathbb{R}^3 \setminus \{0\}$ and $q_n^i = p^i Z_n^{\frac{1}{v-1}}$.

We now proceed as above, arriving at (4.13). Note that the inequality (4.13) holds for any $N \geq 1$. In fact, if $N = 1$, the inequality simplifies significantly: the double sums are not present, and only the $i = 1$ terms remain. Passing to the limit as in (4.15) and recalling $m_n^0 \rightarrow \mathcal{L}$, we then have

$$\limsup_{n \rightarrow \infty} F_{N, (\mathcal{L}, m^1, \dots, m^N)}(\xi_n^1, \dots, \xi_n^N) \leq F_{N, (\mathcal{L}, m^1, \dots, m^N)}(p^1, \dots, p^N),$$

for any choice of distinct nonzero vectors p^1, \dots, p^N in \mathbb{R}^3 . Now, as the ξ_n^i are bounded below, the left hand side of the above inequality is finite. However, the function $F_{N, (\mathcal{L}, m^1, \dots, m^N)}$ is unbounded below, and thus we may choose p^1, \dots, p^N so as to contradict the inequality. We conclude that $|x_n^1| \ll Z_n^{\frac{1}{v-1}}$.

Finally, for $m^0 = \mathcal{L}$ and $N \geq 2$, we prove the asymptotic distribution of the concentration centers. For this, we return to the definitions of $\bar{R}_n, \bar{\rho}_n$ in the Proof of Lemma IV.4 (c), in which we proved that $\bar{R}_n \geq c Z_n^{\frac{1}{v-1}}$. We recall that the components G_n^0, H_n^0 defined in (4.3) (but using $\bar{\rho}_n$ in the cutoff $\chi_{\bar{\rho}_n}$) will enclose neighborhoods of both $x_n^0 = 0$ and x_n^1 , and hence their masses combine in G_n^0, H_n^0 , as in (4.12). By the same arguments as in Ref. 6, Proposition 8, all minimizing sequences of the interaction energy $\bar{F}_{N, (m^1, m^2, \dots, m^N)}$ converge to a minimizer $(y^2, \dots, y^N) \in \bar{\Sigma}_N$. Define $q_n^0 = 0$ and $q_n^i = y^i Z_n^{\frac{1}{v-1}}$, $i = 2, \dots, N$. Applying (4.8) with these choices, we have

$$\begin{aligned} & \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{|x_n^i - x_n^j|} + (m^0 + m^1 - \mathcal{L} + o(1)) \sum_{i=2}^N \frac{m_n^i}{|x_n^i|} - Z_n \sum_{i=2}^N \frac{m_n^i}{|x_n^i|^v} \\ & \leq \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{|q_n^i - q_n^j|} + (m^0 + m^1 - \mathcal{L} + o(1)) \sum_{i=2}^N \frac{m_n^i}{|q_n^i|} - Z_n \sum_{i=2}^N \frac{m_n^i}{|q_n^i|^v} + \bar{\epsilon}_{1,n} + \bar{\epsilon}_{2,n}, \end{aligned}$$

with [as in part (i)] $Z_n^{\frac{1}{v-1}} \bar{\epsilon}_{1,n}, Z_n^{\frac{1}{v-1}} \bar{\epsilon}_{2,n} \rightarrow 0$. Multiplying the above inequality by $Z_n^{\frac{1}{v-1}}$, we pass to the limit and obtain an inequality for $\bar{F}_{N, (m^1, m^2, \dots, m^N)}$,

$$\limsup_{n \rightarrow \infty} \bar{F}_{N, (m^1, m^2, \dots, m^N)}(\xi_n^2, \dots, \xi_n^N) \leq \bar{F}_{N, (m^1, m^2, \dots, m^N)}(y^2, \dots, y^N).$$

Again, the renormalized centers $(\xi_n^2, \dots, \xi_n^N)$ give a minimizing sequence for $\bar{F}_{N, (m^1, m^2, \dots, m^N)}$ and must converge to a minimizer. This completes the Proof of Theorem I.4. \square

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APPENDIX A: PROOF OF THE CONCENTRATION THEOREM

In this section, we prove the Concentration Theorem I.1. The use of concentration–compactness techniques in Thomas–Fermi-type problems goes back at least to Lions,³ for whom these problems were an important motivation for the development of the general theory. The result of the Concentration Theorem I.1 is essentially contained in the work of Lions,³ although not as a single theorem and with many details left to the reader. Since we make extensive use of this Theorem in proving the main results of this paper, main results of this paper, we provide a more complete proof here (with specific references to steps appearing in other articles).

Proof of Theorem I.1. We first present the proof with $V \not\equiv 0$; the case $V \equiv 0$ requires only a simple modification. Let $\{u_n\}_{n \in \mathbb{N}}$ be a minimizing sequence for \mathcal{E}_V with $\|u_n\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = M$. Since \mathcal{E}_V is coercive, $\{u_n\}_{n \in \mathbb{N}}$ is bounded in $\mathcal{H}^1(\mathbb{R}^3)$. Hence, there exists $u^0 \in \mathcal{H}^1(\mathbb{R}^3)$ and a subsequence for which $u_n \rightharpoonup u^0$ weakly in $\mathcal{H}^1(\mathbb{R}^3)$. At this point, it is not clear if u^0 is nontrivial; this will be shown later. Let $m^0 := \|u^0\|_{\mathcal{L}^2(\mathbb{R}^3)}^2$ and $x_n^0 = 0$. If $m^0 = M$, then the sequence converges strongly in \mathcal{L}^2 , and u^0 minimizes $I_V(M)$, and the procedure terminates with $N = 0$.

If instead $m^0 < M$, we define the remainder $u_n^0(x) := u_n(x) - u^0(x + x_n^0)$. Note that by weak convergence, $\|u_n^0\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \rightarrow M - m^0$ and by weak convergence and the Brezis–Lieb Lemma, the energy decouples in the limit (see Refs. 2 and 5),

$$\lim_{n \rightarrow \infty} [\mathcal{E}_V(u_n) - \mathcal{E}_V(u^0) - \mathcal{E}_0(u_n^0)] = 0,$$

and thus

$$I_V(M) = \lim_{n \rightarrow \infty} \mathcal{E}_V(u_n) = \mathcal{E}_V(u^0) + \lim_{n \rightarrow \infty} \mathcal{E}_0(u_n^0) \geq I_V(m^0) + I_0(M - m^0).$$

By the binding inequality (2.1), we have

$$I_V(m^0) + I_0(M - m^0) \geq I_V(M) \geq \mathcal{E}_V(u^0) + \lim_{n \rightarrow \infty} \mathcal{E}_0(u_n^0) \geq I_V(m^0) + I_0(M - m^0), \quad (\text{A1})$$

and hence we obtain equality of each expression,

$$\mathcal{E}_V(u^0) = I_V(m^0) \quad \text{and} \quad \lim_{n \rightarrow \infty} \mathcal{E}_0(u_n^0) = I_0(M - m^0),$$

that is, the remainder sequence $\{u_n^0\}_{n \in \mathbb{N}}$ is a minimizing sequence for $I_0(M - m^0)$.

We next consider the residual sequence $\{u_n^0\}_{n \in \mathbb{N}}$ and show it concentrates after translation. First, we must eliminate the possibility of “vanishing” in the concentration–compactness framework.⁸ To this end, for any bounded sequence, we define (as in Nam–van den Bosch⁵)

$$\omega(\{v_n\}) := \sup \left\{ \|v\|^2 \mid \exists y_n \in \mathbb{R}^3 \text{ and a subsequence such that } v_n(\cdot - y_n) \rightharpoonup v \text{ in } \mathcal{H}^1(\mathbb{R}^3) \right\}.$$

We claim that $\omega(\{u_n^0\}) > 0$. Indeed, applying Ref. 8, Lemma I.1, if $\omega(\{u_n^0\}) = 0$, then $u_n^0 \rightarrow 0$ in $\mathcal{L}^q(\mathbb{R}^3)$ norm, $\forall 2 < q < 6$, so, in particular, $\int_{\mathbb{R}^3} (u_n^0)^{\frac{q}{3}} \rightarrow 0$. In addition, by (1.2), we have $\int_{\mathbb{R}^3} V|u_n^0|^2 \rightarrow 0$, and hence $I_V(M) = \lim_{n \rightarrow \infty} \mathcal{E}_V(u_n^0) \geq 0$, which contradicts Proposition II.1. Hence “vanishing” cannot occur.

We can, therefore, choose a sequence $x_n^1 \in \mathbb{R}^3$ for which $u_n^0(\cdot - x_n^1) \rightharpoonup u^1$, for some $u^1 \in \mathcal{H}^1(\mathbb{R}^3)$, with mass $m^1 := \|u^1\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \geq \frac{1}{2}\omega(\{u_n^0\}) > 0$. As $u_n^0 \rightarrow 0$, we must have $|x_n^1| \rightarrow \infty$. In case $m^0 = M - m^1$, the sequence converges strongly in \mathcal{L}^2 , and u^1 minimizes $I_V(M - m^1)$, and we obtain (1.8)–(1.11), with $N = 1$.

If $m^1 < M - m^0$, we again define the remainder sequence, $u_n^1(x) := u_n^0(x) - u^1(x + x_n^1)$. By definition, $u_n^1 \rightarrow 0$, $u^1(\cdot - x_n^1) \rightarrow 0$, and $\|u_n^1\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \rightarrow M - m^0 - m^1$, and the energy splits

$$\mathcal{E}_0(u_n^0) = \mathcal{E}_0(u^1) + \mathcal{E}_0(u_n^1) + o(1).$$

By the same argument as in (A1), this implies that $\mathcal{E}_0(u^1) = I_0(m^1)$, $I_0(M - m^0) = I_0(m^1) + I_0(M - m^0 - m^1)$, and $\{u_n^1\}_{n \in \mathbb{N}}$ is a minimizing sequence for $I_0(M - m^0 - m^1)$. Substituting for $I_0(M - m^0)$ in (A1), we conclude

$$I_V(M) = I_V(m^0) + I_0(m^1) + I_0(M - m^0 - m^1).$$

We iterate the above process: for each $k = 2, 3, \dots$, we obtain translations $\{x_n^k\}$ in \mathbb{R}^3 , $|x_n^k| \rightarrow \infty$, functions $u^k \in \mathcal{H}^1(\mathbb{R}^3)$ with

$$\|u^k\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 := m^k \geq \frac{1}{2}\omega(\{u_n^{k-1}\}), \quad (\text{A2})$$

and remainder sequences

$$u_n^k(x) := u_n^{k-1}(x) - u^k(x + x_n^k) = u_n(x) - u^0(x) - \sum_{i=1}^k u^i(x + x_n^i),$$

satisfying

$$\begin{aligned} \|u_n^k\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 &= M - \left(m^0 + \sum_{i=1}^k m^i \right) + o(1), \\ u_n^k(\cdot - x_n^k) &\rightarrow 0, \quad \text{weakly in } \mathcal{H}^1(\mathbb{R}^3), \\ I_V(M) &= I_V(m^0) + \sum_{i=1}^k I_0(m^i), \quad \text{and hence} \\ \mathcal{E}_0(u^k) &= I_V(m^k). \end{aligned}$$

Next, we show that $|x_n^k - x_n^i| \rightarrow \infty$ for all $i \neq k$. Suppose not, and take the smallest $k > i$ for which $|x_n^k - x_n^i|$ remains bounded along some subsequence (so $|x_n^i - x_n^j| \rightarrow \infty$ for all $i < j < k$). Taking a further subsequence, $(x_n^k - x_n^i) \rightarrow \xi$ for some $\xi \in \mathbb{R}^3$. Now, note that $u_n^i(x) = u_n^k(x) + \sum_{j=i+1}^k u^j(x + x_n^j)$ and hence

$$u_n^i(x - x_n^i) = u_n^k(x - x_n^i) + u^k(x - x_n^i + x_n^i) + \sum_{j=i+1}^k u^j(x - x_n^i + x_n^j). \quad (\text{A3})$$

Since $|x_n^j - x_n^i| \rightarrow \infty$ for $i < j < k$, $u^j(\cdot - x_n^i + x_n^j) \rightarrow 0$, while $u^k(\cdot - x_n^i + x_n^k) \rightarrow u^k(\cdot + \xi)$. $u_n^k(\cdot - x_n^i) \rightarrow 0$, and hence we pass to the limit in (A3) to obtain $u_n^i(\cdot - x_n^i) \rightarrow u^i(\cdot + \xi) \neq 0$, a contradiction. Hence, (1.11) is verified.

We claim that this process must terminate at some finite step $k = N$, for which $M = m^0 + \sum_{i=1}^N m^i$. Indeed, if $m^i > 0$ for all $i \in \mathbb{N}$, since $M \geq \sum_{i=0}^k m^i$ for all k , we have $\lim_{k \rightarrow \infty} m^k = 0$. By (A2), we conclude that $\lim_{k \rightarrow \infty} \omega(\{u_n^k\}) = 0$, i.e., the remaining mass after k steps, $(M - \sum_{i=0}^k m^i)$ may be made arbitrarily small. However, by the concavity of $I_0(M)$ for small [see Appendix or Ref. 5, Lemma 9 (iii)] there exists $M_c > 0$ such that minimizing sequences for I_0 do not split for $M < M_c$. This proves statements (1.8)–(1.10).

For $V \neq 0$, we now show that $m^0 > 0$, and hence the translations $x_n^0 = 0$ are trivial in this case. Indeed, if $m^0 = 0$, consider the sequence $\tilde{u}_n = u_n(\cdot - x_n^1)$. As \mathcal{E}_0 is translation invariant, and $\mathcal{E}_V(u^1) < \mathcal{E}_0(u^1)$, a simple calculation shows $\lim_{n \rightarrow \infty} \mathcal{E}_V(\tilde{u}_n) < I_V$, which is not possible. For $V \equiv 0$, the functional \mathcal{E}_0 is translation invariant. Hence, we may begin the process at the Step $k = 1$, defining $\omega(\{u_n\})$ and identifying a first set of translates $\{x_n^0\}$ as above. By translation invariance, $\tilde{u}_n = u_n(\cdot - x_n^1)$ is also a minimizing sequence for $I_0(M)$, and the weak limit $u^0 = w - \lim_{n \rightarrow \infty} \tilde{u}_n$ will be nontrivial. The rest of the proof continues as in the case of nontrivial V .

It remains to show that each u^i solves the Euler–Lagrange equation with the same Lagrange multiplier μ . By the Ekeland variational principle¹³ (see also Ref. 14, Corollary 5.3), we may find a minimizing sequence $\{v_n\}_{n \in \mathbb{N}}$, with $\|v_n\|_{\mathcal{H}^1(\mathbb{R}^3)}^2 = M$ and $\|v_n - u_n\| \rightarrow 0$, for which the Euler–Lagrange equation is solved up to an small error in $\mathcal{H}^{-1}(\mathbb{R}^3)$. That is, $\exists \mu_n \in \mathbb{R}$ with

$$D\mathcal{E}_V(v_n) - \mu_n v_n \rightarrow 0 \quad \text{in } \mathcal{H}^{-1} \text{ norm.}$$

The Lagrange multipliers may be expressed as

$$\mu_n M = \langle D\mathcal{E}_V(v_n), v_n \rangle + o(1) \|v_n\|_{\mathcal{H}^1(\mathbb{R}^3)} = \langle D\mathcal{E}_V(v_n), v_n \rangle + o(1),$$

as minimizing sequences are bounded. By Lemma II.3, $|\mu_n|$ is uniformly bounded, and hence (after extracting a sequence), we may assume $\mu_n \rightarrow \mu$ for some $\mu \in \mathbb{R}$. As $u_n(\cdot - x_n^i) \rightharpoonup u^i$ weakly in $\mathcal{H}^1(\mathbb{R}^3)$, the same is true for $\tilde{v}_n := v_n(\cdot - x_n^i) \rightharpoonup u^i$, $i = 0, \dots, N$. Hence, for every $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$\langle D\mathcal{E}_V(u^0) - \mu u^0, \varphi \rangle = \lim_{n \rightarrow \infty} \langle D\mathcal{E}_V(\tilde{v}_n) - \mu_n \tilde{v}_n, \varphi \rangle = 0,$$

and similarly, $D\mathcal{E}_0(u^i) - \mu u^i = 0$, $i = 1, \dots, N$. □

APPENDIX B: CONCAVITY FOR SMALL MASS

We show that $I_0(M)$ is concave for small values of M . This is another property which the TFDW-type functionals share with Gamow's liquid drop model.

Proposition B.1. $I_0(M)$ is strictly concave for M sufficiently small.

Proof. Nam and Van Den Bosch⁵ showed $I_0(M)$ is attained for M small enough by exploiting

$$I_0(M) = \inf\{F_u(M); u \in \mathcal{H}^1(\mathbb{R}^3), \|u\|_{\mathcal{H}^1(\mathbb{R}^3)} = 1\}, \quad M > 0,$$

where

$$F_u(M) := -\frac{M^{\frac{5}{3}} \left(C_u - M^{\frac{2}{3}} D_u \right)_+^2}{4(A_u + M^{\frac{2}{3}} B_u)},$$

with

$$\begin{aligned} A_u &:= \int_{\mathbb{R}^3} |\nabla u(x)|^2 dx, & B_u &:= c_1 \int_{\mathbb{R}^3} |u(x)|^{\frac{10}{3}} dx, \\ C_u &:= c_2 \int_{\mathbb{R}^3} |u(x)|^{\frac{8}{3}} dx, & D_u &:= \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u^2(x) u^2(y)}{|x-y|} dx dy. \end{aligned}$$

Indeed, they proved $M \ll 1 \mapsto I_0(M)$ is strictly subadditive by showing that $M \ll 1 \mapsto F_u(M)/M$ is strictly increasing, uniformly in u . The latter was established by making use of the inequalities

$$B_u \leq CM^{\frac{2}{3}} A_u, \quad D_u \leq CM^{\frac{2}{3}} C_u, \quad u \in \mathcal{H}^1(\mathbb{R}^3). \quad (\text{B1})$$

(B1) follow from Hölder's inequality, Sobolev's inequality, Hardy–Littlewood's inequality, and the interpolation inequality in Lebesgue spaces.

Then, let us fix any $\alpha \in (0, 1)$, and $M_1, M_2 \ll 1$. By (B1),

$$\frac{d^2F}{dM^2} = \frac{d^2}{dM^2} \left[-\frac{M^{\frac{5}{3}}(C_u - M^{\frac{2}{3}}D_u)^2}{4(A_u + M^{\frac{2}{3}}B_u)} \right] = -\frac{2G_u(M)}{9M^{\frac{1}{3}}(A_u + M^{\frac{2}{3}}B_u)^3}, \quad M \ll 1,$$

where

$$\begin{aligned} G_u(M) := & 14M^{\frac{8}{3}}B_u^2D_u^2 + M^2(37A_uB_uD_u^2 - 10B_u^2C_uD_u) + M^{\frac{4}{3}}(27A_u^2D_u^2 - 30A_uB_uC_uD_u) \\ & + M^{\frac{2}{3}}(-28A_u^2C_uD_u + A_uB_uC_u^2) + 5A_u^2C_u^2 \\ & > A_u^2C_u^2(-10M^2 - 30M^{\frac{4}{3}} - 28M^{\frac{2}{3}} + 5) > 0, \end{aligned}$$

uniformly in u . Therefore, $F_u(M)$ is strictly concave for $M \ll 1$ uniformly in u . As a consequence, for some $u^* = u^*_{\alpha, M_1, M_2}$,

$$\begin{aligned} I_0(\alpha M_1 + (1 - \alpha)M_2) &= F_{u^*}(\alpha M_1 + (1 - \alpha)M_2) \\ &> \alpha F_{u^*}(M_1) + (1 - \alpha)F_{u^*}(M_2) \\ &\geq \alpha I_0(M_1) + (1 - \alpha)I_0(M_2). \end{aligned}$$

Since α, M_1 , and M_2 were arbitrary, we conclude that I_0 is strictly concave for $M \ll 1$. \square

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