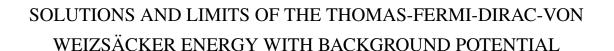
# SOLUTIONS AND LIMITS OF THE THOMAS-FERMI-DIRAC-VON WEIZSÄCKER ENERGY WITH BACKGROUND POTENTIAL



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A Thesis Submitted to the Department of Mathematics and Statistics and the School of Graduate Studies in Partial Fulfilment of the Requirements for the Degree Doctor of Philosophy

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#### **Abstract**

We study energy-driven nonlocal pattern forming systems with opposing interactions. Selections are drawn from the area of Quantum Physics, and nonlocalities are present via Coulombian type interactions. More precisely, we study Thomas-Fermi-Dirac-Von Weizsäcker (TFDW) type models, which are mass-constrained variational problems. The TFDW model is a physical model describing ground state electron configurations of many-body systems.

First, we consider minimization problems of the TFDW type, both for general external potentials and for perturbations of the Newtonian potential satisfying mild conditions. We describe the structure of minimizing sequences, and obtain a more precise characterization of patterns in minimizing sequences for the TFDW functionals regularized by long-range perturbations.

Second, we consider the TFDW model and the Liquid Drop Model with external potential, a model proposed by Gamow in the context of nuclear structure. It has been observed that the TFDW model and the Liquid Drop Model exhibit many of the same properties, especially in regard to the existence and nonexistence of minimizers. We show that, under a "sharp interface" scaling of the coefficients, the TFDW energy with constrained mass Gamma-converges to the Liquid Drop model, for a general class of external potentials. Finally, we present some consequences for global minimizers of each model.

Acknowledgements

To my loved ones

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#### **Declaration of Academic Achievement**

My supervisor, Dr. Lia Bronsard, my co-supervisor, Dr. Stanley Alama, and myself, conducted the research presented in this dissertation. In recognition of this fact, I have chosen to use the personal pronoun "we" where applicable throughout the text. Original results based on published work joint with my supervisor and my co-supervisor are presented in chapters two to five.

## **Chapter 1**

#### Introduction

In computational Chemistry and Physics, behaviour of atoms and molecules should be governed by the many-body Schrödinger theory. However, using this theory is unfeasible, both analytically and computationally, when there is a large number of particles. Thus, approximate theories have been developed to study properties of atoms and molecules, and the most widely used ones can be classified into two main classes: wavefunction methods, and density functional methods. The Thomas-Fermi-Dirac-von Weizsäcker (TFDW) theory is an example of the latter. In the TFDW theory, properties of atoms and molecules are encoded in the electron density instead of the more complex wavefunction. The first density functional theory was the TF theory (see [56, 19],) a theory that captures the behavior of the ground state energy of molecules in the large nuclear charge limit [35]. But negative ions, molecules with more electrons than protons, were absent in this theory, and there were issues with stability of molecules in the TF theory [55]. Then, two corrections were incorporated (see [57, 16]) hence making the accuracy of the TFDW theory comparable to that of the Hartre Fock theory [6], an accurate density matrix theory (statistical ensemble of various quantum states,) when there are many protons.

Throughout this thesis we are concerned with a class of energy functionals which include the TFDW model. More precisely, we consider variational problems of the form

$$\mathscr{I}_{V}^{p,q}(M) := \inf\{\mathscr{E}_{V}^{p,q} \; ; \; u \in \mathscr{H}^{1}(\mathbb{R}^{3}), \|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} = M\}, \quad M > 0,$$
 (1.1)

where the energy  $\mathcal{E}_{V}^{p,q}$  is defined as

$$\mathscr{E}_{V}^{p,q}(u) := \int_{\mathbb{R}^{3}} \left( c_{W} \|\nabla u\|^{2} + c_{TF} |u|^{p} - c_{D} |u|^{q} - Vu^{2} \right) d\overrightarrow{x} + \frac{1}{2} \int_{\mathbb{R}^{3}} \int_{\mathbb{R}^{3}} \frac{u^{2}(\overrightarrow{x}) u^{2}(\overrightarrow{y})}{\|\overrightarrow{x} - \overrightarrow{y}\|} d\overrightarrow{x} d\overrightarrow{y},$$

with  $c_W, c_{TF}, c_D > 0, 2 < q < p \le 6$ , and

$$V \ge 0, \quad V \in \mathcal{L}^{\frac{3}{2}}(\mathbb{R}^3) + \mathcal{L}^{\infty}(\mathbb{R}^3), \text{ and } V(\overrightarrow{x}) \xrightarrow[\|\overrightarrow{x}\| \to \infty]{} 0.$$
 (1.2)

Conditions above ensure  $\mathscr{I}_V^{p,q}(M)$  is finite for each M > 0,  $\mathscr{E}_V^{p,q}$  is coercive in  $\mathscr{H}^1(\mathbb{R}^3)$  on the constraint set (see Proposition 3,) and

$$u \in \mathscr{H}^1(\mathbb{R}^3) \mapsto \int_{\mathbb{R}^3} V u^2 d\vec{x}$$

is weakly continuous (see Proposition 5.)

The TFDW model corresponds to particular choices of  $c_W, c_{TF}$  and  $c_D, p = \frac{10}{3}, q = \frac{8}{3}$ , and

$$V_{TFDW}(\vec{x}) := \sum_{k=1}^{K} \frac{\alpha_k}{\|\vec{x} - \vec{r}_k\|},\tag{1.3}$$

with  $K \in \mathbb{N}$ ,  $\{\alpha_k\}_{k=1}^K \subset \mathbb{R}^+$  and  $\{\overrightarrow{r}_k\}_{k=1}^K \subset \mathbb{R}^3$  all fixed.  $\mathcal{E}_{V_{TFDW}}^{\frac{10}{3}, \frac{8}{3}}(u)$  is to be thought of as the energy of a system of M electrons interacting with K nuclei fixed at positions  $\overrightarrow{r}_k$ . Each nucleus has charge  $\alpha_k > 0$ , and the total nuclear charge is denoted

$$\mathscr{Z} := \sum_{k=1}^{K} \alpha_k > 0, \tag{1.4}$$

and plays a key role in existence results (see the works of Frank, Nam, and Van Den Bosch [23], and Lieb [33] for a survey.) We note that chemical and physical systems are usually found in their most stable state, and that corresponds to the lowest energy possible. The infimum corresponds to the ground state energy, and an optimal *u* corresponds to a state or configuration of optimal energy.

Background potentials of the form

$$V_{\nu}(\vec{x}) := \sum_{k=1}^{K} \frac{\alpha_k}{\|\vec{x} - \vec{r}_j\|^{\nu}},\tag{1.5}$$

with  $K \in \mathbb{N}$ ,  $\{\alpha_k\}_{k=1}^K \subset \mathbb{R}^+$ ,  $\{\overrightarrow{r}_k\}_{k=1}^K \subset \mathbb{R}^3$ , and  $0 < \nu < 2$ , are also of mathematical interest.

In the TFDW model, the gradient term in the energy is the von-Weizsäcker term; it corresponds to the kinetic energy of particles very close to nuclei, the leading order correction. The term with the  $\frac{10}{3}$  in it also corresponds to the kinetic energy. The Dirac term is the term with  $\frac{8}{3}$  in it, which represents the exchange energy between electrons, the second order correction. In regard to other terms,  $V_{TFDW}$  is a Coulombian potential that corresponds to the one-body attractive interaction between electrons and nuclei, while the nonlocal term models the two-body repulsive interaction between electrons. Here u plays the role of electron distribution. We note that  $\mathcal{Z}$  and M do not necessarily have to be integers. Also, appropriate values of coefficients would have to be chosen in order for the TFDW model to be an accurate approximation to Schrödinger's theory.

The second chapter of the thesis contains preliminary results, some of which are original. The main contribution of the third chapter of this thesis is the characterization of minimizing sequences for  $\mathscr{I}_V^{p,q}$ , both with V general and with V chosen to be a perturbation of the molecular potential  $V_{TFDW}$ .

Even though the energy  $\mathscr{E}_V^{p,q}$  is coercive, existence of a minimizer for  $\mathscr{I}_V^{p,q}(M)$  is a highly nontrivial problem, due to a lack of compactness at infinity and the nonconvexity of  $\mathscr{E}_V^{p,q}$ . Lions devised a method for studying compactness of minimizing sequences in unbounded domains for a diverse array of problems in Physics, including functionals of the form  $\mathscr{I}_{V_{TFDW}}^{p,q}$ . The method is called the concentration-compactness method and it relies on a Lemma that tells us that there are only three options when we have a sequence of functions with fixed mass in  $\mathbb{R}^3$ : there is convergence up to a subsequence and translations, or there is vanishing, or there is splitting of mass into at least two pieces moving infinitely far away from one another. The proof of the concentration Lemma relies on a concentration function that measures "the largest piece of mass that stays in a bounded region". In our setting, convergence ensures the existence of minimizers and we can prove that translations can be bypassed, vanishing cannot happen because  $\mathscr{I}_V^{p,q} < 0$ , and if there is splitting then the energy splits accordingly (see Proposition 9.) Lions [37] used his method to prove that there exists a minimizer for  $\mathscr{I}_{V_{TFDW}}^{p,q}(M)$  if  $M \leq \mathscr{L}$ , while Le Bris [31] proved existence of minimizers for  $\mathscr{I}_{V_{TFDW}}^{10,8}(M)$  in the case  $M \leq \mathscr{L} + \varepsilon$  for some  $\varepsilon = \varepsilon(\mathscr{L}) > 0$ . We can extend the latter with little to no changes to the following result we do not prove in this thesis:

**Theorem 1.** (Le Bris [31, Theorem 1]) Let V satisfy (1.2) and

$$V(\vec{x}) \ge V_{TFDW}(\vec{x}) = \sum_{k=1}^{K} \frac{\alpha_k}{\|\vec{x} - \vec{r}_k\|}, \quad pointwise \ almost \ everywhere \ in \ \mathbb{R}^3, \tag{1.6}$$

for some  $K \in \mathbb{N}$ ,  $\{\alpha_k\}_{k=1}^K \subset \mathbb{R}^+$  and  $\{\vec{r}_k\}_{k=1}^K \subset \mathbb{R}^3$ . Then,  $\mathscr{I}_V^{p,q}(M)$  is attained for  $0 < M \le \mathscr{Z} + \varepsilon$  for some  $\varepsilon = \varepsilon(\mathscr{Z})$ .

For *V* more general, we can easily extend a proof by Lions [37] to the following result we do not prove in this thesis:

**Theorem 2.** (Lions [37, Corollary II.2, part i)]) Let V satisfy (1.2). Then,  $\mathscr{I}_{V}^{p,q}(M)$  is attained for M sufficiently small.

In regard to nonexistence of minimizers for  $\mathscr{J}_{V_{TFDW}}^{\frac{10}{3}, \frac{8}{3}}(M)$ , Nam and Van Den Bosch proved that  $\mathscr{J}_{V_{TFDW}}^{\frac{10}{3}, \frac{8}{3}}(M)$  is not attained if both M is sufficiently large and  $\mathscr{Z}$  is sufficiently small, while Frank, Nam, and Van Den Bosch [46] proved nonexistence of a minimizer for  $M > \mathscr{Z} + C$ , for some universal C > 0, in the case where there is only one nucleus (i.e., K = 1 in (1.3).) In experiments, it has been observed that this constant is two. It makes sense there is a bound on the number of electrons which can be bound by nuclei because when nuclei are not sufficiently charged, then electrons are left free to repel each other and escape.

There is a special class of potentials V for which the existence problem for  $\mathscr{I}_V^{\frac{10}{3},\frac{8}{3}}$  is completely understood. We say that V is a long-range potential if V satisfies (1.2) and

$$\liminf_{t \to \infty} \left[ t \left( \inf_{\|\vec{x}\| = t} V(\vec{x}) \right) \right] = \infty.$$
(1.7)

For instance, the homogeneous potentials  $V^{\nu}(\vec{x}) = \|\vec{x}\|^{-\nu}$  are of long-range for  $0 < \nu < 1$ . For long-range potentials, Alama *el al.* [3] showed that  $\mathscr{I}_{V}^{\frac{10}{3},\frac{8}{3}}(M)$  is attained for <u>every</u> M > 0. We can extend their result with little to no changes to the following result we do not prove in this thesis:

**Theorem 3.** (Alama et al. [3, Theorem 2]) Let 2 , and <math>V satisfy (1.2) and (1.7). Then,  $\mathscr{I}_{V}^{p,q}(M)$  is attained for every M > 0.

Thus, we may perturb the TFDW potential via a long-range potential of the form  $V_V$  as in (1.5), and think of this as a "regularization" of the TFDW model. We, thus, define a family of long-range potentials,

$$V_Z(\overrightarrow{x}) := V_{TFDW}(\overrightarrow{x}) + \frac{Z}{\|\overrightarrow{x}\|^{\nu}}, \qquad 0 < \nu < 1,$$

with parameter Z>0. By taking a sequence  $Z_n \xrightarrow[n\to\infty]{} 0^+$  we recover the TFDW model  $\mathscr{I}_{V_{TFDW}}^{10}$ , but via a special minimizing sequence  $\{u_n\}_{n\in\mathbb{N}}$  composed of minimizers of the long-range problem,  $\mathscr{E}_{V_n}^{10}$ ,  $u_n = \mathscr{I}_{V_n}^{10}$ . The energy  $\mathscr{I}_0^{10}$ ,  $u_n = \mathscr{I}_0^{10}$ ,  $u_n = \mathscr{I}_0^{10}$ ,  $u_n = \mathscr{I}_0^{10}$ , with  $||\vec{x}_n|| \xrightarrow[n\to\infty]{} \infty$ . The existence properties for  $\mathscr{I}_0^{10}$ ,  $u_n = u_n = u_n$  are analogous to those of  $|u_n|$ , the infimum is attained for sufficiently small  $u = u_n = u_n = u_n$ . We see [39].)

If a function  $u \in \mathcal{H}^1(\mathbb{R}^3)$  attains the minimum in  $\mathscr{I}_V^{p,q}(M)$  (respectively,  $u_0 \in \mathcal{H}^1(\mathbb{R}^3)$  attains the minimum in  $\mathscr{I}_0^{p,q}(M)$ ,) the minimizers satisfy the partial differential equations (PDEs)

$$-c_W \Delta u + c_{TF} \frac{p}{2} u |u|^{p-2} - c_D \frac{q}{2} u |u|^{q-2} - Vu + (u^2 \star ||\cdot||^{-1}) u = \mu u, \tag{1.8}$$

$$-c_W \Delta u + c_{TF} \frac{p}{2} u |u|^{p-2} - c_D \frac{q}{2} u |u|^{q-2} + u^2 \star ||\cdot||^{-1} u = \mu u, \tag{1.9}$$

with Lagrange multiplier  $\mu$  induced by the mass constraint (see Propositions 10 and 11.)

As mentioned above, the existence question is complicated by noncompactness due to translations of mass to infinity and the lack of concavity of the energy functional. However, minimizing sequences may be characterized using a general Concentration-Compactness structure (see [36], [37].) The following Theorem is proved in section 1 of chapter 3.

**Concentration Theorem 4.** Let  $\{u_n\}_{n\in\mathbb{N}}$  be a minimizing sequence for  $\mathscr{I}_V^{p,q}(M)$ , where V satisfies (1.2). Assume q < 3 in the case  $V \equiv 0$ .

Then, there exist  $N \in \mathbb{N} \cup \{0,\infty\}$ , masses  $\{m^i\}_{i=0}^N \subset \mathbb{R}^+$ , translations  $\{\vec{x}_n^i\}_{n\in\mathbb{N}} \subset \mathbb{R}^3$ , and functions  $\{u^i\}_{i=0}^N \subset \mathcal{H}^1(\mathbb{R}^3)$  such that, up to a subsequence,

$$u_n(\cdot) - \sum_{i=0}^N u^i \left( \cdot - \overrightarrow{x}_n^i \right) \xrightarrow[n \to \infty]{} 0 \text{ in } \mathcal{L}^2(\mathbb{R}^3), \tag{1.10}$$

$$\mathcal{I}_{V}^{p,q}(m^{0}) = \mathcal{E}_{V}^{p,q}(u^{0}), \quad \mathcal{I}_{0}^{p,q}(m^{i}) = \mathcal{E}_{0}^{p,q}(u^{i}), i > 0, 
where \quad ||u^{i}||_{\mathcal{L}^{2}(\mathbb{R}^{3})}^{2} = m^{i};$$
(1.11)

$$\sum_{i=0}^{N} m^{i} = M, \quad \mathscr{I}_{V}^{p,q}(m^{0}) + \sum_{i=0}^{N} \mathscr{I}_{0}^{p,q}(m^{i}) = \mathscr{I}_{V}^{p,q}(M), \tag{1.12}$$

$$\|\vec{x}_n^i - \vec{x}_n^j\| \xrightarrow[n \to \infty]{} \infty, \quad i \neq j.$$
 (1.13)

The functions  $u^i$  satisfy (1.8) for i = 1,...,N, and  $u^0$  satisfies (1.9), each with the <u>same</u> Lagrange multiplier  $\mu \leq 0$ .

Moreover,

1. if  $V \not\equiv 0$ , then we can take  $\vec{x}_n^0 = \vec{0}$ , while

2. if 
$$p = \frac{10}{3}$$
 and  $q = \frac{8}{3}$ , then  $N < \infty$  and the convergence in (1.10) takes place in  $\mathcal{H}^1(\mathbb{R}^3)$ .

If a minimizer exists, then no splitting is necessary, and there exist minimizing sequences with N=0. This occurs for  $V=V_{TFDW}$  when the mass is not much larger than the total charge (see Theorem 1,) or for V in the class of long-range potentials (see Theorem 3,) for instance. In contrast, we expect splitting with large mass M, and the pieces resulting from noncompactness each minimize  $\mathcal{I}_V^{p,q}$  or  $\mathcal{I}_0^{p,q}$  for its given mass, that is,

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

where

$$\mathscr{M}_{V}^{p,q}:=\left\{M>0\;;\;\mathscr{I}_{V}^{p,q}(M)\;\text{has a minimizer}\;u\in\mathscr{H}^{1}(\mathbb{R}^{3}),\;\int_{\mathbb{R}^{3}}u^{2}=M
ight\}.$$

It is an open question to determine whether  $\mathcal{M}_{V}^{p,q}$  is an interval, for any choice of background potential V and powers p and q.

Let us explain the basic idea behind Theorem 4. Minimizing sequences  $\{u_n\}_{n\in\mathbb{N}}$  for  $\mathscr{I}_V^{p,q}(M)$  may lose compactness due to splitting into widely spaced components, each of which tends to a minimizer of  $\mathscr{I}_V^{p,q}$  or (for those components which translate off to infinity)  $\mathscr{I}_0^{p,q}$ . Asymptotically, all of the mass M is accounted for by this splitting. Although the pieces eventually move infinitely far away, they retain some information of the original minimization problem as they share the same Lagrange multiplier.

Concentration results like this one have appeared in numerous papers. For the TFDW model, a very similar result is outlined in [37], and a proof of the exact decomposition of energy (1.12) for the case  $V \equiv 0$ ,  $p = \frac{10}{3}$ , and  $q = \frac{8}{3}$  is given in [46, Lemma 9]. The finiteness of the components in the case  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$  is a result of the concavity of the energy  $\mathcal{E}_0^{\frac{10}{3},\frac{8}{3}}$  for small masses, as proved in Proposition 7.

We obtain more precise information on the splitting structure of sequences coming from perturbing  $\mathscr{I}_{VTFDW}^{p,q}$ . In particular, when mass splits, the piece that remains in a bounded region has mass  $m^0 \geq \mathscr{Z}$ , the total nuclear charge in case  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$ . The proof of the following Theorem can be found in section 2 of chapter 3.

**Theorem 5.** Assume V satisfies (1.2) and (1.6). Then, with the notation of Theorem 4, for any minimizing sequence  $\{u_n\}_{n\in\mathbb{N}}$  of  $\mathscr{I}_V^{p,q}(M)$ , either  $M\in\mathscr{M}_V^{p,q}$  or splitting occurs with  $m^0\geq\mathscr{Z}$ , with  $\mathscr{Z}$  as in (1.4).

Heuristically, this is a satisfying result when  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$ : after splitting, the nuclei should still capture as many electrons as the total nuclear charge  $\mathscr{Z}$ . We expect that nuclei should be able to retain strictly more, to form a negatively charged ion.

Next, we examine more closely the loss of compactness which may occur for the long-range regularized families  $V_n$  satisfying (1.14) with 0 < v < 1 and with  $p = \frac{10}{3}, q = \frac{8}{3}$ . First, minimizers of  $\mathscr{I}_{V_n}^{\frac{10}{3}, \frac{8}{3}}(M)$  form a minimizing sequence for  $\mathscr{I}_{V_{TFDW}}^{\frac{10}{3}, \frac{8}{3}}(M)$ , so when M is large in comparison with  $\mathscr{Z}$ , compactness is lost and mass splits off to infinity as described in Theorem 4.

**Proposition 1.** Let  $Z_n \xrightarrow[n \to \infty]{} 0^+$  and

$$V_n(\vec{x}) = V_{TFDW}(\vec{x}) + \frac{Z_n}{\|\vec{x}\|^{\nu}}, \tag{1.14}$$

with 0 < v < 1, and  $\mathscr{Z}$  as in (1.4). Suppose that  $u_n$  minimizes  $\mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M)$ ,  $n \in \mathbb{N}$ . Then,

- (i)  $\{u_n\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathcal{J}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M)$ .
- (ii) Either  $M \in \mathcal{M}_{V_{TFDW}}^{\frac{10}{3}, \frac{8}{3}}$  or splitting occurs with  $m^0 \geq \mathcal{Z}$ .

The nonlocal term in  $\mathcal{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}$  exerts a repulsive effect on the components  $u^i$ , while the vanishing long-range potential provides a degree of containment. The combination of attractive and repulsive terms has generally led 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 [11, 2].)

Nonetheless, for potentials  $V_n$  of the form (1.14), the interactions between the fleeing components  $u^i$  appear in the energy at order  $Z_n^{\frac{1}{1-\nu}}$ . As a result, we need some information about the spatial decay of the minimizers of  $\mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}$  away from the centers of the support in order to control the errors in an expansion of the energy in terms of  $Z_n \xrightarrow[n \to \infty]{} 0^+$ . In the liquid drop problem, the splitting is into characteristic functions of disjoint bounded domains, and this issue does not arise. To calculate interactions we require exponential decay of the solutions, which is connected to the delicate question of the negativity of the Lagrange multiplier  $\mu$ . We obtain exponential decay when  $\mu < 0$ ,

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

for any  $0 < \lambda < \sqrt{-\mu}$ . We know that  $\mu \le 0$  because  $\mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M)$  is strictly decreasing in M and in fact we 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  $M \in \mathscr{M}_{V}^{\frac{10}{3},\frac{8}{3}}$ . The strict negativity is known for the cases  $V \equiv 0$  with sufficiently small mass, or with  $V = V_{TFDW}$  with  $M < \mathscr{Z} + \kappa$  with  $\kappa = \kappa(V_{TFDW}) > 0$  (see Proposition 11.)

Let us state our result on the distribution of masses in the case of splitting. The proof of this result can be found in section 3 of chapter 3. But first, we define the set

$$\mathcal{M}_{V}^{*} := \left\{ M \in \mathcal{M}_{V}^{\frac{10}{3}, \frac{8}{3}} ; \text{ every minimizer } u \text{ of } \mathcal{I}_{V_{TFDW}}^{\frac{10}{3}, \frac{8}{3}}(M) \text{ satisfies (1.8) with } \mu < 0. \right\}$$

**Theorem 6.** Let  $u_n$  minimize  $\mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M)$  with  $V_n$  satisfying (1.14) with 0 < v < 1 and  $Z_n \xrightarrow[n \to \infty]{} 0^+$ . Let  $N \in \mathbb{N}$ ,  $\{m^i\}_{i=0}^N$  and  $\{\vec{x}_n^0\}_{n \in \mathbb{N}}, \ldots, \{\vec{x}_n^N\}_{n \in \mathbb{N}}$  be as in Theorem 4. Assume  $m^0 \in \mathscr{M}_{V_{TFDW}}^*$ . Then, up to a subsequence and relabeling, either

(i)  $m^0 > Z$  and

$$Z_n^{\frac{1}{1-\nu}} \overrightarrow{x}_n^i \xrightarrow[n \to \infty]{} \overrightarrow{y}^i, \quad i = 1, \dots, N,$$

where  $(\vec{y}^1, \dots, \vec{y}^N)$  minimizes the interaction energy

$$F_{N,(m^0,m^1,...,m^N)}(\overrightarrow{w}^1,\ldots,\overrightarrow{w}^N) := \sum_{1 \leq i < j} \frac{m^i m^j}{\|\overrightarrow{w}^i - \overrightarrow{w}^j\|} + \left(m^0 - \mathscr{Z}\right) \sum_{i=1}^N \frac{m^i}{\|\overrightarrow{w}^i\|} - \sum_{i=1}^N \frac{m^i}{\|\overrightarrow{w}^i\|^V}$$

over

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

or.

(ii)  $m^0 = Z$ ,  $Z_n^{\frac{1}{1-\nu}} \overrightarrow{x}_n^1 \xrightarrow[n \to \infty]{0}$  and if  $N \ge 2$  we have:

$$Z_n^{\frac{1}{1-\nu}} \overrightarrow{x}_n^i \xrightarrow[n \to \infty]{} \overrightarrow{y}^i, \quad i = 2, \dots, N,$$

where  $(\vec{y}^2, \dots, \vec{y}^N)$  minimizes the interaction energy

$$\overline{F}_{N,(m^1,m^2,...,m^N)}(\vec{w}^2,...,\vec{w}^N) := \sum_{2 \le i < j} \frac{m^i m^j}{|||\vec{w}^i - \vec{w}^j||} + m^1 \sum_{i=2}^N \frac{m^i}{||\vec{w}^i||} - \sum_{i=2}^N \frac{m^i}{||\vec{w}^i||^V}$$

over

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

- **Remark 1.** 1. The specific choice of powers  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$  in the nonlinear potential well  $W(u) = c_{TF}|u|^p c_D|u|^q$  is physically appropriate for the TFDW model, but from the point of view of analysis other choices might be possible. Theorem 6 can be extended to the case 2 < q < 3 and q with no major modifications provided that <math>N in Theorem (4) is finite. A necessary condition for  $N < \infty$  is that  $\mathscr{I}_0^{p,q}(M)$  is strictly subadditive for  $M \ll 1$ , but it is unclear whether this is the case for general p and q.
  - 2. 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 cancelled by the attractive effect of the nuclear potential  $V_{TFDW}$ . 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  $Z^{-\frac{1}{1-\nu}}$ . 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.

- 3. If  $m^0 = \mathcal{Z}$ , then  $m^0 \in \mathcal{M}^*_{V_{TEDW}}$  automatically (see Proposition 11.)
- 4. The proof of the compactness of all minimizing sequences of  $\inf F_{N,(m^0,m^1,\dots,m^N)}$  and  $\inf \overline{F}_{N,(m^1,m^2,\dots,m^N)}$  follows with little modification from the proof of [2, Proposition 8] (see Proposition 16.)
- 5. By Theorem 4, each of the components  $u^i$  shares the same Lagrange multiplier  $\mu$ , and hence it suffices to have that any one of the components satisfy (1.8) with  $\mu < 0$ .
- 6. We do not know whether the condition  $\mu < 0$  could be relaxed. We make use of  $\mu < 0$  for uniform exponential decay of the functions  $\{u_n\}_{n\in\mathbb{N}}$  away from  $\vec{x}_n^i$ , but some weaker uniform decay away from the mass centers may be sufficient. It is unclear how rapidly minimizers of (1.1) decay when  $\mu = 0$ .

Graphically, we are thinking of the following situation:

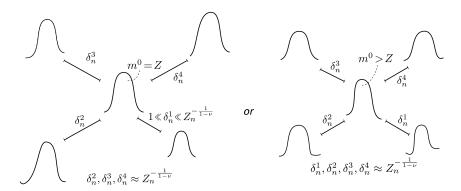


Figure 1.1: Splitting, in the case there are four pieces in total (N = 3)

From now on we denote

$$D(f,g) := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{f(\overrightarrow{x})g(\overrightarrow{y})}{\|\overrightarrow{x} - \overrightarrow{y}\|} d\overrightarrow{x} d\overrightarrow{y},$$

for any pair of functions  $f, g : \mathbb{R}^3 \to \mathbb{R}$ .

We build a bridge between the TFDW mode and the Liquid Drop Model in chapters four and five of this thesis. The Liquid Drop model was conceived by George Gamow, a Russian theoretical physicist, during his visit to Bohr. Mathematicians became more interested in the Liquid Drop Model about fifteen years ago when studying the Ohta-Kawasaki functional. The purpose of the Liquid Drop Model is to predict three features: the shape of nuclei (observed ones are spherical,) the existence of nuclei with the least energy per nucleon, and the nonexistence of nuclei with too many protons. Nuclei are to be thought of as fluid bodies that are incompressible and uniformly charged.

The Liquid Drop Model (with potential) is also a variational problem: for sets  $\Omega \subset \mathbb{R}^3$  of finite perimeter and fixed volume  $|\Omega| = M$ , we minimize the energy

$$E_{LD}(\Omega) := \operatorname{Per}_{\mathbb{R}^3}(\Omega) - \int_{\Omega} V d\overrightarrow{x} + D(\mathbb{1}_{\Omega}, \mathbb{1}_{\Omega}).$$

In this model, the first term represents the perimeter of  $\partial\Omega$ , which may be calculated as the total variation of the measure  $\|\nabla\mathbbm{1}_{\Omega}\|$ , with  $\mathbbm{1}_{\Omega}\in BV(\mathbb{R}^3;\{0,1\})$ . When  $V\equiv 0$ , this is Gamow's problem. The constraint value M represents the number of nucleons bound by the strong nuclear force. Mathematically, the energy that is being minimized corresponds to the sum of surface tension and the Coulombic repulsion interaction term over sets of fixed nuclear mass, that is, a fixed number of neutrons.

As variational problems, the TFDW and Liquid Drop Models have much in common. Each problem features a competition between local attractive terms (gradient and potential terms) and a common nonlocal repulsive term. As such, each problem is characterized by subtle problems of existence and nonexistence due to the translation invariance of the problem "at infinity": for large values of the "mass" constraint M, minimizing sequences may fail to converge due to splitting of mass which escapes to infinity, the "dichotomy" case in the concentration-compactness principle of Lions [36]. (See e.g., [9, 11, 20, 21, 23, 28, 29, 37, 39, 40, 46].) While this similarity has often been remarked, and we often speak of the Liquid Drop Model as a sort of "sharp interface" version of TFDW, no direct analytic connection between the two has been made. If we think of the Liquid Drop model as sharp interface toy model for the TFDW model, then we are thinking of an atom as having piece-wise constant density, and the kinetic energy corresponds to surface tension.

In the second part of this thesis we prove that, after an appropriate "sharp interface" scaling and normalization, a TDFW energy converges to the Liquid Drop Model with potential, in the context of  $\Gamma$ -convergence. In order to establish this connection we select the constants in the TFDW type energy so as to set up a sharp interface limit. We emphasize that this choice of scaling is not physically natural for the application to ionization phenomena, but is motivated purely mathematically.

We introduce a length-scale parameter  $\varepsilon > 0$ , and choose constants  $c_W = \frac{\varepsilon}{2}$ ,  $c_{TF} = \frac{1}{2\varepsilon}$  and  $c_D = \frac{1}{\varepsilon}$ . We note that for fixed  $\varepsilon$ , the qualitative behavior of the minimization problem for TFDW type models is not affected by the specific choices of the constants  $c_W, c_{TF}, c_D$ , and the values we select here match the standard choice of constants in the Liquid Drop Model. In addition, we complete the square in the nonlinear potential by adding in a multiple of the constrained  $\mathscr{L}^2$  norm, which is a constant in the minimization problem and thus has no effect on the existence of minimizers or the Euler-Lagrange equations. That is, we rewrite the nonlinear potential as,

$$\int_{\mathbb{R}^3} \frac{1}{2\varepsilon} \left( |u|^{\frac{10}{3}} - 2|u|^{\frac{8}{3}} \right) d\overrightarrow{x} = \int_{\mathbb{R}^3} \frac{1}{2\varepsilon} u^2 \left( |u|^{\frac{2}{3}} - 1 \right)^2 d\overrightarrow{x} - \frac{M}{2\varepsilon},$$

where  $M = \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^2$  according to the constraint. Thus we recognize the triple well potential,

$$W(u) := u^2 \left( |u|^{\frac{2}{3}} - 1 \right)^2,$$

vanishing at |u| = 0, 1, and a version of the TFDW type energy in the rescaled and normalized form,

$$\mathscr{E}_{\varepsilon}^{V}(u) := \int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \|\nabla u\|^2 + \frac{1}{2\varepsilon} W(u) - V u^2 \right] dx + D(u^2, u^2), \quad \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M. \tag{1.15}$$

As  $\varepsilon \to 0^+$  we expect that sequences  $\{u_\varepsilon\}_{\varepsilon>0}$  of uniformly bounded energy converge almost everywhere to one of the wells of the potential W, that is, in the limit  $u(\vec{x}) \in \{0,\pm 1\}$ . As  $\mathscr{E}^V_\varepsilon(|u|) = \mathscr{E}^V_\varepsilon(u)$ , we expect minimizers of  $\mathscr{E}^V_\varepsilon$  to have fixed sign, but families  $\{u_\varepsilon\}_{\varepsilon>0}$  with bounded energy might well take both positive and negative values. Hence, we define the limiting liquid drop functional for  $u \in BV(\mathbb{R}^3; \{0,\pm 1\})$  as

$$\mathscr{E}_0^V(u) := \frac{1}{8} \int_{\mathbb{R}^3} \|\nabla u\| - \int_{\mathbb{R}^3} V u^2 d\vec{x} + D(u^2, u^2). \tag{1.16}$$

The first term is the total variation of the measure  $\|\nabla u\|$ , and for  $u = \mathbb{1}_{\Omega}$  it measures the perimeter of  $\partial\Omega$ . If u takes both values  $\pm 1$ , then

$$\int_{\mathbb{R}^3} \|\nabla u\| = \int_{\mathbb{R}^3} \|\nabla u_+\| + \|\nabla u_-\|,$$

which measures the perimeter of  $\{\vec{x} \in \mathbb{R}^3 : u(\vec{x}) = 1\}$  and that of  $\{\vec{x} \in \mathbb{R}^3 : u(\vec{x}) = -1\}$ , whereas the other terms yield the same value for u and  $|u| = u^2$ .

For the second part of this thesis we make the following general hypotheses regarding the background potential V:

$$V \in \mathscr{L}^{\frac{5}{2}}(\mathbb{R}^3) + \mathscr{L}^{\infty}(\mathbb{R}^3) \text{ and } V(\overrightarrow{x}) \xrightarrow[\|\overrightarrow{x}\| \to \infty]{} 0.$$
 (1.17)

The hypothesis (1.17) is slightly stronger than is typical for problems of TFDW type, in which a weaker local integrability is assumed, V satisfying (1.2) (see e.g., [8, 46].) Having  $V \in \mathcal{L}_{loc}^{\frac{3}{2}}(\mathbb{R}^3)$  is a natural condition for using the squared gradient to control  $V|u|^2$  via the Sobolev embedding. However, given the singularly perturbed nature of  $\mathcal{E}^V_{\varepsilon}$ , control on the Dirichlet energy is lost as  $\varepsilon \to 0^+$ , and we must rely on the  $\mathcal{L}^{\frac{10}{3}}$  norm instead; hence the need for the more stringent  $\mathcal{L}^{\frac{5}{2}}(\mathbb{R}^3) + \mathcal{L}^{\infty}(\mathbb{R}^3)$  demanded in (1.17).

We define domains for the functionals which incorporate the mass constraint,

$$\begin{split} \mathscr{H}^M &:= \left\{ u \in \mathscr{H}^1(\mathbb{R}^3); \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M \right\}, \\ \mathscr{X}^M &:= \left\{ u \in BV(\mathbb{R}^3, \{0, \pm 1\}); \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M \right\}, \end{split}$$

and define the infima values

$$e^V_{\varepsilon}(M) := \inf \left\{ \mathscr{E}^V_{\varepsilon}(u) \, ; \, u \in \mathscr{H}^M \right\}, \qquad e^V_0(M) := \inf \left\{ \mathscr{E}^V_0(u) \, ; \, u \in \mathscr{X}^M \right\},$$

for the constrained TFDW and liquid drop problems. Given that the existence problem for both the TFDW type and the Liquid Drop models is very subtle (see the first chapter of this thesis and papers [11], [46], [2], [1], and [12],) the target space and  $\Gamma$ -limit incorporate the concentration structure of minimizing sequences for the Liquid Drop Model: while minimizing sequences for either TFDW or liquid drop may not converge, they

do concentrate at one or more mass centers, and if there is splitting of mass the separate pieces diverge away via translation. We define the energy "at infinity",  $\mathcal{E}_0^0(u)$ , taking potential  $V \equiv 0$ , with infimum value  $e_0^0(M)$ . From this we then define the appropriate  $\Gamma$ -limit as

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^{\infty}) := \begin{cases} \mathscr{E}_0^V(u^0) + \sum_{i=1}^{\infty} \mathscr{E}_0^0(u^i), & \{u^i\}_{i=0}^{\infty} \in \mathscr{H}_0^M, \\ \infty, & otherwise, \end{cases}$$

$$(1.18)$$

on the space of limiting configurations,

$$\mathscr{H}_0^M := \left\{ \{u^i\}_{i=0}^{\infty} \subset BV(\mathbb{R}^3, \{0, \pm 1\}); \ \sum_{i=0}^{\infty} \int_{\mathbb{R}^3} \|\nabla u^i\| < \infty, \ \sum_{i=0}^{\infty} \|u^i\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M \right\}.$$

Let us state our  $\Gamma$ -convergence result with respect to the notion of convergence given by (1.19)-(1.20). This result is proved in chapter 4.

**Theorem 7.**  $\mathscr{E}^V_{\varepsilon}$   $\Gamma$ -converges to  $\mathscr{F}^V_0$ , in the sense that:

(i) (Compactness and Lower-bound) For any sequence  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$ , if  $\{u_{\varepsilon_k}\}_{k \in \mathbb{N}} \subset \mathscr{H}^M$  and  $\sup_k \mathscr{E}^V_{\varepsilon_k}(u_{\varepsilon_k}) < \infty$ , then there exist a subsequence (still denoted  $\varepsilon_k$ ,) a collection  $\{u^i\}_{i=0}^{\infty} \in \mathscr{H}_0^M$ , and translations  $\{\vec{x}_k^i\}_{k \in \mathbb{N}} \subset \mathbb{R}^3$ , with  $\{\vec{x}_k^0\}_{k \in \mathbb{N}} = \{\vec{0}\}$ , so that

$$\left| u_{\varepsilon_k}(\cdot) - \sum_{i=0}^{\infty} u^i(\cdot - \vec{x}_k^i) \right| \xrightarrow[k \to \infty]{} 0 \text{ in } \mathcal{L}^2(\mathbb{R}^3), \tag{1.19}$$

$$\|\vec{x}_k^i - \vec{x}_k^j\| \xrightarrow[k]{} \infty, \quad i \neq j,$$
 (1.20)

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^{\infty}) \le \liminf_{k \to \infty} \mathscr{E}_{\varepsilon_k}^V(u_{\varepsilon_k}). \tag{1.21}$$

(ii) (Upper-bound) Given  $\{u^i\}_{i=0}^{\infty} \in \mathcal{H}_0^M$  and a sequence  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$ , there exist functions  $\{u_{\varepsilon_k}\}_{k \in \mathbb{N}} \subset \mathcal{H}_0^M$  and translations  $\{\vec{x}_k^i\}_{k \in \mathbb{N}} \subset \mathbb{R}^3$ , with  $\{\vec{x}_k^0\}_{k \in \mathbb{N}} = \{\vec{0}\}$ , such that equations (1.19) and (1.20) hold, and

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^\infty) \geq \limsup_{k \to \infty} \mathscr{E}_{\varepsilon}^V(u_{\varepsilon_k}).$$

The compactness and lower semicontinuity with respect to the notion of convergence given by (1.19)-(1.20) proved in (i) combine two different approaches in the calculus of variations. Local convergence of the singular limits uses BV bounds in the flavor of the Cahn-Hilliard problems, as studied in [44, 52]. There, authors consider a fluid under isothermal conditions and confined to a bounded container in  $\mathbb{R}^3$  whose Gibbs free energy, per unit volume, is a prescribed function W of the density distribution u. The classical problem of determining stable configurations of the fluid is to minimize the total energy of the fluid. To recover the physically reasonable criterion that the interface has minimal area, the gradient term is added with a coefficient  $\varepsilon^2$  that vanishes.

On the other hand, the lack of global compactness imposes a concentration-compactness structure [36, 37, 21, 2], in order to recover all of the mass escaping to infinity. This form of the  $\Gamma$ -limit, as a sum of disassociated variational problems splitting on different scales is common in droplet breakup for di-block copolymers; see [11, 4].

For the recovery sequence and upper bound (ii), the presence of an infinite number of  $\{u^i\}_{i=0}^{\infty}$  presents some obstacles not normally seen in Cahn-Hilliard-type problems, where the setting is usually a bounded domain or a flat torus. Indeed, for (ii) of Theorem 7 we must consider  $\{u^i\}_{i=0}^{\infty}$  with infinitely many nontrivial components, and then it is only possible at any fixed  $\varepsilon > 0$  to construct a trial function approximating  $u^i$  when the scale of its support is large compared to  $\varepsilon$ .

There are various implications of Theorem 7 to minimization problems in various settings on minimizers of TFDW type and of the liquid drop problem. We note that  $\mathscr{E}^V_{\varepsilon}(|u|) = \mathscr{E}^V_{\varepsilon}(u)$ ,  $\mathscr{E}^V_0(|u|) = \mathscr{E}^V_0(u)$ , and so we restrict to the cone of nonnegative functions  $\mathscr{H}^M_+$ ,  $\mathscr{X}^M_+$ ,  $\mathscr{H}^M_{0,+}$  as the domain for each.

We think of a  $\Gamma$ -limit as a framework in which minimizers of the  $\varepsilon$  functionals should converge to minimizers of the limiting energy (see, e.g., [30],) but given the complexity of the question of the existence of minimizers for each model, this is a subtle point. The notion of *generalized minimizers*, introduced for the case  $V \equiv 0$  in [29, Definition 4.3], provides a useful means of discussing the structure of minimizing sequences which may lose compactness:

**Definition 1.** Suppose that V satisfies (1.17) and M > 0. A <u>generalized minimizer</u> of  $\mathcal{E}_0^V(M)$  is a finite collection  $\{u^0, u^1, \dots, u^N\}$ ,  $u^i \in BV(\mathbb{R}^3, \{0, 1\})$ , such that:

1. 
$$||u^i||_{\mathcal{L}^2(\mathbb{R}^3)}^2 := m^i$$
,  $i = 0, 1, ..., N$ , with  $\sum_{i=0}^N m^i = M$ ;

2.  $u^0$  attains the minimum  $e_0^V(m^0)$  and  $u^i$  attains  $e_0^0(m^i)$ , i = 1, ..., N;

3. 
$$e_0^V(M) = e_0^V(m^0) + \sum_{i=1}^N e_0^0(m^i)$$
.

Alama *et al.* showed in [2] that we may associate a generalized minimizer as above to *any* minimizing sequence for the Liquid Drop Model with (or without) potential V. In this way, up to translation ferrying the components  $u^i$  to infinity, the collection of all generalized minimizers of  $\mathcal{E}_0^V$  with constrained mass M completely characterizes the minimizing sequences of  $\mathcal{E}_0^V$ .

We naturally associate to a generalized minimizer  $\{u^0,u^1,\dots,u^N\}$  an element  $\{u^i\}_{i=0}^\infty$  of  $\mathscr{H}_0^M$  by taking  $u^i=0$  for all  $i\geq N+1$ , and then we have  $\mathscr{F}_0^V(\{u^i\}_{i=0}^\infty)=e_0^V(M)$ . In what follows, when convenient, we abuse notation and set  $\mathscr{F}_0^V(\{u^i\}_{i=0}^N)$  to be the value of the limiting energy for a generalized minimizer. We may thus address the convergence of minimizers of  $\mathscr{E}_{\varepsilon}^V$  (should they exist) in terms of generalized minimizers of  $\mathscr{E}_0^V$ , using Theorem 7:

**Theorem 8.** Let M > 0 and assume that there exists  $\varepsilon_n \xrightarrow[n \to \infty]{} 0^+$  for which  $e_{\varepsilon_n}^V(M)$  is attained at  $u_n \in \mathcal{H}_+^M$  for each  $n \in \mathbb{N}$ . Then, there exists a subsequence (not relabeled) and a generalized minimizer  $\{u^0, \dots, u^N\}$  of

 $\mathcal{E}_0^V$  for which (1.19) and (1.20) hold for i = 0, ..., N, and

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^N) = e_0^V(M) = \lim_{n \to \infty} e_{\varepsilon_n}^V(M).$$

A slightly more general version of Theorem 8 is proved in Lemma 17, and both results can be found in chapter 5.

As mentioned before, there is a special class of potentials V for which the existence problem  $\inf \mathscr{E}^V_{\mathcal{E}}$  is completely understood for each  $\mathcal{E}$ ; namely, long-range V. We proved that the global minimum is attained for any M>0 for TFDW type models in Theorem 3, and the same is true for liquid drop functionals [3]. For this class of problem, we prove global convergence of minimizers in  $\mathscr{L}^2(\mathbb{R}^3)$  in chapter 5:

**Corollary 1.** Assume that V satisfies (1.17) and (1.7), and for M > 0 and  $\varepsilon > 0$ , let  $u_{\varepsilon} \in \mathcal{H}_{+}^{M}$  be a minimizer of  $e_{\varepsilon}^{V}(M)$ . Then, for any sequence  $\varepsilon_{n} \xrightarrow[n \to \infty]{} 0^{+}$  there exists a subsequence (not relabeled) and a minimizer  $u^{0} \in \mathcal{X}_{+}^{M}$  of  $e_{0}^{V}(M)$  with  $u_{\varepsilon_{n}} \xrightarrow[n \to \infty]{} u^{0}$  in  $\mathcal{L}^{2}(\mathbb{R}^{3})$ .

Atomic or molecular potentials V are the most important examples for TFDW as they are related to the Ionization Conjecture [37, 31, 23, 40, 46]. We consider the atomic case,

$$V(\overrightarrow{x}) = V_Z(\overrightarrow{x}) = \frac{Z}{\|\overrightarrow{x}\|},$$

with  $Z \ge 0$  representing a constant nuclear charge in the case  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$ . With slight abuse of notation, we denote by  $\mathscr{E}^Z_{\varepsilon}$ ,  $\mathscr{E}^Z_0$  the energies (1.15) and (1.16), respectively, with the atomic choice  $V = V_Z = Z/\|\vec{x}\|$ , and

$$e^Z_{\varepsilon}(M) \colon= \inf \left\{ \mathscr{E}^Z_{\varepsilon}(u) \, \colon u \in \mathscr{H}^M_+ \right\}, \quad e^Z_0(M) \colon= \inf \left\{ \mathscr{E}_0(u) \, \colon u \in \mathscr{X}^M_+ \right\}.$$

For this choice of potential in the liquid drop setting, Lu and Otto [40] proved that there exists  $\mu_0 > 0$  for which the ball  $\mathbb{B}_M = B_{r_M}(\vec{0})$ ,  $r_M = \sqrt[3]{\frac{3M}{4\pi}}$ , centered at the origin of volume M is the unique (up to translations for Z = 0), strict minimizer of  $e_0^Z(M)$  for all  $0 < M < Z + \mu_0$ . The corresponding existence result for TFDW is much weaker, as stated in Theorem 1. A natural conjecture is that the intervals of existence converge, that is,  $\mu_{\varepsilon} \xrightarrow{\rho_0 + \rho_1} \mu_0$ . Using Theorem 7, we can prove the following in chapter 5:

**Theorem 9.** Let  $V(\vec{x}) = \frac{Z}{\|\vec{x}\|}$  and Z > 0.

- (a) For any  $M \in (0, Z + \mu_{\varepsilon})$ ,  $e_{\varepsilon}^{Z}(M)$  is attained at  $u_{\varepsilon} \in \mathscr{H}_{+}^{M}$  for each  $\varepsilon > 0$ , and  $u_{\varepsilon} \xrightarrow[\varepsilon \to 0^{+}]{} \mathbb{1}_{\mathbb{B}_{M}}$  in  $\mathscr{L}^{2}(\mathbb{R}^{3})$ .
- (b) For all  $M \in (Z, Z + \mu_0)$  and  $\varepsilon > 0$ ,  $\exists M_{\varepsilon} \leq M$  with  $M_{\varepsilon} \xrightarrow[\varepsilon \to 0^+]{} M$  such that  $e_{\varepsilon}^{Z}(M_{\varepsilon})$  attains a minimizer  $u_{\varepsilon} \in \mathscr{H}_{+}^{M_{\varepsilon}}$ . Moreover,  $u_{\varepsilon} \xrightarrow[\varepsilon \to 0^+]{} \mathbb{1}_{\mathbb{B}_{M}}$  in  $\mathscr{L}^{2}(\mathbb{R}^{3})$ .

Theorem 9 is related to the classical Kohn-Sternberg [30] result on the existence of local minimizers of the  $\varepsilon$ -problem in an  $\mathscr{L}^2$ -neighborhood of an isolated local minimizer of the  $\Gamma$ -limit. We find minimizers for  $\mathscr{E}^Z_{\varepsilon}$  which converge to the ball of mass M as  $\varepsilon \to 0^+$  in  $\mathscr{L}^2(\mathbb{R}^3)$ , which would have the given mass M except for the possibility of vanishingly small pieces splitting off and diverging to infinity as  $\varepsilon \to 0^+$ . If we could

find a uniform (in  $\varepsilon > 0$ ) lower bound on the quantity of diverging mass in the case of splitting, then we would be able to eliminate this possibility completely and assert that  $M_{\varepsilon} = M$  in (b), as conjectured above.

My studies have left a wealth of questions unanswered that have motivated me to consider continuations of my work in multiple directions, including exploring collective behaviour and nonlocal PDEs further.

I would like to investigate local minimizers or nonminimizing critical points of TFDW type models further by using the Lyapunov-Schmidt reduction method. Naturally, knowing more about spectral properties of TFDW type equations would be very important, and this falls into the areas of spectral properties of Schrödinger equations and nonlocal equations. HF, TFW, and some of TFDW equations have been studied by Lions [37] by using min-max critical point theory, fixed point theory, and critical point theory and index bounds. On the other hand, the Lyapunov-Schmidt reduction has been used to study local minimizers and nonminimizing critical points for sharp interface energies of Ohta-Kawasaki models in works like the ones by Cristoferi [15], and Ren and Wei [50]. Functions we may start studying as candidates for critical points of the atomic TFDW model relate to the atomic TFDW functional restricted to radial functions. Indeed, we can show that the radial atomic TFDW problem always has minimizers; Lieb [33] showed that minimizers for the atomic TFDW are radial if  $M \le Z$ , and Nam and Van Den Bosch [46] proved that such minimizers are not radially symmetric if M is sufficiently large.

It is possible to extend my studies to models with similar structure. Examples of such models come not only from considering V and W more general, but also the repulsive term is not necessarily Coulombic, nor the model 3D. Super-Coulombic interactions between closely spaced atoms and molecules, like  $1/|x-y|^3$ , have been observed in 2D hyperbolic media [7, 14]; that is, highly anisotropic media with hyperbolic dispersion. Extensions to more general nonlocal terms have been recently explored for the Liquid Drop Model with background potential by Alama et al. [2], and for Riesz-type problems generalizing the Liquid Drop model by Novaga and Pratelli [47]. On the other hand, models with coercive background potentials; i.e., potentials that do not decay but grow at infinity, are likely to lead to new patterns, as well. One such problem was recently studied by Générau and Oudet [25] in the context of the Liquid Drop Model, where they proved that there exists a minimizer for all masses such that for certain interactions, as the mass blows up, minimizers eventually coalesce into a large ball, and that balls centered at the origin are the only minimizers for large M, again, for certain interactions. Even though the Liquid Drop Model with background potential and the TFDW model are close to one another, analyses for the latter may differ due to the fact that minimizers are not necessarily compactly supported. Therefore, some information about the spatial decay of minimizers may be required, which leads to questions on properties of solutions of the PDE associated with the problem and related spectral problems. Among other directions that could be explored there are TF type functionals. An example of such functionals, more precisely the TFDW energy for graphene at the neutrality point, was recently studied by Lu et al. [38].

There are many interesting questions about the structure of minimizing sequences for TFDW type models that remain open. For instance, one of the questions concerns the existence of minimizing sequences that

undergo splitting and end up with a prescribed structure. Also, it is unclear how components into which minimizing sequences may break decay. In regard to the first issue, we can generate minimizing sequences by minimizing perturbations that "regularize" the problem. Since those minimizers are eigenfunctions of PDEs that differ by little, it is natural to try to generate combinations of eigenfunctions of such equations in a way that the prescribed structure is imposed. However, complications arise very quickly due to the complexity of the PDE; namely, such equation is nonlinear and nonlocal, and its spectral properties are not fully understood. As for the second issue, components decay exponentially if, for instance, zero is not a Lagrange Multiplier of the equations associated with the system; this seems to be a difficult spectral problem. Another question is how different "regularizations" via potentials that decay slow enough may impact the structure of minimizers as there are multiple ways to introduce these perturbations.

Lastly, there are long-standing questions in the TFDW theory, for instance the nonexistence of highly negative molecules, and a better understanding of qualitative properties of minimizers. In regard to qualitative properties, works on Choquard equations by Ma and Zhao [42], and Moroz and Schaftingen [43] may be relevant for further explorations in the PDE direction, while works on a quantitative Pólya-Szegö principle by Cianchi *et al.* [13], and spherical flocking by Frank and Lieb [22] may be relevant for further exploration in the direction of the Calculus of Variations.

**Note:** C denotes a generic constant hereafter; C might vary from one line to the other.

## **Chapter 2**

## **Energy estimates**

In this chapter we establish some basic estimates, which give relations between the various terms in the TFDW energy, both for arbitrary functions in  $\mathcal{H}^1(\mathbb{R}^3)$  and for minimizers. We treat various cases of p > q, including the physically relevant  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$ . The study of (1.1) with q > p instead of p > q differs greatly.

Throughout this chapter, we assume V satisfies (1.2).

#### 2.1 On nonlinearity

By considering powers 6 > p > q > 2 we cover the original TFDW model. The choices  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$  are particularly convenient because of the origins of  $\mathscr{I}_{V_{TFDW}}^{10}$ , in Physics, and because we know more about  $\mathscr{I}_0^{10}$ ,  $\frac{8}{3}$  than we do about  $\mathscr{I}_0^{p,q}$  with p and q more general (see Proposition 7.) By understanding the energy "at infinity" better, we are then able to carry out a more detailed analysis of the structure of minimizing sequences for  $\mathscr{I}_V^{10}$ ,  $\frac{8}{3}$  (see Theorems 4-6.)

On the other hand, considering p < q leads to very different analyses. More precisely, in such case it is possible to have either  $\mathscr{I}_V^{p,q} \equiv -\infty$  or  $\mathscr{I}_0^{p,q}(M) = 0$  (see Proposition right below.) If the latter occurs, then the concentration-compactness structure of minimizing sequences might be simpler (see [37, Corollary II.1].)

**Proposition 2.** *Suppose that* 2 .*The following hold:* 

- (i) If  $q > \frac{10}{3}$ , then  $\mathscr{I}_V^{p,q}(M) = -\infty$  for all M > 0.
- (ii) If  $q \leq \frac{10}{3}$ , then for M sufficiently small, both  $\mathcal{I}_0^{p,q}(M) = 0$  and  $\mathcal{I}_0^{p,q}(M)$  is not attained.

*Proof.* In order to prove (i), we note that the transformation

$$u \in \mathcal{L}^2(\mathbb{R}^3) \to u_{\sigma}(\vec{x}) := \sigma^{3/2} u(\sigma \vec{x}), \sigma > 0,$$
 (2.1)

keeps the  $\mathcal{L}^2$  norm invariant, and for  $u \in \mathcal{H}^1(\mathbb{R}^3)$ ,

$$\int_{\mathbb{R}^3} \|\nabla u_{\sigma}\|^2 d\vec{x} = \int_{\mathbb{R}^3} \|\nabla(\sigma^{3/2} u(\sigma \vec{x}))\|^2 d\vec{x} = \int_{\mathbb{R}^3} \|\sigma^{5/2} (\nabla u)(\sigma \vec{x})\|^2 d\vec{x} = \sigma^2 \int_{\mathbb{R}^3} \|\nabla u\|^2 d\vec{x},$$

$$\int_{\mathbb{R}^3} |u_{\sigma}|^r d\overrightarrow{x} = \int_{\mathbb{R}^3} |\sigma^{3/2} u(\sigma \overrightarrow{x})|^r d\overrightarrow{x} = \sigma^{3r/2-3} \int_{\mathbb{R}^3} |u|^r d\overrightarrow{x}, \quad r \ge 1,$$

and

$$D(u_{\sigma}^2, u_{\sigma}^2) = \sigma \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{[\sigma^{3/2} u(\sigma \vec{x})]^2 [\sigma^{3/2} u(\sigma \vec{y})]^2}{\|\sigma \vec{x} - \sigma \vec{y}\|} d\vec{x} d\vec{y} = \sigma D(u^2, u^2).$$

Consequently,

$$\begin{split} \mathscr{E}_{V}^{p,q}(u_{\sigma}) &< \mathscr{E}_{0}^{p,q}(u_{\sigma}) \\ &= \int_{\mathbb{R}^{3}} (c_{W}\sigma^{2} \|\nabla u\|^{2} + c_{TF}\sigma^{3p/2-3} |u|^{p} - c_{D}\sigma^{3q/2-3} |u|^{q}) d\overrightarrow{x} + \frac{1}{2} D(u^{2}, u^{2}) \xrightarrow[\sigma \to \infty]{} -\infty. \end{split}$$

As for statement (ii),  $\mathscr{I}_0^{p,q} \leq 0$  follows from applying the transformation (2.1) and taking  $\sigma \to 0^+$ . Moreover, if we also have  $c_W = c_{TF} = c_D = 1$ , then Hölder's inequality and Sobolev's inequality give

$$\int_{\{\vec{x}\in\mathbb{R}^3:|u(\vec{x})|\geq 1\}} |u|^q d\vec{x} \leq \int_{\{\vec{x}\in\mathbb{R}^3:|u(\vec{x})|\geq 1\}} |u|^{\frac{10}{3}} d\vec{x} 
\leq \left(\int_{\{\vec{x}\in\mathbb{R}^3:|u(\vec{x})|\geq 1\}} u^2 d\vec{x}\right)^{\frac{2}{3}} \left(\int_{\{\vec{x}\in\mathbb{R}^3:|u(\vec{x})|\geq 1\}} u^6 d\vec{x}\right)^{\frac{1}{3}} 
\leq \left(\int_{\mathbb{R}^3} u^2 d\vec{x}\right)^{\frac{2}{3}} \left(\int_{\mathbb{R}^3} u^6 d\vec{x}\right)^{\frac{1}{3}} \leq \frac{1}{3} \left(\frac{2}{\pi}\right)^{\frac{4}{3}} \left(\int_{\mathbb{R}^3} u^2 d\vec{x}\right)^{\frac{2}{3}} \int_{\mathbb{R}^3} ||\nabla u||^2 d\vec{x}.$$

As a result, for u in the domain of  $\mathcal{E}_0^{p,q}$  and M sufficiently small, we have

$$\begin{split} \mathscr{E}_{0}^{p,q}(u) &\geq \int_{\mathbb{R}^{3}} \|\nabla u\|^{2} d\vec{x} + \int_{\mathbb{R}^{3}} (|u|^{p} - |u|^{q}) d\vec{x} \\ &= \int_{\mathbb{R}^{3}} \|\nabla u\|^{2} d\vec{x} + \int_{\{|u| \geq 1\}} (|u|^{p} - |u|^{q}) d\vec{x} + \int_{\{|u| < 1\}} (|u|^{p} - |u|^{q}) d\vec{x} \\ &\geq \int_{\mathbb{R}^{3}} \|\nabla u\|^{2} d\vec{x} + \int_{\{|u| \geq 1\}} (|u|^{p} - |u|^{q}) d\vec{x} \geq \left[1 - \frac{1}{3} \left(\frac{2}{\pi}\right)^{\frac{4}{3}} M^{\frac{2}{3}}\right] \int_{\mathbb{R}^{3}} \|\nabla u\|^{2} d\vec{x} > 0, \end{split}$$

Then,  $\mathscr{I}_0^{p,q}(M) = 0$ , and the infimum cannot be attained. The proof we just gave does not change significantly if  $c_W, c_{TF}$ , and  $c_D$  are more general.

#### 2.2 Some bounds for terms in $\mathcal{E}_V^{p,q}$ and coercivity

We use the following results to prove that  $\mathcal{E}_V^{p,q}$  is coercive.

We begin by estimating the nonlinear terms.

**Lemma 1.** Given  $\varepsilon > 0$  and  $1 \le r < q < p < \infty$ ,

$$\int_{\mathbb{R}^3} |u|^q d\overrightarrow{x} \le \varepsilon \int_{\mathbb{R}^3} |u|^p d\overrightarrow{x} + \frac{p-q}{p-r} \left[ \frac{q-r}{\varepsilon(p-r)} \right]^{\frac{q-r}{p-q}} \int_{\mathbb{R}^3} |u|^r d\overrightarrow{x}, \quad u \in \mathcal{L}^q(\mathbb{R}^3). \tag{2.2}$$

In particular,

$$\int_{\mathbb{R}^3} |u|^{\frac{8}{3}} d\vec{x} \leq \varepsilon \int_{\mathbb{R}^3} |u|^{\frac{10}{3}} d\vec{x} + \frac{1}{4\varepsilon} \int_{\mathbb{R}^3} u^2 d\vec{x}, \quad \varepsilon > 0, u \in \mathscr{L}^{\frac{8}{3}}(\mathbb{R}^3).$$

*Proof.* By the interpolation inequality in Lebesgue spaces,

$$\int_{\mathbb{R}^3} |u|^q d\vec{x} \le \left( \int_{\mathbb{R}^3} |u|^r d\vec{x} \right)^{\frac{1}{p}q\theta} \left( \int_{\mathbb{R}^3} |u|^p d\vec{x} \right)^{\frac{1}{p}q(1-\theta)},\tag{2.3}$$

where

$$\frac{1}{q} = \frac{1}{r}\theta + \frac{1}{p}(1-\theta),$$

or, equivalently,

$$\theta = \frac{r(p-q)}{q(p-r)},$$

implying

$$\frac{1}{r}q\theta = \frac{p-q}{p-r}, \quad \frac{q}{p}(1-\theta) = \frac{q}{p}\frac{q(p-r)-r(p-q)}{q(p-r)} = \frac{q-r}{p-r} < 1.$$

Therefore, (2.3) reads

$$\int_{\mathbb{R}^3} |u|^q d\vec{x} \leq \left( \int_{\mathbb{R}^3} |u|^r d\vec{x} \right)^{\frac{p-q}{p-r}} \left( \int_{\mathbb{R}^3} |u|^p d\vec{x} \right)^{\frac{q-r}{p-r}}.$$

and Young's inequality applies to ensure

$$\int_{\mathbb{R}^{3}} |u|^{q} d\vec{x} \leq \frac{p-q}{p-r} \left[ \frac{q-r}{\varepsilon(p-r)} \right]^{\frac{q-r}{p-q}} \left( \int_{\mathbb{R}^{3}} |u|^{r} d\vec{x} \right)^{\frac{p-q}{p-r} \left(\frac{p-r}{q-r}\right)'} + \varepsilon \int_{\mathbb{R}^{3}} |u|^{p} d\vec{x} 
= \frac{p-q}{p-r} \left[ \frac{q-r}{\varepsilon(p-r)} \right]^{\frac{q-r}{p-q}} \int_{\mathbb{R}^{3}} |u|^{r} d\vec{x} + \varepsilon \int_{\mathbb{R}^{3}} |u|^{p} d\vec{x}.$$

Next, we consider bounds on the external potential.

**Lemma 2.** Given  $\varepsilon > 0$ ,

$$\int_{\mathbb{R}^3} V u^2 d\vec{x} \le \varepsilon \int_{\mathbb{R}^3} \|\nabla u\|^2 d\vec{x} + C_{\varepsilon} \int_{\mathbb{R}^3} u^2 d\vec{x}, \quad u \in \mathscr{H}^1(\mathbb{R}^3), \tag{2.4}$$

where  $C_{\varepsilon} \xrightarrow[\varepsilon \to 0^+]{} \infty$ .

Moreover, in the case  $V = V_V$  as in (1.5), we can take

$$C_{\varepsilon} := \frac{1}{3} \left(\frac{2}{\pi}\right)^{\frac{4}{3}} \left(\frac{4\pi}{6-3\nu}\right)^{\frac{2}{3}} \left(\frac{\max_{k=1,\dots,K} \alpha_k}{\varepsilon}\right)^{\frac{2-\nu}{\nu}} Z.$$

Finally, in the case  $V = V_v$  with v taking certain values we can tell more:

$$\int_{\mathbb{D}^3} V_{\nu} u^2 d\vec{x} \leq \varepsilon \|\nabla u\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 + C\sqrt{D(u,u)}, \quad \varepsilon > 0, u \in \mathscr{H}^1(\mathbb{R}^3), 2^{-1} < \nu < 2.$$

*Proof.* We follow techniques from [34, section 11.3].

Let us rewrite  $V = V_{3/2} + V_{\infty}$  where  $V_{3/2} \in \mathcal{L}^{\frac{3}{2}}(\mathbb{R}^3)$  and  $V_{\infty} \in \mathcal{L}^{\infty}(\mathbb{R}^3)$ . Since

$$\begin{split} \mathcal{L}(\{\vec{x} \in \mathbb{R}^3 : |f(\vec{x})| > t\}) &\leq t^{-\frac{3}{2}} \|f\|_{\mathcal{L}^{\frac{3}{2}}(\{\vec{x} \in \mathbb{R}^3 : |f(\vec{x})| > t\})}^{\frac{3}{2}} \\ &\leq t^{-\frac{3}{2}} \|f\|_{\mathcal{L}^{\frac{3}{2}}(\mathbb{R}^3)}^{\frac{3}{2}}, \quad f \in \mathcal{L}^{\frac{3}{2}}(\mathbb{R}^3), t > 0, \end{split}$$

we have that

$$\mathscr{L}(\{\vec{x} \in \mathbb{R}^3 : |V_{3/2}(\vec{x})| > t\}) = o\left(t^{-\frac{3}{2}}\right) \text{ as } t \to \infty.$$

As a result,

$$\|[V_{3/2} - t(\varepsilon)]_+\|_{\mathscr{L}^{\frac{3}{2}}(\mathbb{R}^3)} = \|V_{3/2} - t(\varepsilon)\|_{\mathscr{L}^{\frac{3}{2}}(\{\vec{x} \in \mathbb{R}^3: V_{3/2}(\vec{x}) > t(\varepsilon)\})} < 3\left(\frac{\pi}{2}\right)^{\frac{4}{3}}\varepsilon$$

for some  $t(\varepsilon) > 0$ . Therefore, by Hölder's inequality and Sobolev's inequality,

$$\int_{\mathbb{R}^{3}} Vu^{2} d\vec{x} = \int_{\mathbb{R}^{3}} [V_{3/2} - t(\varepsilon)] u^{2} d\vec{x} + t(\varepsilon) \int_{\mathbb{R}^{3}} u^{2} d\vec{x} + \int_{\mathbb{R}^{3}} V_{\infty} u^{2} d\vec{x} 
\leq \int_{\mathbb{R}^{3}} [V_{3/2} - t(\varepsilon)]_{+} u^{2} d\vec{x} + t(\varepsilon) \int_{\mathbb{R}^{3}} u^{2} d\vec{x} + \int_{\mathbb{R}^{3}} V_{\infty} u^{2} d\vec{x} 
\leq \|(V_{3/2} - t(\varepsilon))_{+}\|_{\mathscr{L}^{\frac{3}{2}}(\mathbb{R}^{3})} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + C\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} 
\leq \varepsilon \|\nabla u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} + C\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}.$$
(2.5)

Next suppose  $V = V_v$  for 0 < v < 2. Then, by Hölder's inequality and Sobolev's inequality,

$$\int_{\mathbb{R}^3} Vu^2 d\vec{x} = \left( \int_{\cup B_{\delta}(\vec{r}_j)} + \int_{\mathbb{R}^3 \setminus \cup B_{\delta}(\vec{r}_j)} \right) Vu^2 d\vec{x}$$

$$\begin{split} &\leq \|V\|_{\mathscr{L}^{\frac{3}{2}}(\cup B_{\delta}(\overrightarrow{r}_{j}))} \|u\|_{\mathscr{L}^{6}(\cup B_{\delta}(\overrightarrow{r}_{j}))}^{2} + \|V\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3}\setminus \cup B_{\delta}(\overrightarrow{r}_{j}))} \|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3}\setminus \cup B_{\delta}(\overrightarrow{r}_{j}))}^{2} \\ &= \left(\frac{2\pi}{3-\frac{3}{2}\nu}\delta^{3-\frac{3}{2}\nu}\right)^{\frac{2}{3}} Z\|u\|_{\mathscr{L}^{6}(\cup B_{\delta}(\overrightarrow{r}_{j}))}^{2} + \max_{k=1,\dots,K}\alpha_{k}\delta^{-\nu}\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3}\setminus \cup B_{\delta}(\overrightarrow{r}_{j}))}^{2} \\ &= \left(\frac{4\pi}{6-3\nu}\right)^{\frac{2}{3}} \delta^{2-\nu}Z\|u\|_{\mathscr{L}^{6}(\cup B_{\delta}(\overrightarrow{r}_{j}))}^{2} + \max_{k=1,\dots,K}\alpha_{k}\delta^{-\nu}\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3}\setminus \cup B_{\delta}(\overrightarrow{r}_{j}))}^{2} \\ &\leq \left(\frac{4\pi}{6-3\nu}\right)^{\frac{2}{3}} \delta^{2-\nu}Z\|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \max_{k=1,\dots,K}\alpha_{k}\delta^{-\nu}\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} \\ &\leq \frac{1}{3}\left(\frac{2}{\pi}\right)^{\frac{4}{3}} \left(\frac{4\pi}{6-3\nu}\right)^{\frac{2}{3}} \delta^{2-\nu}Z\|\nabla u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} + \max_{k=1,\dots,K}\alpha_{k}\delta^{-\nu}\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}, \quad \delta > 0. \end{split}$$

Equation (2.4) is established by choosing  $\delta$  appropriately.

Next, given  $\delta>0$  to be fixed, pick any smooth  $\eta:\mathbb{R}^3\to[0,1]$  for which

$$\mathbb{1}_{B_{\delta}(\overrightarrow{0})} \eta \equiv 1, \quad \mathbb{1}_{\mathbb{R}^3 \setminus B_{2\delta}(\overrightarrow{0})} \eta \equiv 0,$$

and let

$$V_1(\vec{x}) := ||\vec{x}||^{-\nu} \eta(\vec{x}) \text{ and } V_2(\vec{x}) = ||\vec{x}||^{-\nu} [1 - \eta(\vec{x})].$$

Then, by definition of  $\eta$  and since  $3 - \frac{3}{2}v > 0$ ,

$$\mathbb{1}_{\mathbb{R}^3\setminus B_{2\delta}(\overrightarrow{0})}V_1\equiv 0,\quad V_1\in \mathscr{L}^{\frac{3}{2}}(\mathbb{R}^3),$$

and

$$\mathbb{1}_{B_{S}(\vec{0})}V_{2} \equiv 0, \quad V_{2} \in \mathcal{W}^{2,r}(\mathbb{R}^{3}), r \gg 1, \quad and \quad -\Delta V_{2} \in \mathcal{L}^{\frac{6}{5}}(\mathbb{R}^{3}),$$

the latter coming from  $3 - \frac{6}{5}(v+2) < 0$ . Also, from

$$-\Delta \left(u^2 \star \|\overrightarrow{x}\|^{-1}\right) = 4\pi u^2,$$

and by Sobolev's inequality, we have

$$\left|\left|u^{2}\star\right|\|\cdot\|^{-1}\right|\right|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2}\leq\frac{1}{3}\left(\frac{2}{\pi}\right)^{\frac{4}{3}}\left|\left|\nabla\left(u^{2}\star\|\cdot\|^{-1}\right)\right|\right|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}=\frac{4\pi}{3}\left(\frac{2}{\pi}\right)^{\frac{4}{3}}D(u^{2},u^{2}).$$

Consequently, by Hölder's inequality and Sobolev's inequality,

$$\int_{\mathbb{R}^{3}} \frac{u^{2}(\vec{x})}{\|\vec{x}\|^{v}} d\vec{x} = \int_{\mathbb{R}^{3}} V_{1} u^{2} d\vec{x} + \int_{\mathbb{R}^{3}} V_{2} u^{2} d\vec{x} 
\leq \|V_{1}\|_{\mathscr{L}^{\frac{3}{2}}(\mathbb{R}^{3})} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \int_{\mathbb{R}^{3}} V_{2} u^{2} d\vec{x}$$

$$\begin{split} &= \|V_{1}\|_{\mathscr{L}^{\frac{3}{2}}(\mathbb{R}^{3})} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \frac{1}{4\pi} \int_{\mathbb{R}^{3}} V_{2} \left[ -\Delta \left( u^{2} \star \| \cdot \|^{-1} \right) \right] d\vec{x} \\ &= \left\| \frac{\eta(\cdot)}{\| \cdot \|^{\nu}} \right\|_{\mathscr{L}^{\frac{3}{2}}(\mathbb{R}^{3})} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \frac{1}{4\pi} \int_{\mathbb{R}^{3}} (-\Delta V_{2})(\vec{x}) \left( u^{2} \star \| \cdot \|^{-1} \right) (\vec{x}) d\vec{x} \\ &\leq \left\| \| \cdot \|^{-\nu} \right\|_{\mathscr{L}^{\frac{3}{2}}(B_{2\delta}(\vec{0}))} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \frac{1}{4\pi} \| -\Delta V_{2} \|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \|u^{2} \star \| \cdot \|^{-1} \|_{\mathscr{L}^{6}(\mathbb{R}^{3})} \\ &= \left[ \frac{4\pi}{3 - \frac{3}{2}\nu} (2\delta)^{3 - \frac{3}{2}\nu} \right]^{\frac{2}{3}} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \frac{1}{4\pi} \| -\Delta V_{2} \|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \|u^{2} \star \| \cdot \|^{-1} \|_{\mathscr{L}^{6}(\mathbb{R}^{3})} \\ &= \left( \frac{8\pi}{6 - 3\nu} \right)^{\frac{2}{3}} (2\delta)^{2 - \nu} \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \frac{1}{4\pi} \| -\Delta V_{2} \|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \|u^{2} \star \| \cdot \|^{-1} \|_{\mathscr{L}^{6}(\mathbb{R}^{3})} \\ &\leq \frac{1}{3} \left( \frac{2}{\pi} \right)^{\frac{4}{3}} \left( \frac{8\pi}{6 - 3\nu} \right)^{\frac{2}{3}} (2\delta)^{2 - \nu} \|\nabla u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} \\ &+ \frac{1}{4\pi} \sqrt{\frac{1}{3} \left( \frac{2}{\pi} \right)^{\frac{4}{3}}} \| -\Delta V_{2} \|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \|\nabla \left( u^{2} \star \| \cdot \|^{-1} \right) \|_{\mathscr{L}^{2}(\mathbb{R}^{3})} \\ &= \frac{1}{3} \left( \frac{2}{\pi} \right)^{\frac{4}{3}} \left( \frac{8\pi}{6 - 3\nu} \right)^{\frac{2}{3}} (2\delta)^{2 - \nu} \|\nabla u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} \\ &+ \frac{1}{4\pi} \sqrt{\frac{8\pi}{3} \left( \frac{2}{\pi} \right)^{\frac{4}{3}}} \left\| -\Delta \left[ \frac{1 - \eta(\cdot)}{\| \cdot \|^{\nu}} \right] \right\|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \sqrt{D(u^{2}, u^{2})}. \end{split}$$

Now we can prove coercivity of the TFDW energy, which is essential for proving compactness of minimizing sequences.

**Proposition 3.** (Coercivity) For each  $u \in \mathcal{H}^1(\mathbb{R}^3)$ , we have

$$\mathscr{E}_{V}^{p,q}(u) + C \int_{\mathbb{R}^{3}} u^{2} d\vec{x} \ge \frac{1}{2} \int_{\mathbb{R}^{3}} (c_{W} \|\nabla u\|^{2} + c_{TF} |u|^{p}) d\vec{x} + \frac{1}{2} D(u^{2}, u^{2}). \tag{2.6}$$

*Proof.* This is an immediate consequence of equations (2.2) and (2.4) both with  $\varepsilon = \frac{1}{2}$ .

We make use of the following Proposition throughout the thesis:

**Proposition 4.** Let  $u \in \mathcal{H}^1(\mathbb{R}^3)$  with  $||u||^2_{\mathcal{L}^2(\mathbb{R}^3)} = M$  and  $\mathscr{E}^{p,q}_V(u) \leq 0$ . Then,

$$||u||_{\mathscr{H}^{1}(\mathbb{R}^{3})}^{2} + D(u^{2}, u^{2}) + \int_{\mathbb{R}^{3}} Vu^{2} d\overrightarrow{x} \leq CM.$$

*Proof.* This is an immediate consequence of Proposition 3 and (2.5).

**Remark 2.** We note that boundedness of a sequence in  $\mathcal{H}^1(\mathbb{R}^3)$  implies boundedness of the same sequence in  $\mathcal{L}^r(\mathbb{R}^3)$  for  $2 \le r \le 6$ .

Next, we study the nonlocal relation. We use the following result to prove that  $\mathcal{I}_0^{\frac{10}{3},\frac{8}{3}}(M)$  is strictly concave down for M sufficiently small (see part (vi) of Proposition 7).

**Lemma 3.** Given 12/5 < r < 3, we have that

$$D(u^{2}, u^{2}) \leq C \|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{\frac{2(5r-12)}{3(r-2)}} \|u\|_{\mathscr{L}^{r}(\mathbb{R}^{3})}^{\frac{2r}{3(r-2)}}, \quad u \in \mathscr{L}^{2}(\mathbb{R}^{3}) \cap \mathscr{L}^{r}(\mathbb{R}^{3}),$$

where

$$C \le \frac{3}{2} \left( \frac{4}{3} \pi \right)^{\frac{1}{3}} \frac{2(5r-6)}{3r^2} \left\{ \left[ \frac{r}{3(r-2)} \right]^{\frac{1}{3}} + \left( \frac{r}{6-2r} \right)^{\frac{1}{3}} \right\}$$

*In particular, when*  $r = \frac{8}{3}$  *we obtain* 

$$D(u^2, u^2) \le C \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^{\frac{4}{3}} \|u\|_{\mathscr{L}^{\frac{8}{3}}(\mathbb{R}^3)}^{\frac{8}{3}}, \quad u \in \mathscr{L}^2(\mathbb{R}^3) \cap \mathscr{L}^{\frac{8}{3}}(\mathbb{R}^3),$$

where

$$C \le \frac{11}{8} (3 + 3^{\frac{2}{3}}) \left(\frac{\pi}{12}\right)^{\frac{1}{3}} \approx 4.5.$$

Furthermore, if also  $q \leq \frac{8}{3}$ ,  $u_M$  is a minimizer for  $\mathscr{I}_V^{p,q}(M)$ , and M is sufficiently small, then

$$D(u^2, u^2) \le CM^{\frac{5q-12}{3(q-2)}} \|u\|_{\mathscr{L}^q(\mathbb{R}^3)}^q. \tag{2.7}$$

Proof. Since

$$\frac{2}{r} + \frac{1}{3} + \frac{5r - 6}{3r} = 2,$$

we can make use of Hardy-Littlewood's inequality to obtain

$$D(u^{2}, u^{2}) \leq C \|u^{2}\|_{\mathscr{L}^{\frac{r}{2}}(\mathbb{R}^{3})} \|u^{2}\|_{\mathscr{L}^{\frac{3r}{5r-6}}(\mathbb{R}^{3})} = C \|u\|_{\mathscr{L}^{r}(\mathbb{R}^{3})}^{2} \|u\|_{\mathscr{L}^{\frac{6r}{5r-6}}(\mathbb{R}^{3})}^{2}.$$

$$(2.8)$$

On the other hand, by the interpolation inequality,

$$||u||_{\mathscr{L}^{\frac{6r}{5r-6}}(\mathbb{R}^3)} \leq ||u||_{\mathscr{L}^2(\mathbb{R}^3)}^{\theta} ||u||_{\mathscr{L}^r(\mathbb{R}^3)}^{1-\theta},$$

where

$$\frac{5r-6}{6r} = \frac{1}{2}\theta + \frac{1}{r}(1-\theta) = \left(\frac{1}{2} - \frac{1}{r}\right)\theta + \frac{1}{r} = \frac{r-2}{2r}\theta + \frac{1}{r},$$

or, equivalently,

$$\theta = \frac{2r}{r-2} \left( \frac{5r-6}{6r} - \frac{1}{r} \right) = \frac{2r}{r-2} \frac{5r-12}{6r} = \frac{5r-12}{3(r-2)}.$$

Then,

$$\|u\|_{\mathscr{L}^{\frac{6r}{5r-6}}(\mathbb{R}^3)} \le \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^{\frac{5r-12}{3(r-2)}} \|u\|_{\mathscr{L}^r(\mathbb{R}^3)}^{\frac{6-2r}{3(r-2)}}.$$
(2.9)

By inserting (2.9) into (2.8) we obtain

$$D(u^2, u^2) \leq C \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^{\frac{2(5r-12)}{3(r-2)}} \|u\|_{\mathscr{L}^r(\mathbb{R}^3)}^{2\left[1 + \frac{6-2r}{3(r-2)}\right]} = C \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^{\frac{2(5r-12)}{3(r-2)}} \|u\|_{\mathscr{L}^r(\mathbb{R}^3)}^{\frac{2r}{3(r-2)}}.$$

Finally, (2.7) follows from Proposition 4 and the fact that when  $q \leq \frac{8}{3}$  and M is sufficiently small,

$$\frac{2q}{3(q-2)} \ge q, \text{ and } \|u\|_{\mathscr{L}^q(\mathbb{R}^3)} \ll 1,$$

hence 
$$\|u\|_{\mathscr{L}^q(\mathbb{R}^3)}^{\frac{2q}{3(q-2)}} \le \|u\|_{\mathscr{L}^q(\mathbb{R}^3)}^q$$
.

The following proposition states that the background potential term in the TFDW energy is weakly sequentially continuous. This result plays an important role in characterizing the structure of minimizing sequences of  $\mathscr{I}_{V}^{p,q}$  described in Theorem 4.

**Proposition 5.** If  $u_n \xrightarrow[n \to \infty]{} u$  in  $\mathcal{H}^1(\mathbb{R}^3)$ , then

$$\int_{\mathbb{R}^3} V u_n^2 d\vec{x} \xrightarrow[n \to \infty]{} \int_{\mathbb{R}^3} V u^2 d\vec{x}.$$

*Proof.* We follow ideas from [33, Theorem 11.4].

Let us rewrite  $V = V_{3/2} + V_{\infty}$  where  $V_{3/2} \in \mathcal{L}^{\frac{3}{2}}(\mathbb{R}^3)$  and  $V_{\infty} \in \mathcal{L}^{\infty}(\mathbb{R}^3)$ . We have that for R > 0,

$$\begin{split} \left| \int_{\mathbb{R}^{3}} V(u_{n}^{2} - u^{2}) d\vec{x} \right| &\leq \int_{\mathbb{R}^{3}} V|u_{n}^{2} - u^{2}| d\vec{x} \\ &= \left( \int_{B_{R}(\vec{0})} V_{3/2} |u_{n}^{2} - u^{2}| d\vec{x} + \int_{B_{R}(\vec{0})} V_{\infty} |u_{n}^{2} - u^{2}| d\vec{x} + \int_{\mathbb{R}^{3} \backslash B_{R}(\vec{0})} V|u_{n}^{2} - u^{2}| d\vec{x} \right) \\ &\leq \left( \int_{B_{R}(\vec{0}) \cap \{\vec{x} \in \mathbb{R}^{3} : |V_{3/2}| \geq R\}} |V_{3/2}| |u_{n}^{2} - u^{2}| d\vec{x} + \int_{B_{R}(\vec{0}) \cap \{\vec{x} \in \mathbb{R}^{3} : |V_{3/2}| \leq R\}} |V_{3/2}| |u_{n}^{2} - u^{2}| d\vec{x} \right) \\ &+ \int_{B_{R}(\vec{0})} |V_{\infty}| |u_{n}^{2} - u^{2}| d\vec{x} + \int_{\mathbb{R}^{3} \backslash B_{R}(\vec{0})} V|u_{n}^{2} - u^{2}| d\vec{x} \right) \\ &\leq \|V_{3/2}\|_{\mathscr{L}^{\frac{3}{2}}(\{\vec{x} \in \mathbb{R}^{3} : |V_{3/2}(\vec{x})| \geq R\})} \|u_{n}^{2} - u^{2}\|_{\mathscr{L}^{3}(\mathbb{R}^{3})} + (R + C) \int_{B_{R}(\vec{0})} |u_{n}^{2} - u^{2}| d\vec{x} \\ &+ \int_{\mathbb{R}^{3} \backslash B_{R}(\vec{0})} V|u_{n}^{2} - u^{2}| d\vec{x}, \\ &\leq \|V_{3/2}\|_{\mathscr{L}^{\frac{3}{2}}(\{\vec{x} \in \mathbb{R}^{3} : |V_{3/2}(\vec{x})| \geq R\})} (\|u_{n}\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2} + \|u\|_{\mathscr{L}^{6}(\mathbb{R}^{3})}^{2}) + (R + C) \int_{B_{R}(\vec{0})} |u_{n}^{2} - u^{2}| d\vec{x} \\ &+ \int_{\mathbb{R}^{3} \backslash B_{R}(\vec{0})} V|u_{n}^{2} - u^{2}| d\vec{x}, \end{split}$$

On the other hand, it is possible to choose a radius R > 0 such that all terms on the right hand side are small for n large thanks to the Dominated Convergence Theorem, Sobolev's inequality,

$$||u_n||_{\mathscr{H}^1(\mathbb{R}^3)} \leq C,$$

the Rellich-Kondrakov compactness Theorem, and (1.2). Thus the conclusion follows.

Finally, the following result plays an important role in the proof of Theorem 7. We could have stated Proposition 5 as a corollary of the following:

**Proposition 6.** Assume V satisfies (1.17), and  $\{u_n\}_{n\in\mathbb{N}}$ ,  $\{v_n\}_{n\in\mathbb{N}}$  are sequences which are bounded in  $\mathcal{L}^2(\mathbb{R}^3)\cap \mathcal{L}^{\frac{10}{3}}(\mathbb{R}^3)$  and such that  $(u_n-v_n)\xrightarrow[n\to\infty]{}0$  in  $\mathcal{L}^2_{loc}(\mathbb{R}^3)$ . Then,

$$\int_{\mathbb{R}^3} V\left(|u_n|^2 - |v_n|^2\right) d\overrightarrow{x} \xrightarrow[n \to \infty]{} 0.$$

*Proof.* Let  $\delta > 0$  be given. By (1.17) we may decompose  $V = V_1 + V_2 + V_3$ , where

$$V_1(\vec{x}) = V(\vec{x})[1 - \mathbb{1}_{B_R}(\vec{x})], \quad V_2(\vec{x}) = [V(\vec{x}) - t] + \mathbb{1}_{B_R}(\vec{x}), \quad V_3(\vec{x}) = \min\{V(\vec{x}), t\} \mathbb{1}_{B_R}(\vec{x}),$$

with R large enough that  $||V_1||_{\mathscr{L}^{\infty}(\mathbb{R}^3)} < \delta$ ; t large enough that  $||V_2||_{\mathscr{L}^{\frac{5}{2}}(\mathbb{R}^3)} < \delta$ . Note that  $V_3$  is compactly supported and uniformly bounded. We then consider each part separately:

$$\begin{split} \int_{\mathbb{R}^{3}} V_{1} \big| |u_{n}|^{2} - |v_{n}|^{2} \big| d\overrightarrow{x} &\leq \delta(\|u_{n}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} + \|v_{n}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}) \leq c\delta; \\ \int_{\mathbb{R}^{3}} V_{2} \big| |u_{n}|^{2} - |v_{n}|^{2} \big| d\overrightarrow{x} &\leq \|V_{2}\|_{\mathscr{L}^{\frac{5}{2}}(\mathbb{R}^{3})} (\|u_{n}\|_{\mathscr{L}^{\frac{10}{3}}(\mathbb{R}^{3})} + \|v_{n}\|_{\mathscr{L}^{\frac{10}{3}}(\mathbb{R}^{3})}) \leq c\delta; \\ \int_{\mathbb{R}^{3}} V_{3} \big| |u_{n}|^{2} - |v_{n}|^{2} \big| d\overrightarrow{x} &\leq \|V_{3}\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})} \int_{B_{P}} ||u_{n}|^{2} - |v_{n}|^{2} \big| d\overrightarrow{x} \xrightarrow[n \to \infty]{} 0. \end{split}$$

As  $\delta > 0$  is arbitrary, the result follows.

#### **2.3** Basic properties of $\mathscr{I}_{V}^{p,q}$

In this section we present properties of  $\mathscr{I}_{V}^{p,q}$  we use in later chapters.

**Proposition 7.** *The following hold:* 

- (i) For any M > 0,  $\mathcal{I}_0^{p,q}(M) \le 0$ .
- (ii) The following "binding inequality" holds:

$$\mathscr{I}_{V}^{p,q}(M) \le \mathscr{I}_{V}^{p,q}(M) + \mathscr{I}_{0}^{p,q}(M-m), \quad 0 \le m \le M.$$
 (2.10)

In particular,  $\mathcal{I}_{V}^{p,q}$  is always nonincreasing.

*Proof.* Statement (i) follows from (2.1) by taking  $\sigma \to 0^+$ .

Next, let  $v_1, v_2 \in C_0^{\infty}(\mathbb{R}^3)$  satisfy

$$\int_{\mathbb{R}^3} v_1^2 d\vec{x} = m, \quad \int_{\mathbb{R}^3} v_2^2 d\vec{x} = M - m,$$

pick any  $\vec{x}_0 \in \mathbb{R}^3 \setminus \{\vec{0}\}\$ , and set

$$w_n(\cdot) := v_1(\cdot) + v_2(\cdot + n\overrightarrow{x}_0), n \in \mathbb{N}.$$

Then, up to a subsequence,

$$\begin{split} \int_{\mathbb{R}^{3}} \|\nabla w_{n}\|^{2} d\vec{x} &= \int_{supp\ v_{1}} \|\nabla v_{1}(\vec{x}) + \nabla(v_{2}(\vec{x} + n\vec{x}_{0}))\|^{2} d\vec{x} + \int_{\mathbb{R}^{3} \setminus supp\ v_{1}} \|\nabla(v_{2}(\vec{x} + n\vec{x}_{0}))\|^{2} d\vec{x} \\ &= \int_{supp\ v_{1}} \|\nabla v_{1}\|^{2} d\vec{x} + \int_{\mathbb{R}^{3}} \|(\nabla v_{2})(\vec{x} + n\vec{x}_{0})\|^{2} d\vec{x} \\ &= \int_{\mathbb{R}^{3}} \|\nabla v_{1}\|^{2} d\vec{x} + \int_{\mathbb{R}^{3}} \|\nabla v_{2}\|^{2} d\vec{x}, \end{split}$$

$$\begin{split} \int_{\mathbb{R}^{3}} |w_{n}|^{r} d\overrightarrow{x} &= \int_{supp\ v_{1}} |v_{1}(\overrightarrow{x}) + v_{2}(\overrightarrow{x} + n\overrightarrow{x}_{0})|^{r} d\overrightarrow{x} + \int_{\mathbb{R}^{3} \setminus supp\ v_{1}} |v_{2}(\overrightarrow{x} + n\overrightarrow{x}_{0})|^{r} d\overrightarrow{x} \\ &= \int_{supp\ v_{1}} |v_{1}|^{r} d\overrightarrow{x} + \int_{\mathbb{R}^{3}} |v_{2}(\overrightarrow{x} + n\overrightarrow{x}_{0})|^{r} d\overrightarrow{x} \\ &= \int_{supp\ v_{1}} |v_{1}|^{r} d\overrightarrow{x} + \int_{supp\ v_{2}} |v_{2}|^{r} d\overrightarrow{x}, \quad r \geq 1, \end{split}$$

$$\begin{split} \int_{\mathbb{R}^3} V w_n^2 d \, \vec{x} &= \int_{\mathbb{R}^3} V v_1^2 d \, \vec{x} + 2 \int_{\mathbb{R}^3} V(\vec{x}) v_1(\vec{x}) v_2(\vec{x} + n \, \vec{x}_0) d \, \vec{x} + \int_{\mathbb{R}^3} V(\vec{x}) [v_2(\vec{x} + n \, \vec{x}_0)]^2 d \, \vec{x} \\ &= \int_{\mathbb{R}^3} V v_1^2 d \, \vec{x} + 2 \int_{supp\ v_1} V(\vec{x}) v_1(\vec{x}) v_2(\vec{x} + n \, \vec{x}_0) d \, \vec{x} + \int_{\mathbb{R}^3} V(\vec{x} - n \, \vec{x}_0) v_2^2(\vec{x}) d \, \vec{x} \\ &= \int_{\mathbb{R}^3} V v_1^2 d \, \vec{x} + \int_{supp\ v_2} V(\vec{x} - n \, \vec{x}_0) v_2^2(\vec{x}) d \, \vec{x}, \end{split}$$

and

$$\begin{split} D(w_n^2, w_n^2) &= \int_{supp\ v_1} \int_{supp\ v_1} \frac{|v_1(\vec{x}) + v_2(\vec{x} + n\vec{x}_0)|^2 |v_1(\vec{y}) + v_2(y + n\vec{x}_0)|^2}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \\ &+ \int_{\mathbb{R}^3 \setminus supp\ v_1} \int_{\mathbb{R}^3 \setminus supp\ v_1} \frac{|v_2(\vec{x} + n\vec{x}_0)|^2 |v_2(y + n\vec{x}_0)|^2}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \\ &+ \int_{\mathbb{R}^3 \setminus supp\ v_1} \int_{supp\ v_1} \frac{|v_1(\vec{x}) + v_2(\vec{x} + n\vec{x}_0)|^2 |v_2(y + n\vec{x}_0)|^2}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \\ &+ \int_{supp\ v_1} \int_{\mathbb{R}^3 \setminus supp\ v_1} \frac{|v_2(\vec{x} + n\vec{x}_0)|^2 |v_1(\vec{y}) + v_2(y + n\vec{x}_0)|^2}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \\ &= \int_{supp\ v_1} \int_{supp\ v_1} \frac{v_1^2(\vec{x})v_1^2(\vec{y})}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \\ &+ \int_{\mathbb{R}^3 \setminus supp\ v_1} \int_{\mathbb{R}^3 \setminus supp\ v_1} \frac{|v_2(\vec{x} + n\vec{x}_0)|^2 |v_2(y + n\vec{x}_0)|^2}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \end{split}$$

$$+2 \int_{\mathbb{R}^{3} \setminus supp \ v_{1}} \int_{supp \ v_{1}} \frac{v_{1}^{2}(\vec{x})|v_{2}(y+n\vec{x}_{0})|^{2}}{\|\vec{x}-\vec{y}\|} d\vec{x} d\vec{y}$$

$$= \int_{supp \ v_{1}} \int_{supp \ v_{1}} \frac{v_{1}^{2}(\vec{x})v_{1}^{2}(\vec{y})}{\|\vec{x}-\vec{y}\|} d\vec{x} d\vec{y} + \int_{\mathbb{R}^{3} \setminus supp \ v_{1}+n\vec{x}_{0}} \int_{\mathbb{R}^{3} \setminus supp \ v_{1}+n\vec{x}_{0}} \frac{v_{2}^{2}(\vec{x})v_{2}^{2}(\vec{y})}{\|\vec{x}-\vec{y}\|} d\vec{x} d\vec{y}$$

$$+2 \int_{\mathbb{R}^{3} \setminus supp \ v_{1}+n\vec{x}_{0}} \int_{supp \ v_{1}} \frac{v_{1}^{2}(\vec{x})v_{2}^{2}(\vec{y})}{\|\vec{x}-\vec{y}+n\vec{x}_{0}\|} d\vec{x} d\vec{y}$$

$$= \int_{supp \ v_{1}} \int_{supp \ v_{1}} \frac{v_{1}^{2}(\vec{x})v_{1}^{2}(\vec{y})}{\|\vec{x}-\vec{y}\|} d\vec{x} d\vec{y} + \int_{supp \ v_{2}} \int_{supp \ v_{2}} \frac{v_{2}^{2}(\vec{x})v_{2}^{2}(\vec{y})}{\|\vec{x}-\vec{y}\|} d\vec{x} d\vec{y}$$

$$+2 \int_{supp \ v_{2}} \int_{supp \ v_{1}} \frac{v_{1}^{2}(\vec{x})v_{2}^{2}(\vec{y})}{\|\vec{x}-\vec{y}+n\vec{x}_{0}\|} d\vec{x} d\vec{y} .$$

Consequently, the dominated convergence Theorem applies to ensure

$$\mathscr{I}_{V}^{p,q}(M) \le \lim_{n \to \infty} \mathscr{E}_{V}^{p,q}(w_n) = \mathscr{E}_{V}^{p,q}(v_1) + \mathscr{E}_{0}^{p,q}(v_2), \tag{2.11}$$

and we can optimize the right hand side of (2.11) to obtain (2.10).

We can say that the energy "at infinity" vanishes under certain conditions. As pointed out in the first section of this chapter, the study of TFDW problems with vanishing energy "at infinity" might be simpler.

#### **Proposition 8.** Assume that

$$g(t) := c_{TF}|t|^p - c_D|t|^q + \frac{2\sqrt{c_W}}{C}|t|^3 \ge 0, \quad t \in \mathbb{R},$$
(2.12)

where C satisfies

$$\int_{\mathbb{R}^3} |u|^3 d\vec{x} \le \frac{C}{2} \sqrt{\int_{\mathbb{R}^3} \|\nabla u\|^2 d\vec{x}} \sqrt{D(u^2, u^2)}, \quad u \in \mathcal{H}^1(\mathbb{R}^3).$$
 (2.13)

Then,  $\mathcal{I}_0^{p,q} \equiv 0$  and the infimum cannot be attained.

Moreover.

- i) both  $\mathcal{I}_0^{p,\frac{10}{3}}(M) = 0$  and the infimum is not attained for  $M \ll 1$ ,
- ii) (2.12) holds if and only if

$$q = 3, \quad \frac{c_D}{\sqrt{c_W}} \le \frac{2}{C},\tag{2.14}$$

or

$$q > 3$$
,  $\frac{c_{TF}}{\sqrt{c_W}} \left(\frac{c_D}{c_{TF}}\right)^{\frac{p-3}{p-q}} < \frac{2(p-3)}{C(p-q)} \left(\frac{p-3}{q-3}\right)^{\frac{q-3}{p-q}}$ . (2.15)

*Proof.* In virtue of (2.13),

$$\mathscr{E}_{0}^{p,q}(u) \geq \int_{\mathbb{R}^{3}} \left( c_{W} \|\nabla u\|^{2} - \frac{2\sqrt{c_{W}}}{C} |u|^{3} \right) d\vec{x} + \frac{1}{2} D(u^{2}, u^{2})$$

$$\geq c_W \int_{\mathbb{R}^3} \|\nabla u\|^2 d\vec{x} - \sqrt{c_W \int_{\mathbb{R}^3} \|\nabla u\|^2 d\vec{x}} \sqrt{D(u^2, u^2)} + \frac{1}{2} D(u^2, u^2)$$

$$= \left(\sqrt{c_W \int_{\mathbb{R}^3} \|\nabla u\|^2 d\vec{x}} - \frac{1}{2} \sqrt{D(u^2, u^2)}\right)^2 + \frac{1}{4} D(u^2, u^2) > 0, \quad u \in \mathscr{H}^1(\mathbb{R}^3) \setminus \{0\}$$

As a result,  $\mathscr{I}_0^{p,q} \ge 0$ , which joint with the nonpositivity of  $\mathscr{I}_0^{p,q}$  implies  $\mathscr{I}_0^{p,q} \equiv 0$ . Moreover, from the equation above we can see that the infimum cannot be attained.

Next, we establish (i). We note that

$$\int_{\mathbb{R}^{3}} |u|^{\frac{10}{3}} d\vec{x} \leq \left( \int_{\mathbb{R}^{3}} u^{2} d\vec{x} \right)^{\frac{1}{2} \frac{10}{3} \theta} \left( \int_{\mathbb{R}^{3}} |u|^{6} d\vec{x} \right)^{\frac{1}{6} \frac{10}{3} (1 - \theta)} \leq C M^{\frac{5}{3} \theta} \left( \int_{\mathbb{R}^{3}} \|\nabla u\|^{2} \right)^{\frac{5}{3} (1 - \theta)}, \quad (2.16)$$

by the interpolation inequality in Lebesgue spaces and Sobolev's inequality, where

$$\frac{3}{10} = \frac{1}{2}\theta + \frac{1}{6}(1 - \theta),$$

or, equivalently,  $\theta = 2/5$ . Then, (2.16) reads

$$\int_{\mathbb{R}^3} |u|^{\frac{10}{3}} d\vec{x} \le CM^{\frac{2}{3}} \int_{\mathbb{R}^3} ||\nabla u||^2 d\vec{x},$$

thus

$$\mathscr{E}_{0}^{p,q}(u) \geq \int_{\mathbb{R}^{3}} \left[ (c_{W} - c_{D}CM^{\frac{2}{3}}) \|\nabla u\|^{2} + c_{TF}|u|^{p} \right] d\overrightarrow{x} + \frac{1}{2}D(u^{2}, u^{2}), \quad u \in \mathscr{H}^{1}(\mathbb{R}^{3}),$$

and when  $M \ll 1$ ,

$$\mathscr{E}_0(u) > 0, u \in \mathscr{H}^1(\mathbb{R}^3), \|u\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M.$$

The latter joint with the nonpositivity of  $\mathscr{I}_0^{p,\frac{10}{3}}$  implies  $\mathscr{I}_0^{p,\frac{10}{3}} \equiv 0$ . Moreover, the infimum cannot be attained. This proves (i).

Finally, in regards to (ii), q < 3 is discarded because g(t) < 0 for  $t \ll 1$  in this case. Regarding the other two posibilities for q, first note that

$$\lim_{|t|\to\infty}g(t)=\infty$$

Then,

$$q = 3 \Rightarrow g(t) = c_{TF}|t|^p + \left(\frac{2\sqrt{c_W}}{C} - c_D\right)|t|^3, \forall t \in \mathbb{R}, \Rightarrow \left(g(t) \ge 0, \forall t \in \mathbb{R}, \Leftrightarrow c_D \le \frac{2\sqrt{c_W}}{C}\right);$$

that is, if (2.14) holds, then (2.12) holds. Moreover, if (2.15) holds, then g(0) = 0 and for

$$t \in \mathbb{R} \setminus \{0\} \mapsto f(t) := \frac{g(t)}{c_{TF}|t|^3},$$

it is true that

$$(f(t) \ge 0 \Leftrightarrow g(t) \ge 0, \forall t \in \mathbb{R} \setminus \{0\}), \quad \lim_{|t| \to \infty} f(t) = \infty.$$

Also, f has only one critical point, say  $t_0$ , and it satisfies

$$(p-3)t_0^{p-4} - \frac{c_D}{c_{TF}}(q-3)t_0^{q-4} = 0 \Leftrightarrow t_0^{p-3} = \frac{c_D(q-3)}{c_{TF}(p-3)}t_0^{q-3} \Leftrightarrow t_0 = \left[\frac{c_D(q-3)}{c_{TF}(p-3)}\right]^{\frac{1}{p-q}},$$

then

$$f(t_0) = \left[\frac{c_D(q-3)}{c_{TF}(p-3)} - \frac{c_D}{c_{TF}}\right] t_0^{q-3} + \frac{2\sqrt{c_W}}{c_{TF}C}$$

$$= \frac{c_D(q-p)}{c_{TF}(p-3)} t_0^{q-3} + \frac{2\sqrt{c_W}}{c_{TF}C}$$

$$= \frac{c_D(q-p)}{c_{TF}(p-3)} \left[\frac{c_D(q-3)}{c_{TF}(p-3)}\right]^{\frac{q-3}{p-q}} + \frac{2\sqrt{c_W}}{c_{TF}C} > 0.$$

As a result, (2.12) also holds if we assume (2.15) holds.

The following Lemma is used in the proof of the Concentration-compactness Theorem in the case p = 10/3 and q = 8/3 (see Theorem 4), in the study of vanishing of the energy at "infinity" (see Corollary right after the Lemma), and in the study of the minimization problem over the class of radial functions (see section 4 in chapter 3):

#### **Lemma 4.** *The following hold:*

- 1.  $\mathscr{I}_0^{\frac{10}{3},\frac{8}{3}}(M)$  is strictly concave for  $M \ll 1$ . In particular, this implies that  $\mathscr{I}_0^{\frac{10}{3},\frac{8}{3}}(M)$  is strictly subadditive for  $M \ll 1$ , hence no splitting occurs for sufficiently small masses (i.e. there exist minimizers).
- 2. If  $q \le 3$ , K = 1,  $\overrightarrow{r}_0 = \overrightarrow{0}$  and either Z = 0 or c = 2q 4, then

$$M \in \mathbb{R}^+ \mapsto \frac{\mathscr{I}_V^{p,q}(M)}{M^{2q-3}}$$

is nondecreasing.

3. Let q < 2.4 and K = 1,  $\vec{r}_0 = \vec{0}$ . Then,

$$M \in \mathbb{R}^+ \mapsto rac{\mathscr{I}_V^{p,q}(M)}{M\%}$$

is nonincreasing for

$$V \equiv 0, \quad \gamma_0 \in \left[0, \frac{12 - 5q}{8 - 3q}\right) (\in [0, 1)),$$

or

$$V \not\equiv 0, \quad v \in \left[\frac{2q-4}{4-q}, \frac{3q-6}{q}\right] \subseteq (0,1), \quad \gamma_0 = \frac{3}{2} \frac{(q-2)^2}{2c+6-3q} + \frac{q}{2} \in [0,1).$$

*Proof.* Nam and Van Den Bosch [46] showed  $\mathscr{I}_0^{\frac{10}{3},\frac{8}{3}}(M)$  is attained for M small enough by exploiting the fact that

$$\mathscr{I}_0(M) = \inf\{F_u(M); u \in \mathscr{H}^1(\mathbb{R}^3), \|u\|_{\mathscr{L}^2(\mathbb{R}^3)} = 1\}, \quad M > 0,$$

where

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

with

$$A_{u} := c_{W} \int_{\mathbb{R}^{3}} \|\nabla u\|^{2} d\vec{x}, \quad B_{u} := c_{TF} \int_{\mathbb{R}^{3}} |u|^{\frac{10}{3}} d\vec{x},$$

$$C_{u} := c_{D} \int_{\mathbb{R}^{3}} |u|^{\frac{8}{3}} d\vec{x}, \qquad D_{u} := \frac{1}{2} D(u^{2}, u^{2}).$$

Indeed, they proved  $M \ll 1 \mapsto \mathscr{I}_0^{\frac{10}{3},\frac{8}{3}}(M)$  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

$$B_u \le CM^{\frac{2}{3}}A_u, \ D_u \le CM^{\frac{2}{3}}C_u, \ u \in \mathcal{H}^1(\mathbb{R}^3).$$
 (2.17)

(2.17) 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 (2.17),

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

where

$$G_{u}(M) := 14M^{\frac{8}{3}}B_{u}^{2}D_{u}^{2} + M^{2}(37A_{u}B_{u}D_{u}^{2} - 10B_{u}^{2}C_{u}D_{u}) + M^{\frac{4}{3}}(27A_{u}^{2}D_{u}^{2} - 30A_{u}B_{u}C_{u}D_{u})$$
$$+ M^{\frac{2}{3}}(-28A_{u}^{2}C_{u}D_{u} + A_{u}B_{u}C_{u}^{2}) + 5A_{u}^{2}C_{u}^{2}$$

$$> A_{\mu}^{2}C_{\mu}^{2}(-10M^{2}-30M^{\frac{4}{3}}-28M^{\frac{2}{3}}+5)>0,$$

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

$$\begin{split} \mathscr{I}_0(\alpha M_1 + (1-\alpha)M_2) &= F_{u^*}(\alpha M_1 + (1-\alpha)M_2) \\ &> \alpha F_{u^*}(M_1) + (1-\alpha)F_{u^*}(M_2) \\ &\geq \alpha \mathscr{I}_0(M_1) + (1-\alpha)\mathscr{I}_0(M_2). \end{split}$$

Since  $\alpha$ ,  $M_1$ , and  $M_2$  were arbitrary, we conclude that  $\mathscr{I}_0^{\frac{10}{3},\frac{8}{3}}$  is strictly concave for  $M\ll 1$ .

Now we turn to the proof of statement 2. Given  $\alpha$  and  $\beta$  positive,  $\alpha < \beta$ , choose any function  $u \in \mathcal{H}^1(\mathbb{R}^3)$  with  $||u||^2_{\mathcal{L}^2(\mathbb{R}^3)} = \beta$ . Set  $v := \gamma^2 u(\gamma)$  where  $\gamma := \alpha/\beta < 1$ . Then,

$$\begin{split} \int_{\mathbb{R}^3} v^2 d\overrightarrow{x} &= \int_{\mathbb{R}^3} |\gamma^2 u(\gamma \cdot)|^2 d\overrightarrow{x} = \gamma \int_{\mathbb{R}^3} u^2 d\overrightarrow{x} = \alpha, \\ \int_{\mathbb{R}^3} \|\nabla v\|^2 d\overrightarrow{x} &= \int_{\mathbb{R}^3} \|\nabla (\gamma^2 u(\gamma \cdot))\|^2 d\overrightarrow{x} = \int_{\mathbb{R}^3} \|\gamma^3 (\nabla u)(\gamma \cdot)\|^2 d\overrightarrow{x} = \gamma^3 \int_{\mathbb{R}^3} \|\nabla u\|^2 d\overrightarrow{x}, \\ \int_{\mathbb{R}^3} |v|^r d\overrightarrow{x} &= \int_{\mathbb{R}^3} |\gamma^2 u(\gamma \cdot)|^r d\overrightarrow{x} = \gamma^{2r-3} \int_{\mathbb{R}^3} |u|^r d\overrightarrow{x}, \quad r \ge 1, \\ \int_{\mathbb{R}^3} V v^2 d\overrightarrow{x} &= \gamma^{4+\nu} \int_{\mathbb{R}^3} \frac{Z u(\gamma \overrightarrow{x})}{\|\gamma \overrightarrow{x}\|^\nu} d\overrightarrow{x} = \gamma^{1+\nu} \int_{\mathbb{R}^3} V u^2 d\overrightarrow{x} = \gamma^{2q-3} \int_{\mathbb{R}^3} V u^2, d\overrightarrow{x} \end{split}$$

and

$$D(v^2, v^2) = \gamma \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{[\gamma^2 u(\gamma \vec{x})]^2 [\gamma^2 u(\gamma \vec{y})]^2}{\|\gamma \vec{x} - \gamma \vec{y}\|} d\vec{x} d\vec{y} = \gamma^3 D(u^2, u^2).$$

Consequently,

$$\begin{split} \mathscr{I}_{V}^{p,q}(\alpha) &\leq \mathscr{E}_{V}^{p,q}(v) \\ &= \int_{\mathbb{R}^{3}} (c_{W} \gamma^{3} \|\nabla u\|^{2} d\overrightarrow{x} + c_{TF} \gamma^{2p-3} |u|^{p} d\overrightarrow{x} - c_{D} \gamma^{2q-3} |u|^{q} d\overrightarrow{x} - \gamma^{2q-3} V u^{2}) d\overrightarrow{x} + \frac{1}{2} \gamma^{3} D(u^{2}, u^{2}) \\ &\leq \gamma^{2q-3} \mathscr{E}_{V}^{p,q}(u). \end{split}$$

Thus the conclusion follows.

Regarding statement 3, for  $s, \alpha \in \mathbb{R}$  satisfying

$$2s-3\alpha=1$$
,

$$\begin{split} \mathscr{I}_{V}^{p,q}(M) &= \inf_{\substack{w \in \mathscr{H}^{1}(\mathbb{R}^{3}) \\ \|w\|_{\mathscr{L}^{2}(\mathbb{R}^{3})} = 1}} \left\{ \mathscr{E}_{V}^{p,q}(M^{s}w(M^{\alpha}\cdot)) \right\} \\ &= \inf_{\substack{w \in \mathscr{H}^{1}(\mathbb{R}^{3}) \\ \|w\|_{\mathscr{L}^{2}(\mathbb{R}^{3})} = 1}} \left\{ \int_{\mathbb{R}^{3}} (c_{W}M^{1+2\alpha} \|\nabla w\|^{2} + c_{TF}M^{\frac{3}{2}(p-2)\alpha + \frac{p}{2}} |w|^{p} - c_{D}M^{\frac{3}{2}(q-2)\alpha + \frac{q}{2}} |w|^{q}) d\vec{x} \right. \\ &\quad + M^{\alpha c+1} \int_{\mathbb{R}^{3}} Vw^{2} d\vec{x} + M^{2+\alpha} \frac{1}{2} D(w^{2}, w^{2}) \right\} \\ &= M^{70} \inf_{\substack{w \in \mathscr{H}^{1}(\mathbb{R}^{3}) \\ \|w\|_{\mathscr{L}^{2}(\mathbb{R}^{3})} = 1}} \left\{ \int_{\mathbb{R}^{3}} (c_{W}M^{\left(5 - \frac{3}{2}q\right)\alpha + 1 - \frac{q}{2}} \|\nabla w\|^{2} + c_{TF}M^{\frac{3\alpha + 1}{2}(p-q)} |w|^{p} - c_{D}|w|^{q}) d\vec{x} \right. \\ &\quad - M^{\alpha c + 1 - 70} \int_{\mathbb{R}^{3}} Vw^{2} d\vec{x} + M^{\left(4 - \frac{3}{2}q\right)\alpha + 2 - \frac{q}{2}} \frac{1}{2} D(w^{2}, w^{2}) \right\}, \end{split}$$

where

$$\gamma_0 = \frac{3}{2}(q-2)\alpha + \frac{q}{2}.$$

If  $V \equiv 0$  Choose any constant  $\alpha$  such that

$$-\frac{q}{3q-6} \le \alpha \le -\frac{4-q}{8-3q<0}. (2.18)$$

Note that the interval above is well defined thanks to  $q \le 2.4$ , and that as one varies  $\alpha$ ,

$$0 = \frac{3}{2}(q-2)\left(-\frac{q}{3q-6}\right) + \frac{q}{2} \le \gamma_0 \le \frac{3}{2}(q-2)\left(-\frac{4-q}{8-3q}\right) + \frac{q}{2} = \frac{12-5q}{8-3q}.$$

If  $V \not\equiv 0$  Choose a constant  $\alpha$  such that so that the powers of negative terms in  $\mathcal{E}_V^{p,q}$  match; i.e.

$$\alpha = \frac{q-2}{2c+6-3q}. (2.19)$$

Then, as  $v \in \left[\frac{2q-4}{4-q}, \frac{3q-6}{q}\right]$ ,

$$-\frac{(q-2)(8-3q)}{4-q} \leq 2c+6-3q \leq -\frac{(q-2)(3q-6)}{q},$$

so that from (2.19), (2.18) holds again. Also, for this value of  $\alpha$ ,

$$\gamma_0 = \frac{3}{2} \frac{(q-2)^2}{2c+6-3q} + \frac{q}{2}.$$

In any case, we have

$$\left(5 - \frac{3}{2}q\right)\alpha + 1 - \frac{q}{2} < 0 + 0 = 0$$

$$\frac{3\alpha+1}{2}(p-q) \leq \frac{3\left(-\frac{4-q}{8-3q}\right)+1}{2}(p-q) = -\frac{2}{8-3q}(p-q) < 0,$$

and

$$\left(4 - \frac{3}{2}q\right)\alpha + 2 - \frac{q}{2} \le \frac{8 - 3q}{2}\left(-\frac{4 - q}{8 - 3q}\right) + \frac{4 - q}{2} = 0.$$

Consequently, if  $\tilde{M} < M$ ,

$$\begin{split} \mathscr{I}_{V}^{p,q}(M) &= M^{\gamma_{0}} \inf_{\substack{w \in \mathscr{H}^{1}(\mathbb{R}^{3}) \\ \|w\|_{\mathscr{L}^{2}(\mathbb{R}^{3})} = 1}} \left\{ \int_{\mathbb{R}^{3}} (c_{W} M^{\left(5 - \frac{3}{2}q\right)\alpha + 1 - \frac{q}{2}} \|\nabla w\|^{2} + c_{TF} M^{\frac{3\alpha + 1}{2}(p - q)} |w|^{p} - c_{D} |w|^{q}) d\overrightarrow{x} \right. \\ &\qquad \qquad - \int_{\mathbb{R}^{3}} V w^{2} d\overrightarrow{x} + M^{\left(4 - \frac{3}{2}q\right)\alpha + 2 - \frac{q}{2}} \frac{1}{2} D(w^{2}, w^{2}) \right\} \\ &\leq M^{\gamma_{0}} \inf_{\substack{w \in \mathscr{H}^{1}(\mathbb{R}^{3}) \\ \|w\|_{\mathscr{L}^{2}(\mathbb{R}^{3})} = 1}} \left\{ \int_{\mathbb{R}^{3}} (c_{W} \tilde{M}^{\left(5 - \frac{3}{2}q\right)\alpha + 1 - \frac{q}{2}} \|\nabla w\|^{2} + c_{TF} \tilde{M}^{\frac{3\alpha + 1}{2}(p - q)} |w|^{p} - c_{D} |w|^{q}) d\overrightarrow{x} \right. \\ &\qquad \qquad - \int_{\mathbb{R}^{3}} V w^{2} d\overrightarrow{x} + \tilde{M}^{\left(4 - \frac{3}{2}q\right)\alpha + 2 - \frac{q}{2}} \frac{1}{2} D(w^{2}, w^{2}) \right\} = \left( \frac{M}{\tilde{M}} \right)^{\gamma_{0}} \mathscr{I}_{V}^{p,q}(\tilde{M}) \end{split}$$

Finally, we can prove that the energy at "infinity" does not vanish under certain conditions:

**Corollary 2.** If q < 3, then  $\mathscr{I}_0^{p,q} < 0$ .

*Proof.* Following the same reasoning as in the proof of part 2 of Lemma 4 with  $\beta=1$  and u fixed, we find that the leading term in  $\mathcal{E}_0^{p,q}(v)$  is the negative one, so that  $\mathcal{I}_0^{p,q}(\alpha)<0$  for all  $p\in(q,6)$  and all  $\alpha\ll1$ . Consequently, the binding inequality ensures the function is strictly negative on its whole domain. *It is worth to mention that when we choose functions*  $v=\gamma^s u(\gamma)$  *and see what happens with s to force the negative term to be dominant, we find the same condition* q<3 *coming from trying to force* sq-3<2s-1,4s-5 *that leads to* 2/(4-q)<2/(q-2).

The following proposition contains what the concentration-compactness Lemma by Lions gives in relation to minimizing sequences of TFDW type problems. The first part concerns conditions under which there is equality in the binding inequality.

### **Proposition 9.** The following are true:

(i) Let  $\{u_n\}_{n\in\mathbb{N}}$  be a minimizing sequence for  $\mathscr{I}_V^{p,q}(M)$  and assume  $\mathscr{I}_V^{p,q}<0$ . Then, there exist translations  $\{\vec{x}_n^0\}_{n\in\mathbb{N}}$  and a function  $u^0\in\mathscr{H}^1(\mathbb{R}^3)\setminus\{0\}$  such that, up to a subsequence,

$$u_n(\cdot - \overrightarrow{x}_n^0) - u^0 \xrightarrow[n \to \infty]{} 0$$
 in  $\mathscr{H}^1(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ .

Moreover,

$$\mathscr{I}_{V}^{p,q}(M) = \mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(M-m^{0}), \quad \mathscr{I}_{V}^{p,q}(m^{0}) = \mathscr{E}_{V}^{p,q}(u^{0}), \\ \mathscr{I}_{V}^{p,q}(M-m^{0}) = \lim_{n \to \infty} \mathscr{E}_{V}^{p,q}(u_{n}-u^{0}).$$

where  $m^0 := \|u^0\|_{\mathscr{L}^2(\mathbb{R}^3)}^2$ , and we can choose vectors  $\{\vec{x}_n = \vec{0}\}_{n \in \mathbb{N}}$  if  $V \not\equiv 0$ .

(ii) 
$$\mathscr{I}_{V}^{p,q} < \mathscr{I}_{0}^{p,q} \leq 0$$
 for  $V \not\equiv 0$ .

*Proof.* (i) Let us consider  $V \not\equiv 0$  first.

The sequence  $\{u_n\}_{n\in\mathbb{N}}$  is bounded in  $\mathscr{H}^1(\mathbb{R}^3)$  as  $\mathscr{E}_V^{p,q}$  is coercive (see Proposition 3). Then, there exists  $u^0 \in \mathscr{H}^1(\mathbb{R}^3)$  and a (not relabeled) subsequence for which  $u_n \xrightarrow[n \to \infty]{} u^0$  weakly in  $\mathscr{H}^1(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ . By the weak convergence and the Brezis-Lieb Lemma [10],  $\mathscr{E}_V^{p,q}$  decouples in the limit (see [46, 33]),

$$\lim_{n\to\infty} \left[ \mathscr{E}_V^{p,q}(u_n) - \mathscr{E}_V^{p,q}(u^0) - \mathscr{E}_0^{p,q}(u_n - u^0) \right] = 0,$$

and thus

$$\mathscr{I}_V^{p,q} = \lim_{n \to \infty} \mathscr{E}_V^{p,q}(u_n) = \mathscr{E}_V^{p,q}(u^0) + \lim_{n \to \infty} \mathscr{E}_0^{p,q}(u_n^0) \geq \mathscr{I}_V^{p,q}(m^0) + \mathscr{I}_0^{p,q}(M-m^0).$$

On the other hand, by the binding inequality (2.10), we have

$$\mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(M - m^{0}) \ge \mathscr{I}_{V}^{p,q}(M) \ge \mathscr{E}_{V}^{p,q}(u^{0}) + \lim_{n \to \infty} \mathscr{E}_{0}^{p,q}(u^{0}) \ge \mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(M - m^{0}), \tag{2.20}$$

and hence we obtain equality of each expression,

$$\mathscr{E}_{V}^{p,q}(u^0) = \mathscr{I}_{V}^{p,q}(m^0) \quad \text{and} \quad \lim_{n \to \infty} \mathscr{E}_{0}^{p,q}(u_n - u^0) = \mathscr{I}_{0}^{p,q}(M - m^0),$$

that is, the remainder sequence  $\{u_n^0\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_0^{p,q}(M-m^0)$ .

Next, we prove that  $m^0 > 0$ . Suppose this was not the case to get a contradiction.

We eliminate the possibility of "vanishing" in the Concentration-Compactness framework [36], for any bounded sequence we define (as in Nam-van den Bosch [46],)

$$\omega(\{v_n\}_{n\in\mathbb{N}}) := \sup\left\{\|v\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 ; \exists y_n \in \mathbb{R}^3 \text{ and a subsequence such that } v_n(\cdot - y_n) \xrightarrow[n \to \infty]{} v \text{ in } \mathscr{H}^1(\mathbb{R}^3)\right\}. \tag{2.21}$$

We claim that  $\omega(\{u_n\}_{n\in\mathbb{N}}) > 0$ . Indeed, applying [36, Lemma I.1], if  $\omega(\{u_n\}_{n\in\mathbb{N}}) = 0$ , then  $u_n \xrightarrow[n\to\infty]{} 0$  in  $\mathscr{L}^r(\mathbb{R}^3)$  norm, for all 2 < r < 6, so in particular

$$\int_{\mathbb{R}^3} |u_n|^q \xrightarrow[n\to\infty]{} 0.$$

In addition, by Proposition 5 we have

$$\int_{\mathbb{D}^3} V |u_n|^2 d\overrightarrow{x} \xrightarrow[n\to\infty]{} 0,$$

and hence

$$\mathscr{I}_{V}^{p,q}(M) = \lim_{n \in \mathbb{N}} \mathscr{E}_{V}^{p,q}(u_n) \leq \liminf_{n \to \infty} \mathscr{E}_{0}^{p,q}(u_n) \geq 0,$$

which contradicts  $\mathscr{I}_V^{p,q} < 0$ . Hence "vanishing" cannot occur. Then, by definition of  $\omega(\{u_n\}_{n\in\mathbb{N}})$ , we can choose translations  $\{\overrightarrow{x}_n^1\}_{n\in\mathbb{N}}$  so that, up to a subsequence,  $u_n(\cdot - \overrightarrow{x}_n^1) \xrightarrow[n \to \infty]{} u^1 \not\equiv 0$  in  $\mathscr{H}^1(\mathbb{R}^3)$ .

Now, since  $\mathcal{E}_0^{p,q}$  is translation invariant,  $V \not\equiv 0$ , and by Proposition 5, we have

$$\begin{split} \mathscr{I}_{V}^{p,q}(M) &\leq \liminf_{n \to \infty} \mathscr{E}_{V}^{p,q}(u_{n}(\cdot - \overrightarrow{x}_{n}^{1})) \\ &= \liminf_{n \to \infty} \left\{ \mathscr{E}_{0}^{p,q}(u_{n}) - \int_{\mathbb{R}^{3}} V[u_{n}(\overrightarrow{x} - \overrightarrow{x}_{n}^{1})]^{2} d\overrightarrow{x} \right\} \\ &= \liminf_{n \to \infty} \mathscr{E}_{V}^{p,q}(u_{n}) - \int_{\mathbb{R}^{3}} V(u^{1})^{2} d\overrightarrow{x} \\ &= \mathscr{I}_{V}^{p,q}(M) - \int_{\mathbb{D}^{3}} V(u^{1})^{2} d\overrightarrow{x}. \end{split}$$

We reached a contradiction. We then must have that  $m^0 > 0$ .

Finally, we consider  $V \equiv 0$ . In this case, we prove that  $\omega(\{u_n\}_{n\in\mathbb{N}}) > 0$  by using negativity of the energy again, so that it is possible to translations  $\{\vec{x}_n^0\}_{n\in\mathbb{N}}$  so that  $u_n(\cdot - \vec{x}_n^0) \xrightarrow[n \to \infty]{} u^0 \not\equiv 0$  in  $\mathscr{H}^1(\mathbb{R}^3)$ .

(ii) By part (i) and Proposition 10, there exists  $m \in (0, M]$  for which

$$\mathscr{I}_0^{p,q}(M) = \mathscr{I}_0^{p,q}(m) + \mathscr{I}_0^{p,q}(M-m),$$

where  $\mathscr{I}_0^{p,q}(m)$  is attained by a function  $|u_{0,m}| > 0$ . Then,

$$\mathscr{I}_{V}^{p,q}(M) - \mathscr{I}_{0}^{p,q}(m) \leq \mathscr{I}_{V}^{p,q}(u_{0,m}) - \mathscr{I}_{0}^{p,q}(u_{0,m}) = -\int_{\mathbb{R}^{3}} V(\vec{x}) u_{0,m}^{2}(\vec{x}) < 0,$$

because  $V \not\equiv 0$ . Therefore, the binding inequality gives

$$\mathscr{I}_{V}^{p,q}(M) \leq \mathscr{I}_{V}^{p,q}(M) + \mathscr{I}_{0}^{p,q}(M-m) < \mathscr{I}_{0}^{p,q}(m) + \mathscr{I}_{0}^{p,q}(M-m) = \mathscr{I}_{0}^{p,q}(M) \leq 0.$$

Finally, we can compare  $\mathscr{I}_V^{p,q}$  with M as follows.

**Corollary 3.** Let V be as in (1.5). Then, there exist  $K_1, K_2 \in \mathbb{R}^+$  for which

$$-K_1M \le \mathscr{I}_V^{p,q}(M) \le -K_2M.$$

For V more general, we can take  $K_2 = 0$ .

*Proof.* The lower bound follows from coercivity of  $\mathcal{E}_V^{p,q}$ . On the other hand, the upper bound follows from applying the binding inequality multiple times and from

$$\limsup_{M\to 0^+}\frac{\mathscr{I}_V^{p,q}(M)}{M}<0,$$

an inequality we establish in what remains of this proof.

Let us define

$$E_{M,V} := \inf \left\{ \int_{\mathbb{R}^3} (c_W \|\nabla u\|^2 - Vu^2) d\vec{x} \; ; \; u \in \mathcal{H}^1(\mathbb{R}^3), \int_{\mathbb{R}^3} u^2 = M \right\}, \quad M > 0.$$

We can show that  $E_{M,V} < 0$  by applying the transformation  $u \mapsto \sigma^{\frac{3}{2}}u(\sigma \cdot)$  and taking  $\sigma \to 0^+$ . Moreover,  $E_{M,V} = ME_{1,V}$  for M > 0. Then, by applying the concentration-compactness Lemma to a minimizing sequence for any of the  $E_{M,V}$  and by lower semicontinuity of the energy that is being minimized, we obtain that each  $E_{M,V}$  is attained. In particular, there exists  $\phi_1 \in \mathcal{H}^1(\mathbb{R}^3)$  at which  $E_{1,V}$  is attained.

Next, we have

$$\mathscr{I}_{V}^{p,q}(M) \leq \mathscr{E}_{V}^{p,q}(\sqrt{M}\phi_{1}) = ME_{1,V} + M\varepsilon(M),$$

where  $\varepsilon(M) \to 0$  as  $M \to 0^+$ . Hence

$$\limsup_{M\to 0^+} \frac{\mathscr{I}_V^{p,q}(M)}{M} \le E_{1,V} < 0.$$

## **2.4** Basic properties of minimizers of $\mathscr{I}_{V}^{p,q}$

In this section we present some estimates on minimizers and consequences.

**Proposition 10.** If  $\mathscr{I}_0^{p,q}(M)$  is attained at  $u_{0,M}$ , then  $u \in \mathscr{C}^{\infty}(\mathbb{R}^3)$ ,  $0 < |u_{0,M}| \le \left(\frac{q}{p}\frac{c_D}{c_{TF}}\right)^{\frac{1}{p-q}}$ , and (1.9) holds with Lagrange Multiplier  $\mu \le 0$  induced by the mass constraint. Moreover, if either  $q \le \frac{12}{5}$  or both  $q \le \frac{8}{3}$  and  $M \ll 1$ , then  $\mu < 0$ .

**Remark 3.** When the Lagrange multiplier  $\mu < 0$ , we obtain exponential decay (see (66) in [37]): for all  $t < \sqrt{-\mu/c_W}$ , there exists C with

$$|u_{0,M}(\vec{x})| + ||\nabla u_{0,M}(\vec{x})|| \le Ce^{-t||\vec{x}||} \text{ pointwise almost everywhere in } \mathbb{R}^3.$$
 (2.22)

Even if  $\mu_0 = 0$ , we still have  $|u_{0,M}| + \|\nabla u_{0,M}\| \xrightarrow{\|\vec{x}\| \to \infty} 0$ . This follows from (1.9) and Theorem 8.17 uniformly by Gilbarg and Trudinger [26].

*Proof.* Equation (1.9), without the sign of  $\mu$ , corresponds to the Euler-Lagrange equation associated to  $\mathscr{I}_0^{p,q}$ . From the Euler-Lagrange equation we obtain

$$c_W \int_{\mathbb{R}^3} \|\nabla u_{0,M}\|^2 d\vec{x} + c_{TF} \frac{p}{2} \int_{\mathbb{R}^3} |u_{0,M}|^p d\vec{x} - c_D \frac{q}{2} \int_{\mathbb{R}^3} |u_{0,M}|^q d\vec{x} + D(u_{0,M}^2, u_{0,M}^2) = \mu M. \tag{2.23}$$

Next, since  $M \in \mathbb{R}^+ \mapsto \mathscr{I}_0(M)$  is nonincreasing and  $\mathscr{I}_0(M) = \mathscr{E}_0(u_{0,M})$ , the function  $\sigma \in [0,1] \mapsto \mathscr{E}_0(\sigma u_{0,M})$  has a minimum at  $\sigma = 1$ . Then,

$$0 \ge \left. \frac{d}{d\sigma} [\mathscr{E}_0(\sigma u_{0,M})] \right|_{\sigma=1}$$

$$\begin{split} &= \frac{d}{d\sigma} \left[ \int_{\mathbb{R}^3} (c_W \sigma^2 \|\nabla u_{0,M}\|^2 + c_{TF} \sigma^p |u_{0,M}|^p - c_D \sigma^q |u_{0,M}|^q) d\vec{x} + \frac{1}{2} \sigma^4 D(u_{0,M}^2, u_{0,M}^2) \right] \Big|_{\sigma=1} \\ &= \int_{\mathbb{R}^3} (2c_W \|\nabla u_{0,M}\|^2 + c_{TF} p |u_{0,M}|^p - c_D q |u_{0,M}|^q) d\vec{x} + 2D(u_{0,M}^2, u_{0,M}^2) = 2\mu M, \end{split}$$

implying that  $\mu \leq 0$ . In order to obtain  $\mu < 0$  in the case  $q \leq \frac{12}{5}$  we note that

$$0 = \frac{d}{d\sigma} \left[ \mathcal{E}_{0}^{p,q} (\sigma^{3/2} u_{0,M} (\sigma \vec{x})) \right] \Big|_{\sigma=1}$$

$$= \frac{d}{d\sigma} \left[ \int_{\mathbb{R}^{3}} (c_{W} \sigma^{2} \|\nabla u_{0,M}\|^{2} + c_{TF} \sigma^{3p/2-3} |u_{0,M}|^{p} - c_{D} \sigma^{3q/2-3} |u_{0,M}|^{q}) d\vec{x} + \frac{1}{2} \sigma D(u_{0,M}^{2}, u_{0,M}^{2}) \right] \Big|_{\sigma=1} (2.24)$$

$$= \int_{\mathbb{R}^{3}} \left( 2c_{W} \|\nabla u_{0,M}\|^{2} d\vec{x} + c_{TF} \frac{3p-6}{2} |u_{0,M}|^{p} - c_{D} \frac{3q-6}{2} |u_{0,M}|^{q} \right) d\vec{x} + \frac{1}{2} D(u_{0,M}^{2}, u_{0,M}^{2})$$

as  $u_{0,M}$  is a minimizer for  $\mathscr{I}_0^{p,q}(M)$ , or, equivalently,

$$c_{D} \frac{q}{2} \int_{\mathbb{R}^{3}} |u_{0,M}|^{q} d\vec{x} = c_{W} \frac{2q}{3q - 6} \int_{\mathbb{R}^{3}} \|\nabla u_{0,M}\|^{2} d\vec{x} + \frac{c_{TF}}{2} \frac{q(p - 2)}{q - 2} \int_{\mathbb{R}^{3}} |u_{0,M}|^{p} d\vec{x} + \frac{q}{2(3q - 6)} D(u_{0,M}^{2}, u_{0,M}^{2}).$$

$$(2.25)$$

Consequently, plugging (2.25) into (2.23) gives

$$\begin{split} \mu M &= \int_{\mathbb{R}^3} \left[ -c_W \left( \frac{2q}{3q-6} - 1 \right) \|\nabla u_{0,M}\|^2 - \frac{c_{TF}}{2} \left( q \frac{p-2}{q-2} - p \right) |u_{0,M}|^p \right] d\vec{x} \\ &- \left[ \frac{q}{2(3q-6)} - 1 \right] D(u_{0,M}^2, u_{0,M}^2) \\ &= \int_{\mathbb{R}^3} \left( -c_W \frac{6-q}{3q-6} \|\nabla u_{0,M}\|^2 - c_{TF} \frac{p-q}{q-2} |u_{0,M}|^p \right) d\vec{x} - \frac{12-5q}{2(3q-6)} D(u_{0,M}^2, u_{0,M}^2), \end{split}$$

hence  $\mu < 0$  in the case  $q \le \frac{12}{5}$ . Now suppose  $\frac{12}{5} < q \le \frac{8}{3}$  and  $M \ll 1$ . We can rewrite (2.24) as

$$c_{TF} \frac{p}{2} \int_{\mathbb{R}^{3}} |u_{0,M}|^{p} d\vec{x} = \int_{\mathbb{R}^{3}} \left[ -c_{W} \frac{2p}{3p-6} \|\nabla u_{0,M}\|^{2} + \frac{c_{D}}{2} \frac{p(q-2)}{p-2} |u_{0,M}|^{q} \right] d\vec{x} - \frac{p}{2(3p-6)} D(u_{0,M}^{2}, u_{0,M}^{2}),$$
(2.26)

and insert (2.26) into (2.23) to obtain

$$\mu M = \int_{\mathbb{R}^3} \left[ -c_W \left( \frac{2p}{3p - 6} - 1 \right) \|\nabla u_{0,M}\|^2 + \frac{c_D}{2} \left( p \frac{q - 2}{p - 2} - q \right) |u_{0,M}|^p \right] d\vec{x} - \left[ \frac{p}{2(3p - 6)} - 1 \right] D(u_{0,M}^2, u_{0,M}^2)$$

$$= \int_{\mathbb{R}^3} \left( -c_W \frac{6 - p}{3p - 6} \|\nabla u_{0,M}\|^2 - c_D \frac{p - q}{p - 2} |u_{0,M}|^q \right) d\vec{x} - \frac{12 - 5p}{2(3p - 6)} D(u_{0,M}^2, u_{0,M}^2),$$

Then, from (2.7) with r = q we obtain that that  $\mu < 0$  if M is sufficiently small.

We note that if we insert D, or any other term, into the equation for  $-\mu$  we do not improve  $q \leq \frac{12}{5}$ . For

instance, inserting D into (2.23) gives

$$\begin{split} \mu M &= \int_{\mathbb{R}^3} \left[ -3c_W \|\nabla u_{0,M}\|^2 - c_{TF} \left( 3p - 6 - \frac{p}{2} \right) |u_{0,M}|^p + c_D \left( 3q - 6 - \frac{q}{2} \right) |u_{0,M}|^q \right] d\overrightarrow{x} \\ &= \int_{\mathbb{R}^3} \left[ -3c_W \|\nabla u_{0,M}\|^2 - \frac{c_{TF}}{2} (5p - 12) |u_{0,M}|^p + \frac{c_D}{2} (5q - 12) |u_{0,M}|^q \right] d\overrightarrow{x}. \end{split}$$

so we can see that  $q = \frac{12}{5}$  would be a sufficient condition.

Also, we observe that the Pohozaev identity associated with (1.9) does not bring new information about  $\mu$ .

Next, we observe that  $u_{0,M} \in \mathscr{H}^2(\mathbb{R}^3) \subset \mathscr{L}^{\infty}(\mathbb{R}^3)$  as a result of  $-\Delta u_{0,M} \in \mathscr{L}^2(\mathbb{R}^3)$  and by elliptic regularity.  $u_{0,M}(\vec{x}) \xrightarrow[\parallel \vec{x} \parallel \to \infty]{} 0$  and (1.9) ensure

$$-c_W \Delta u_{0,M} = \left(\mu - \frac{5}{3}c_{TF}u_{0,M}^{\frac{4}{3}} + \frac{4}{3}c_Du_{0,M}^{\frac{2}{3}} - u_{0,M}^2 \star \|\cdot\|^{-1}\right)u_{0,M},$$

for some  $\mu < 0$ . Fix  $t \in (0, \sqrt{-\mu/c_W})$ ; then, we have

$$-\Delta u_{0,M} + t^2 u_{0,M} < \left[ \frac{1}{2} \left( t^2 + \frac{\mu}{c_W} \right) + \frac{4}{3} \frac{c_D}{c_W} u_{0,M}^{\frac{2}{3}} \right] u_{0,M},$$

so that for R large enough

$$-\Delta u_{0,M} + t^2 u_{0,M} < 0$$
, pointwise almost everywhere in  $\mathbb{R}^3 \setminus B_R(0)$ .

Next, we can check that

$$-\Delta e^{-t||\vec{x}||} + t^2 e^{-t||\vec{x}||} > 0$$
, pointwise almost everywhere in  $\mathbb{R}^3 \setminus B_R(\vec{0})$ ,

and that there exists C > 0 so that

$$|u_{0,M}|_{\partial B_{R}(\overrightarrow{0})} \leq Ce^{-tR} = Ce^{-t||\overrightarrow{x}||}|_{\partial B_{R}(\overrightarrow{0})}$$

Thus,

$$-\Delta[u_{0,M}(\vec{x}) - Ce^{-t||\vec{x}||}] + t^2[u_{0,M}(\vec{x}) - Ce^{-t||\vec{x}||}] < 0, \text{ pointwise almost everywhere in } \mathbb{R}^3 \setminus B_R(\vec{0}).$$

At this point, we use the maximum principle to assert that  $u_{0,M}(\vec{x})$  is dominated by the supersolution  $v(\vec{x}) = Ce^{-t||\vec{x}||}$  in  $\mathbb{R}^3 \setminus B_R(\vec{0})$ . As the domain is unbounded, this requires some care, but applying Stampacchia's method as in Benguria, Brezis and Lieb [8, Lemma 8] we obtain the desired bound,

$$0 < u_{0,M}(\vec{x}) \le v(\vec{x}) = Ce^{-t||\vec{x}||}, \qquad \vec{x} \in \mathbb{R}^3 \setminus B_R(\vec{0}).$$

The estimate on  $\|\nabla u\|$  follows from standard elliptic estimates; see for instance Theorems 8.22 and 8.32 of [26].

**Proposition 11.** If  $\mathscr{I}_V^{p,q}(M)$  is attained at  $u_M$ , then (1.8) holds with Lagrange multiplier  $\mu \leq 0$  induced by the mass constraint. Furthermore,  $\mu < 0$  if

- (i)  $V \ge V_{TFDW}$  satisfies (1.2) and  $M \le \mathcal{Z} + \kappa$ , for some  $\kappa = \kappa(\mathcal{Z}) > 0$ , or
- (ii) V is of long-range (1.7), or
- (iii) V satisfies (1.2),  $M \ll 1$ , and

$$E := \inf \left\{ \int_{\mathbb{R}^3} (\|\nabla u_M\|^2 - V u_M^2) d\vec{x}; u_M \in \mathcal{H}^1(\mathbb{R}^3), \|u_M\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 = 1 \right\} < 0, \ or,$$

(iv) V is given by (1.5), and  $M \ll 1$ .

**Remark 4.** (i) In the case  $p \le 4$ , (1.8) implies that  $u_M \in C^{0,\alpha}(\mathbb{R}^3)$  for all  $0 < \alpha < 1$ ,  $|u_M| > 0$ , and  $u_M$  is smooth wherever V is.

(ii) When the Lagrange multiplier  $\mu < 0$ , we obtain exponential decay (see (66) in [37]) as in (2.22). Even if  $\mu_0 = 0$ , we still have  $|u_{0,M}| + \|\nabla u_{0,M}\| \xrightarrow{\|\vec{x}\| \to \infty} 0$ . This follows from 1.8 and Theorem 8.17 uniformly by Gilbarg and Trudinger [26].

*Proof.* The proof of (1.8) with  $\mu \le 0$  does not differ from the one of (1.9) with  $\mu \le 0$  substantially.

Statement (i) is the equivalent to part (ii) of Theorem 1 by Le Bris [31], and its prove does not change substantially. More precisely, if  $\mu=0$  and  $M\leq \mathscr{Z}$ , then Newton's Theorem and Lemma 7.18. of Lieb [33] imply that  $u_M\not\in \mathscr{L}^2(\mathbb{R}^3)$ , a contradiction to  $u_M\in \mathscr{H}^1(\mathbb{R}^3)$ . On the other hand, if it is possible to find sequences  $\{\mu_n\}_{n\in\mathbb{N}}=\{0\}$ ,  $\{u_{M_n}\}_{n\in\mathbb{N}}$  and  $M_n\downarrow\mathscr{Z}$  such that  $\mathscr{I}_V^{p,q}(M_n)$  is attained at  $u_{M_n}$ , and  $u_{M_n}$  is associated with the Lagrange multiplier  $\mu_n$ , then  $u_{M_n}\xrightarrow[n\to\infty]{}u_\mathscr{Z}$  in  $\mathscr{H}^1(\mathbb{R}^3)$  and  $\mu_n\xrightarrow[n\to\infty]{}\mu$  where  $u_\mathscr{Z}$  is a minimum of  $\mathscr{I}_V^{p,q}(\mathscr{Z})$  associated with the Lagrange multiplier  $\mu$ . However,  $\mu_n\xrightarrow[n\to\infty]{}0$  and  $\mu\neq 0$  simultaneously. Thus we reach a contradiction.

Statement (ii) is the equivalent to Theorem 2 of Alama *et al.* [3] and its prove does not change substantially. More precisely, if  $\mu = 0$ , then Newton's Theorem and Lemma 7.18. of Lieb [33] imply that  $u_M \notin \mathcal{L}^2(\mathbb{R}^3)$ , a contradiction to  $u_M \in \mathcal{H}^1(\mathbb{R}^3)$ .

Statement (iii) follows by the same reasoning as in the proof of Corollary II.2. of Lions [37]. More precisely, if  $\mathscr{I}_V^{p,q}\left(\frac{1}{n}\right)$  is attained at  $u_{1/n}$ , and  $u_{1/n}$  is associated with the Lagrange multiplier  $\mu_n$ , then  $\sqrt{n}u_{1/n} \xrightarrow[n \to \infty]{} \phi$  in  $\mathscr{H}^1(\mathbb{R}^3)$ , where  $\phi$  is the minimizer for E. Then,  $\mu_n \xrightarrow[n \to \infty]{} E < 0$ .

The following result is instrumental in studying qualitative behaviour of minimizers further. This result allows us to understand the contribution a minimizer makes to the TFDW energy outside and inside balls.

**Proposition 12.** (i) (Localization estimate) Let  $\chi, \eta : \mathbb{R} \to [0, 1]$  be smooth functions satisfying  $\chi^2 + \eta^2 \equiv 1$  on  $\mathbb{R}^3$ , and define  $\Omega := \{\vec{x} \in \mathbb{R}^3 : \chi(\vec{x}) \in (0, 1)\}$ . If  $\mathcal{I}_V^{p,q}(M)$  is attained at  $u_M$ , then

$$D(\chi^{2}u_{M}^{2}, \eta^{2}u_{M}^{2}) \leq \int_{\mathbb{R}^{3}} V \eta^{2} u_{M}^{2} d\vec{x} + \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + c_{W} \left( \|\nabla \chi\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2} + \|\nabla \eta\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2} \right) \right\} \int_{\Omega} u_{M}^{2} d\vec{x}.$$

$$(2.27)$$

(ii) (Annular estimate) If  $\mathcal{I}_V^{p,q}(M)$  is attained at  $u_M$ , then

$$\forall \vec{x}_{0} \in \mathbb{R}^{3}, R \geq 1, \quad \left( \int_{B_{R}(\vec{x}_{0})} u_{M}^{2} d\vec{x} \right) \left( \int_{\mathbb{R}^{3} \setminus B_{2R}(\vec{x}_{0})} \frac{\|\vec{x} - \vec{x}_{0}\|}{\|\vec{x}\|} u_{M}^{2}(\vec{x}) d\vec{x} \right) \\
\leq 12 \int_{\mathbb{R}^{3} \setminus B_{R}(\vec{x}_{0})} \left\{ c_{D} \frac{p - q}{p - 2} \left[ \frac{c_{D}(q - 2)}{c_{TF}(p - 2)} \right]^{\frac{q - 2}{p - q}} + 8c_{W} + \|\vec{x} - \vec{x}_{0}\| V(\vec{x}) \right\} u_{M}^{2}(\vec{x}) d\vec{x}. \quad (2.28)$$

(iii) (Special case of the annular estimate) Let V be as in (1.3). If  $\mathscr{I}_V^{p,q}(M)$  is attained at  $u_M$ , then

$$\forall R \gg 1, \exists C_{R,\mathscr{Z}} \in \mathbb{R}^{+}, \quad \left(\frac{1}{3} \int_{B_{R}(\vec{0})} u_{M}^{2} d\vec{x} - C_{R,\mathscr{Z}}\right) \int_{\mathbb{R}^{3} \setminus B_{2R}(\vec{0})} u_{M}^{2} d\vec{x} 
\leq 4 \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_{W} \right\} \int_{\mathbb{R}^{3} \setminus B_{R}(\vec{x}_{0})} u_{M}^{2} d\vec{x}. \quad (2.29)$$

*Moreover, we can choose constants*  $\{C_{R,\mathscr{Z}}\}_{R\gg 1}$  *so that* 

$$\lim_{R\to\infty} C_{R,\mathscr{Z}}=\mathscr{Z}.$$

*Proof.* We follow ideas by Nam and Van Den Bosch [46, Lemmas 6 and 7].

(i) Since

$$M = \int_{\mathbb{R}^3} u_M^2 d\vec{x} = \int_{\mathbb{R}^3} (\chi^2 + \eta^2) u_M^2 d\vec{x} = \int_{\mathbb{R}^3} \chi^2 u_M^2 d\vec{x} + \int_{\mathbb{R}^3} \eta^2 u_M^2 d\vec{x},$$

we can apply the binding inequality to obtain

$$\mathscr{E}_{V}^{p,q}(u_{M}) = \mathscr{I}_{V}(M) \leq I_{V}^{p,q}\left(\|\chi u_{M}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}\right) + \mathscr{I}_{0}^{p,q}\left(\|\eta u_{M}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}\right) \leq \mathscr{E}_{V}^{p,q}(\chi u_{M}) + \mathscr{E}_{0}^{p,q}(\eta u_{M}).$$

Therefore,

$$0 \geq \mathcal{E}_{V}^{p,q}(u_{M}) - \mathcal{E}_{V}^{p,q}(\chi u_{M}) - \mathcal{E}_{0}^{p,q}(\eta u_{M})$$

$$= c_{W} \int_{\mathbb{R}^{3}} (\|\nabla u_{M}\|^{2} - \|\nabla(\chi u_{M})\|^{2} - \|\nabla(\eta u_{M})\|^{2}) d\vec{x}$$

$$+ \int_{\mathbb{R}^{3}} [c_{TF}(1 - |\chi|^{p} - |\eta|^{p})|u_{M}|^{p} - c_{D}(1 - |\chi|^{q} - |\eta|^{q})|u_{M}|^{q}] d\vec{x}$$

$$- \int_{\mathbb{R}^{3}} V(1 - \chi^{2}) u_{M}^{2} d\vec{x} + \frac{1}{2} \left[ D(u_{M}^{2}, u_{M}^{2}) - D(\chi^{2} u_{M}^{2}, \chi^{2} u_{M}^{2}) - D(\eta^{2} u_{M}^{2}, \eta^{2} u_{M}^{2}) \right]$$

$$= c_{W} \int_{\mathbb{R}^{3}} \left[ -(\|\nabla \chi\|^{2} + \|\nabla \eta\|^{2}) u_{M}^{2} + (1 - \chi^{2} - \eta^{2}) \|\nabla u\|^{2} - \frac{1}{2} \nabla(\chi^{2} + \eta^{2}) \cdot \nabla u_{M}^{2} \right] d\vec{x}$$

$$+ \int_{\mathbb{R}^{3}} [c_{TF}(1 - |\chi|^{p} - |\eta|^{p})|u_{M}|^{p} - c_{D}(1 - |\chi|^{q} - |\eta|^{q})|u_{M}|^{q}] d\vec{x} - \int_{\mathbb{R}^{3}} V \eta^{2} d\vec{x}$$

$$+ \frac{1}{2} \int_{\mathbb{R}^{3}} \int_{\mathbb{R}^{3}} \frac{u_{M}^{2}(\vec{x}) u_{M}^{2}(\vec{y})}{\|\vec{x} - \vec{y}\|} [1 - \chi^{2}(\vec{x}) \chi^{2}(\vec{y}) - \eta^{2}(\vec{x}) \eta^{2}(\vec{y})] d\vec{x} d\vec{y}$$

$$= -c_{W} \int_{\mathbb{R}^{3}} (\|\nabla \chi\|^{2} + \|\nabla \eta\|^{2}) u_{M}^{2} d\vec{x}$$

$$+ \int_{\mathbb{R}^{3}} [c_{TF}(1 - |\chi|^{p} - |\eta|^{p})|u_{M}|^{p} - c_{D}(1 - |\chi|^{q} - |\eta|^{q})|u_{M}|^{q}] d\vec{x}$$

$$- \int_{\mathbb{R}^{3}} V \eta^{2} d\vec{x} + \frac{1}{2} \int_{\mathbb{R}^{3}} \int_{\mathbb{R}^{3}} \frac{u_{M}^{2}(\vec{x}) u_{M}^{2}(\vec{y})}{\|\vec{x} - \vec{y}\|} [1 - \chi^{2}(\vec{x}) \chi^{2}(\vec{y}) - \eta^{2}(\vec{x}) \eta^{2}(\vec{y})] d\vec{x} d\vec{y}.$$

Equation (2.27) follows from estimating each of the terms on the right hand of the inequality above.

First,  $\nabla \chi \, \mathbb{1}_{\mathbb{R}^3 \setminus \Omega} = \nabla \eta \, \mathbb{1}_{\mathbb{R}^3 \setminus \Omega} \equiv 0$  gives

$$\int_{\mathbb{R}^{3}} (\|\nabla \chi\|^{2} + \|\nabla \eta\|^{2}) u_{M}^{2} d\vec{x} = -\int_{\Omega} (\|\nabla \chi\|^{2} + \|\nabla \eta\|^{2}) u_{M}^{2} d\vec{x} 
\geq -\left(\|\nabla \chi\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2} + \|\nabla \eta\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2}\right) \int_{\Omega} u_{M}^{2} d\vec{x}.$$
(2.31)

Second, from

$$0 \leq 1 - |\chi|^q - |\eta|^q \leq 1 - |\chi|^p - |\eta|^p \leq \mathbb{1}_{\Omega}, \quad (1 - |\chi|^r - |\eta|^r) \mathbb{1}_{\mathbb{R}^3 \setminus \Omega} \equiv 0, \quad r \geq 1$$

and

$$|c_{TF}|t|^p - c_D|t|^q \ge -c_D \frac{p-q}{p-2} \left[ \frac{c_D(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} |t|^2, \quad t \in \mathbb{R},$$

we obtain

$$\int_{\mathbb{R}^{3}} \left[ c_{TF} (1 - |\chi|^{p} - |\eta|^{p}) |u_{M}|^{p} - c_{D} (1 - |\chi|^{q} - |\eta|^{q}) |u_{M}|^{q} \right] d\vec{x} 
\geq \int_{\Omega} (1 - |\chi|^{p} - |\eta|^{p}) (c_{TF} |u_{M}|^{p} - c_{D} |u_{M}|^{q}) d\vec{x} 
\geq -c_{D} \frac{p - q}{p - 2} \left[ \frac{c_{D} (q - 2)}{c_{TF} (p - 2)} \right]^{\frac{q - 2}{p - q}} \int_{\Omega} u_{M}^{2} d\vec{x}.$$
(2.32)

Third,

$$1 - \chi^2(\vec{x})\chi^2(\vec{y}) - \eta^2(\vec{x})\eta^2(\vec{y}) = \chi^2(\vec{x})\eta^2(\vec{y}) + \eta^2(\vec{x})\chi^2(\vec{y}), \quad \vec{x}, \vec{y} \in \mathbb{R}^3,$$

so that, by symmetry of the nonlocal term,

$$\frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{u_M^2(\vec{x}) u_M^2(\vec{y})}{\|\vec{x} - \vec{y}\|} [1 - \chi^2(\vec{x}) \chi^2(\vec{y}) - \eta^2(\vec{x}) \eta^2(\vec{y})] d\vec{x} d\vec{y} = D(\chi^2 u_M^2, \eta^2 u_M^2). \quad (2.33)$$

By plugging (2.31), (2.32), and (2.33) back into (2.30) we get

$$\begin{split} 0 &\geq -\left(\|\nabla \chi\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2} + \|\nabla \eta\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2}\right) \int_{\Omega} u_{M}^{2} d\vec{x} - c_{D} \frac{p-q}{p-2} \left[\frac{c_{D}(q-2)}{c_{TF}(p-2)}\right]^{\frac{q-2}{p-q}} \int_{\Omega} u_{M}^{2} d\vec{x} \\ &- \int_{\mathbb{R}^{3}} V \eta^{2} u_{M}^{2} d\vec{x} + D(\chi^{2} u_{M}^{2}, \eta^{2} u_{M}^{2}) \\ &= -\left\{c_{D} \frac{p-q}{p-2} \left[\frac{c_{D}(q-2)}{c_{TF}(p-2)}\right]^{\frac{q-2}{p-q}} + c_{W} \left(\|\nabla \chi\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2} + \|\nabla \eta\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})}^{2}\right)\right\} \int_{\Omega} u_{M}^{2} d\vec{x} \\ &- \int_{\mathbb{R}^{3}} V \eta^{2} u_{M}^{2} d\vec{x} + D(\chi^{2} u_{M}^{2}, \eta^{2} u_{M}^{2}), \end{split}$$

which corresponds to (2.27) but rearranged.

(ii) Let us fix any pair of smooth functions  $f, g : \mathbb{R} \to [0, 1]$  for which

$$f^2 + g^2 \equiv 1$$
,  $f \mathbb{1}_{t \le 0} \equiv 1$ ,  $f \mathbb{1}_{t \ge 1} \equiv 0$ , and  $||f'||, ||g'||_{\mathscr{L}^{\infty}(\mathbb{R}^3)} \le 2$ . (2.34)

Define functions  $\chi_k, \eta_k : \mathbb{R}^3 \to [0,1]$  by

$$\chi_k(\vec{x}) := f(\|\vec{x} - \vec{x}_0\| - R - k), \eta_k(\vec{x}) := g(\|\vec{x} - \vec{x}_0\| - R - k).$$

Each pair  $(\chi_k, \eta_k)$  satisfies hypotheses of part a) of this Lemma with corresponding sets

$$\Omega_k = \{ \overrightarrow{x} \in \mathbb{R}^3 : \chi_k(\overrightarrow{x}) \in (0,1) \} = B_{R+k+1}(\overrightarrow{x}_0) \setminus B_{R+k}(\overrightarrow{x}_0).$$

By applying (2.27) to each pair  $\chi_k$ ,  $\eta_k$  and adding over  $k \in \mathbb{N} \cup \{0\}$  we obtain

$$\begin{split} \sum_{k=0}^{\infty} D(\chi_{k}^{2} u_{M}^{2}, \eta_{k}^{2} u_{M}^{2}) &\leq \sum_{k=0}^{\infty} \left[ \int_{\mathbb{R}^{3}} V \, \eta_{k}^{2} u_{M}^{2} d\vec{x} + C_{k} \int_{B_{R+k+1}(\vec{x}_{0}) \setminus B_{R+k}(\vec{x}_{0})} u_{M}^{2} d\vec{x} \right] \\ &\leq \sum_{k=0}^{\infty} \left\{ \int_{\mathbb{R}^{3}} V \, \eta_{k}^{2} u_{M}^{2} d\vec{x} \right. \\ &\left. + \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_{W} \right\} \int_{B_{R+k+1}(\vec{x}_{0}) \setminus B_{R+k}(\vec{x}_{0})} u_{M}^{2} d\vec{x} \right\} \end{split}$$

$$= \sum_{k=0}^{\infty} \int_{\mathbb{R}^{3}} V \, \eta_{k}^{2} u_{M}^{2} d\vec{x} + \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_{W} \right\} \int_{\mathbb{R}^{3} \setminus B_{R}(\vec{x}_{0})} u_{M}^{2} d\vec{x} , \end{split}$$

where

$$C_k := c_D \frac{p-q}{p-2} \left[ \frac{c_D(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + \|\nabla \chi_k\|_{\mathscr{L}^{\infty}(\mathbb{R}^3)}^2 + \|\nabla \eta_k\|_{\mathscr{L}^{\infty}(\mathbb{R}^3)}^2.$$

Now note that, by definition,

$$\chi_k \mathbb{1}_{B_{R+k}(\vec{x}_0)} \equiv 1, \qquad \chi_k \mathbb{1}_{\mathbb{R}^3 \setminus B_{R+k+1}(\vec{x}_0)} \equiv 0,$$
(2.36)

or, equivalently,

$$\eta_k \mathbb{1}_{B_{R+k}(\vec{x}_0)} \equiv 0, \qquad \eta_k \mathbb{1}_{\mathbb{R}^3 \setminus B_{R+k+1}(\vec{x}_0)} \equiv 1.$$
(2.37)

On the other hand, (2.36), (2.37), and

$$\|\vec{x} - \vec{y}\| \le \|\vec{x}\| + \|\vec{y}\| \le R + k + 1 + \|\vec{y}\| \le 3\|\vec{y}\|, \quad \vec{x} \in B_{R+k+1}(\vec{0}), \vec{y} \in \mathbb{R}^3 \setminus B_{R+k}(\vec{0})$$

give

$$\begin{split} D(\chi_{k}^{2}u_{M}^{2},\eta_{k}^{2}u_{M}^{2}) &= \int_{B_{R+k+1}(\vec{x}_{0})} \int_{\mathbb{R}^{3}\backslash B_{R+k}(\vec{x}_{0})} \frac{\chi_{k}^{2}(\vec{x})u_{M}^{2}(\vec{x})\eta_{k}^{2}(\vec{y})u_{M}^{2}(\vec{y})}{\|\vec{x}-\vec{y}\|} d\vec{x}d\vec{y} \\ &\geq \int_{B_{R+k}(\vec{x}_{0})} \int_{\mathbb{R}^{3}\backslash B_{R+k}(\vec{x}_{0})} \frac{\chi_{k}^{2}(\vec{x})u_{M}^{2}(\vec{x})\eta_{k}^{2}(\vec{y})u_{M}^{2}(\vec{y})}{3\|\vec{y}\|} d\vec{x}d\vec{y} \\ &= \left(\frac{1}{3}\int_{B_{R+k}(\vec{x}_{0})} \chi^{2}u_{M}^{2}d\vec{x}\right) \int_{\mathbb{R}^{3}} \frac{\eta_{k}^{2}(\vec{x})u_{M}^{2}(\vec{x})}{\|\vec{x}\|} d\vec{x} \\ &\geq \left(\frac{1}{3}\int_{B_{R}(\vec{x}_{0})} u_{M}^{2}d\vec{x}\right) \int_{\mathbb{R}^{3}} \frac{\eta_{k}^{2}(\vec{x})u_{M}^{2}(\vec{x})}{\|\vec{x}\|} d\vec{x}, \quad k \in \mathbb{N} \cup \{0\}. \end{split}$$

As a result,

$$\sum_{k \in \mathbb{N}\{0\}} D(\chi_k^2 u_M^2, \eta_k^2 u_M^2) \geq \left(\frac{1}{3} \int_{B_R(\overrightarrow{x}_0)} u_M^2 d\overrightarrow{x}\right) \sum_{k=0}^{\infty} \int_{\mathbb{R}^3} \frac{\eta_k^2(\overrightarrow{x}) u_M^2(\overrightarrow{x})}{\|\overrightarrow{x}\|} d\overrightarrow{x}.$$

Plugging this back into (2.35) gives

$$\left(\frac{1}{3}\int_{B_{R}(\vec{x}_{0})}u_{M}^{2}d\vec{x}\right)\sum_{k=0}^{\infty}\int_{\mathbb{R}^{3}}\frac{\eta_{k}^{2}(\vec{x})u_{M}^{2}(\vec{x})}{\|\vec{x}\|}d\vec{x} \leq \sum_{k=0}^{\infty}\int_{\mathbb{R}^{3}}V\eta_{k}^{2}u_{M}^{2}d\vec{x} + C\int_{\mathbb{R}^{3}\backslash B_{R}(\vec{x}_{0})}u_{M}^{2}d\vec{x}.$$
(2.38)

Next, note that

$$\mathbb{1}_{\mathbb{R}^3 \setminus B_{R+k+1}(\overrightarrow{x}_0)} \le \eta_k^2 \le \mathbb{1}_{\mathbb{R}^3 \setminus B_{R+k}(\overrightarrow{x}_0)}, \quad k \in \mathbb{N} \cup \{0\},$$

$$\sum_{k=0}^{\infty} \mathbb{1}_{\mathbb{R}^3 \setminus B_{R+k}(\vec{x}_0)}(\vec{x}) \le \|\vec{x} - \vec{x}_0\| \mathbb{1}_{\mathbb{R}^3 \setminus B_{R}(\vec{x}_0)}(\vec{x}), \quad \vec{x} \in \mathbb{R}^3$$

and

$$\begin{split} \sum_{k=0}^{\infty} \mathbb{1}_{\mathbb{R}^{3} \backslash B_{R+k+1}(\vec{x}_{0})}(\vec{x}) &\geq \frac{1}{2} (\|\vec{x} - \vec{x}_{0}\| - R) \mathbb{1}_{\mathbb{R}^{3} \backslash B_{R+1}(\vec{x}_{0})}(\vec{x}) \\ &\geq \frac{1}{4} \|\vec{x} - \vec{x}_{0}\| \mathbb{1}_{\mathbb{R}^{3} \backslash B_{2R}(\vec{x}_{0})}(\vec{x}), \quad \vec{x} \in \mathbb{R}^{3}. \end{split}$$

Then,

$$\frac{1}{4} \| \vec{x} - \vec{x}_0 \| \mathbb{1}_{\mathbb{R}^3 \setminus B_{2R}(\vec{x}_0)}(\vec{x}) \le \sum_{k=0}^{\infty} [\eta_k(\vec{x})]^2 \le \| \vec{x} - \vec{x}_0 \| \mathbb{1}_{\mathbb{R}^3 \setminus B_R(\vec{x}_0)}(\vec{x}), \quad \vec{x} \in \mathbb{R}^3.$$

This implies that

$$\sum_{k=0}^{\infty} \int_{\mathbb{R}^3} V \, \eta_k u_M^2 d\vec{x} \le \int_{\mathbb{R}^3 \setminus B_R(\vec{x}_0)} V(\vec{x}) \|\vec{x} - \vec{x}_0\| u_M^2(\vec{x}) d\vec{x}, \tag{2.39}$$

and

$$\sum_{k=0}^{\infty} \int_{\mathbb{R}^3} \frac{\eta_k^2(\vec{x}) u_M^2(\vec{x})}{\|\vec{x}\|} d\vec{x} \ge \frac{1}{4} \int_{\mathbb{R}^3 \setminus B_{2R}(\vec{x}_0)} \frac{\|\vec{x} - \vec{x}_0\| u_M^2(\vec{x})}{\|\vec{x}\|} d\vec{x}. \tag{2.40}$$

Equation (2.28) follows from plugging (2.39) and (2.40) back into (2.38).

(iii) The proof of (2.29) is the same to that of (2.28) with  $\vec{x}_0 = \vec{0}$  up to (2.38). At that point, we use

$$\exists C_{R,\mathscr{Z}} \in \mathbb{R}^+, \forall \overrightarrow{x} \in \mathbb{R}^3 \setminus B_R(\overrightarrow{0}), \quad V(\overrightarrow{x}) \leq \frac{C_{R,\mathscr{Z}}}{\|\overrightarrow{x}\|}$$

to obtain that

$$\left(\frac{1}{3}\int_{B_{R}(\overrightarrow{x}_{0})}u_{M}^{2}d\overrightarrow{x}\right)\sum_{k=0}^{\infty}\int_{\mathbb{R}^{3}}\frac{\eta_{k}^{2}(\overrightarrow{x})u_{M}^{2}(\overrightarrow{x})}{\|\overrightarrow{x}\|}d\overrightarrow{x}$$

$$\leq C_{R,\mathscr{Z}}\sum_{k=0}^{\infty}\int_{\mathbb{R}^{3}}\frac{\eta_{k}^{2}(\overrightarrow{x})u_{M}^{2}(\overrightarrow{x})}{\|\overrightarrow{x}\|}d\overrightarrow{x}+C\int_{\mathbb{R}^{3}\backslash B_{R}(\overrightarrow{x}_{0})}u_{M}^{2}d\overrightarrow{x};$$

or, equivalently,

$$\left(\frac{1}{3} \int_{B_{R}(\vec{x}_{0})} u_{M}^{2} d\vec{x} - C_{R,\mathscr{Z}}\right) \sum_{k=0}^{\infty} \int_{\mathbb{R}^{3}} \frac{\eta_{k}^{2}(\vec{x}) u_{M}^{2}(\vec{x})}{\|\vec{x}\|} d\vec{x} \leq C \int_{\mathbb{R}^{3} \setminus B_{R}(\vec{x}_{0})} u_{M}^{2} d\vec{x}. \tag{2.41}$$

Equation (2.29) follows from using (2.40) with  $\vec{x}_0 = \vec{0}$  to estimate the left hand side of (2.41).

Pick any pair of functions  $f,g:\mathbb{R}\to[0,1]$  satisfying (2.34), and define  $\chi_R,\eta_R:\mathbb{R}^3\to[0,1]$  for  $R\in\mathbb{R}^+$ , by

$$\chi_R(\vec{x}) := f(||\vec{x}|| - R) \text{ and } \eta_R(\vec{x}) := g(||\vec{x}|| - R).$$

For each M > 0, let  $u_M$  be a minimizer for  $\mathscr{I}_V^{p,q}$  and fix  $R_M \in \mathbb{R}^+$  for which

$$\int_{\mathbb{R}^3} \chi_{R_M}^2 u_M^2 d\overrightarrow{x} = \frac{M}{2} = \int_{\mathbb{R}^3} \eta_{R_M}^2 u_M^2 d\overrightarrow{x}.$$

Since  $\chi_{R_M} \mathbb{1}_{B_{R_M}(\vec{0})} \equiv 1$  and  $\chi_{R_M} \mathbb{1}_{\mathbb{R}^3 \setminus B_{R_M+1}(\vec{0})} \equiv 0$ , or, equivalently,

$$\eta_{R_M} \mathbb{1}_{B_{R_M}(\overrightarrow{0})} \equiv 0 \text{ and } \eta_{R_M} \mathbb{1}_{\mathbb{R}^3 \setminus B_{R_M+1}(\overrightarrow{0})} \equiv 1,$$

we have that

$$\int_{B_{R_M+1}(\vec{0})} u_M^2 d\vec{x} \ge \int_{\mathbb{R}^3} \chi_{R_M}^2 u_M^2 d\vec{x} = \frac{M}{2}.$$
 (2.42)

and

$$\int_{\mathbb{R}^3 \setminus B_{R_M}(\overrightarrow{0})} u_M^2 d\overrightarrow{x} \ge \int_{\mathbb{R}^3} \eta_{R_M}^2 u_M^2 d\overrightarrow{x} = \frac{M}{2}.$$
 (2.43)

Here is an estimate of  $R_M$  in terms of M.

### **Lemma 5.** $M \leq CR_M^3$ .

Proof. Hölder's inequality and Proposition 4 give

$$\begin{split} \frac{M}{2} &= \int_{\mathbb{R}^3} \chi_{R_M}^2 u_M^2 d\vec{x} \le \int_{B_{R_M+1}(\vec{0})} u_M^2 d\vec{x} \\ &\le \left[ \frac{4\pi}{3} (R_M+1)^3 \right]^{\frac{p-2}{p}} \left[ \int_{B_{R_M+1}(\vec{0})} |u_M|^p d\vec{x} \right]^{\frac{2}{p}} \le \left[ \frac{4\pi}{3} (R_M+1)^3 \right]^{\frac{p-2}{p}} M^{\frac{2}{p}}. \end{split}$$

Hence the Lemma follows.

Then, we can say that, under certain conditions, the mass of a minimizer concentrates on an annular region.

#### Corollary 4. Suppose that

$$\limsup_{\|\vec{x}\| \to \infty} \|\vec{x}\| V(\vec{x}) < \infty. \tag{2.44}$$

Then, there exists a constant  $C_V$  independent of M such that if  $M \gg 1$ , then

$$\int_{B_{2R_M+2}(\overrightarrow{0})\setminus B_{R_M/2}(\overrightarrow{0})} u_M^2 d\overrightarrow{x} \ge M - C_V.$$

Furthermore, if V is given by (1.3), then we have

$$\frac{1}{3} \int_{B_{R_M/2}(\vec{0})} u_M^2 d\vec{x} \le C_{R_M, \mathcal{Z}} + 8 \left\{ c_D \frac{p-q}{p-2} \left[ \frac{c_D(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_W \right\},\,$$

and

$$\int_{\mathbb{R}^{3}\setminus B_{2R_{M}+2}} u_{M}^{2} d\vec{x} \leq 24 \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_{W} \right\} \frac{1}{1 - 6\frac{C_{R_{M},2^{*}}}{M}},$$

where 
$$C_{R_M,\mathscr{Z}} \xrightarrow[M \to \infty]{} \mathscr{Z} (C_{R,\mathscr{Z}} = \mathscr{Z} \text{ for } V = \frac{\mathscr{Z}}{\|\overrightarrow{x}\|}).$$

*Proof.* We prove the particular case. The general case is very similar.

By (2.29),

$$\forall R \gg 1, \quad \left[\frac{1}{3} \int_{B_{R}(\vec{0})} u_{M}^{2} d\vec{x} - C_{R,\mathscr{Z}}\right] \int_{\mathbb{R}^{3} \setminus B_{2R}(\vec{0})} u_{M}^{2} d\vec{x} \leq 4 \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_{W} \right\} M,$$

where  $\{C_{R,\mathscr{Z}}\}_{R\gg 1}\subset \mathbb{R}^+$  can be chosen so that  $C_{R,\mathscr{Z}}\to \mathscr{Z}$  as  $R\to\infty$ . Then, we can make use of Lemma 5 to obtain that

$$\left[\frac{1}{3} \int_{B_{R_{M}+1}(\vec{0})} u_{M}^{2} d\vec{x} - C_{R_{M}+1,\mathscr{Z}}\right] \int_{\mathbb{R}^{3} \backslash B_{2R_{M}+2}(\vec{0})} u_{M}^{2} d\vec{x} 
\leq 4 \left\{ c_{D} \frac{p-q}{p-2} \left[ \frac{c_{D}(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_{W} \right\} M, \quad M \gg 1,$$

and

$$\left[\frac{1}{3} \int_{B_{R_M/2}(\vec{0})} u_M^2 d\vec{x} - C_{R_M/2,\mathcal{Z}}\right] \int_{\mathbb{R}^3 \backslash B_{R_M}(\vec{0})} u_M^2 d\vec{x} \leq 4 \left\{ c_D \frac{p-q}{p-2} \left[ \frac{c_D(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_W \right\} M, \quad M \gg 1.$$

Then, (2.42) and (2.43) give

$$\left(\frac{M}{6} - C_{R_M+1,\mathscr{Z}}\right) \int_{\mathbb{R}^3 \setminus B_{2R_M+2}(\overrightarrow{0})} u_M^2 d\overrightarrow{x} \leq 4 \left\{ c_D \frac{p-q}{p-2} \left[ \frac{c_D(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_W \right\} M, \quad M \gg 1.$$

and

$$\frac{M}{2} \left[ \frac{1}{3} \int_{B_{R_M/2}(\vec{0})} u_M^2 d\vec{x} - C_{R_M/2, \mathcal{Z}} \right] \leq 4 \left\{ c_D \frac{p-q}{p-2} \left[ \frac{c_D(q-2)}{c_{TF}(p-2)} \right]^{\frac{q-2}{p-q}} + 8c_W \right\} M, \quad M \gg 1,$$

Hence conclusions follow.

Finally, the following two propositions can be proved with no major changes from [46, Lemma 17 and Theorem 3(ii)], correspondingly.

The first result is a consequence of the fact that the mass of a minimizer concentrates on the annular region  $B_{2R_M+2} \setminus B_{R_M/2}$ , as shown before.

**Proposition 13.** There exists a constant  $C_V$  such that if  $u_M$  is a minimizer for  $\mathscr{I}_V^{p,q}(M)$ , then

$$\sup_{\mathbb{R}^3\setminus B_{R_M/2}(\overrightarrow{0})}|u_M|\geq C.$$

And we can use the Proposition above to show the following:

**Proposition 14.** Suppose that V satisfies both (1.2) and (2.44). Then, for M sufficiently large, minimizers of  $\mathscr{I}_{V}^{p,q}(M)$ , if any, are not radial.

## **Chapter 3**

# Structure of minimizing sequences

In this chapter we prove Theorems 4, 5, and 6. Throughout this chapter, we assume V satisfies (1.2).

The use of Concentration-Compactness techniques in Thomas-Fermi-type problems goes back at least to Lions [37], for whom these problems were an important motivation for the development of the general theory.

## 3.1 General background potential

The idea of the Concentration Theorem 4 is partly contained in Lions[37], although it is not stated as a single Theorem, and it leaves many details left to the reader. We provide a complete proof here.

*Proof of Theorem 4.* We first consider  $V \not\equiv 0$ .

By Proposition 9, there is a function  $u^0 \in \mathcal{H}^1(\mathbb{R}^3) \setminus \{0\}$  such that

$$u_n(\cdot - \overrightarrow{x}_n^0) - u^0 \xrightarrow[n \to \infty]{} 0$$
 in  $\mathcal{H}^1(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ ,

and

$$\mathscr{I}_{V}^{p,q}(M) = \mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(M-m^{0}), \quad \mathscr{I}_{V}^{p,q}(m) = \mathscr{E}_{V}^{p,q}(u^{0}),$$

where  $m^0 := ||u^0||_{\mathcal{L}^2(\mathbb{R}^3)}^2$ .

If  $m^0 = M$ , then the sequence converges strongly in  $\mathcal{L}^2(\mathbb{R}^3)$  by the Brezis-Lieb Lemma [10],  $u^0$  minimizes  $\mathcal{I}_V^{p,q}(M)$ , and the procedure terminates, with N = 0.

If  $m^0 < M$ , then we define the remainder sequence

$$u_n^0 := u_n - u^0, \ n \in \mathbb{N}.$$

We note that by the Brezis-Lieb Lemma [10],  $\|u_n^0\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 \xrightarrow[n \to \infty]{} M - m^0$ , while by weak convergence and the Brezis-Lieb Lemma [10] again, the energy decouples in the limit (see [46, 33]),

$$\lim_{n \to \infty} \left[ \mathcal{E}_V^{p,q}(u_n) - \mathcal{E}_V^{p,q}(u^0) - \mathcal{E}_0^{p,q}(u_n^0) \right] = 0,$$

and thus

$$\mathscr{I}_V^{p,q} = \lim_{n \to \infty} \mathscr{E}_V^{p,q}(u_n) = \mathscr{E}_V^{p,q}(u^0) + \lim_{n \to \infty} \mathscr{E}_0^{p,q}(u_n^0) \geq \mathscr{I}_V^{p,q}(m^0) + \mathscr{I}_0^{p,q}(M - m^0).$$

By the binding inequality (2.10), we have

$$\mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(M - m^{0}) \ge \mathscr{I}_{V}^{p,q}(M) \ge \mathscr{E}_{V}^{p,q}(u^{0}) + \lim_{n \to \infty} \mathscr{E}_{0}^{p,q}(u^{0}) \ge \mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(M - m^{0}), \quad (3.1)$$

and hence we obtain equality of each expression,

$$\mathscr{E}_{V}^{p,q}(u^0)=\mathscr{I}_{V}^{p,q}(m^0)\quad\text{and}\quad \lim_{n\to\infty}\mathscr{E}_{0}^{p,q}(u^0_n)=\mathscr{I}_{0}^{p,q}(M-m^0),$$

that is, the remainder sequence  $\{u_n^0\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_0^{p,q}(M-m^0)$ .

Now we 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 [36]. We claim that  $\omega(\{u_n^0\}_{n\in\mathbb{N}})>0$ , where  $\omega$  is given by (2.21). Indeed, applying [36, Lemma I.1], if  $\omega(\{u_n^0\}_{n\in\mathbb{N}})=0$ , then  $u_n^0\xrightarrow[n\to\infty]{}0$  in  $\mathscr{L}^r(\mathbb{R}^3)$  norm, for each 2< r<6, so in particular

$$\int_{\mathbb{R}^3} |u_n^0|^q \xrightarrow[n\to\infty]{} 0$$

and hence

$$\mathscr{I}_0^{p,q}(M-m^0) = \lim_{n \to \infty} \mathscr{E}_0^{p,q}(u_n^0) \ge 0,$$

which contradicts Proposition 7. Hence "vanishing" cannot occur.

Therefore, we can choose a sequence of translations  $\vec{x}_n^1 \in \mathbb{R}^3$  for which  $u_n^0(\cdot - \vec{x}_n^1) \xrightarrow[n \to \infty]{} u^1$  weakly in  $\mathscr{H}^1(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ , for some  $u^1 \in \mathscr{H}^1(\mathbb{R}^3)$ , with mass

$$m^1 := \|u^1\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 \ge \frac{1}{2}\omega(\{u_n^0\}_{n\in\mathbb{N}}) > 0.$$

As  $u_n^0 \xrightarrow[n \to \infty]{} 0$  and by the Rellich-Kondrakov compactness Theorem, we must have that  $\|\vec{x}_n^1\| \xrightarrow[n \to \infty]{} \infty$ .

In case  $m^0 = M - m^1$ , the sequence converges strongly in  $\mathcal{L}^2(\mathbb{R}^3)$  by the Brezis-Lieb Lemma [10],  $u^1$  minimizes  $\mathcal{L}^{p,q}_V(M-m^1)$ , and we obtain (1.10), (1.11), (1.12), and (1.13), with N=1.

If  $m^1 < M - m^0$ , we again define the remainder sequence  $u_n^1(\vec{x}) := u_n^0(\vec{x}) - u^1(\vec{x} + \vec{x}_n^1)$ . By definition,  $u_n^1 \xrightarrow[n \to \infty]{} 0$ ,  $u^1(\cdot - \vec{x}_n^1) \xrightarrow[n \to \infty]{} 0$ , and  $||u_n^1||_{\mathscr{L}^2(\mathbb{R}^3)}^2 \xrightarrow[n \to \infty]{} M - m^0 - m^1$ , and the energy splits,

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

By the same argument as in (3.1), this implies that

$$\mathscr{E}_0^{p,q}(u^1) = \mathscr{I}_0^{p,q}(m^1), \quad \mathscr{I}_0^{p,q}(M-m^0) = \mathscr{I}_0^{p,q}(m^1) + \mathscr{I}_0^{p,q}(M-m^0-m^1),$$

and  $\{u_n^1\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_0^{p,q}(M-m^0-m^1)$ . Substituting for  $\mathscr{I}_0^{p,q}(M-m^0)$  in (3.1) we conclude:

$$\mathscr{I}_{V}^{p,q}(M) = \mathscr{I}_{V}^{p,q}(m^{0}) + \mathscr{I}_{0}^{p,q}(m^{1}) + \mathscr{I}_{0}^{p,q}(M - m^{0} - m^{1}).$$

We can iterate the process we just described to obtain translations  $\{\vec{x}_n^k\}_{n\in\mathbb{N}}$  in  $\mathbb{R}^3$ ,  $\|\vec{x}_n^k\| \xrightarrow[n\to\infty]{} \infty$ , functions  $u^k \in \mathscr{H}^1(\mathbb{R}^3)$  with

$$\|u^k\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 =: m^k \ge \frac{1}{2}\omega(\{u_n^{k-1}\}_{n\in\mathbb{N}}),\tag{3.2}$$

and remainder sequences

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

for each  $k = 2, 3, \dots$  satisfying:

$$\begin{split} M &= \sum_{i=0}^k m^i + \lim_{n \to \infty} \|u_n^k\|_{\mathscr{L}^2(\mathbb{R}^3)}^2, \\ u_n^k(\cdot - \overrightarrow{x}_n^k) \xrightarrow[n \to \infty]{} 0, \quad \text{weakly in } \mathscr{H}^1(\mathbb{R}^3) \text{ and pointwise almost everywhere in } \mathbb{R}^3, \\ \mathscr{I}_V^{p,q}(M) &= \mathscr{I}_V^{p,q}(m^0) + \sum_{i=1}^k \mathscr{I}_0^{p,q}(m^k) + \mathscr{I}_0^{p,q}\left(M - \sum_{i=0}^k m^i\right), \\ \mathscr{E}_0^{p,q}(u^k) &= \mathscr{I}_V^{p,q}(m^k) \text{ and } \lim_{n \to \infty} \mathscr{E}_0^{p,q}(u_n^k) = \mathscr{I}_0^{p,q}\left(M - \sum_{i=0}^k m^i\right). \end{split}$$

At this point we would like to note that the splitting process terminates at some finite step in the case  $p = \frac{10}{3}$  and  $q = \frac{8}{3}$ . Indeed, the concavity of  $\mathcal{I}_0^{p,q}(M)$  for small (see Proposition 7 or [46, Lemma 9 (iii)],) implies that there exists  $M_c > 0$  such that minimizing sequences for  $\mathcal{I}_0^{p,q}$  do not split for  $M < M_c$ . If the process terminates in finitely many steps, then (1.10), (1.11), and (1.12) hold.

If the splitting process does not end, then since  $M \ge \sum_{i=0}^k m^i$  for all k, we have  $\lim_{i\to\infty} m^i = 0$ , and then, by (3.2), we conclude that

$$\lim_{k \to \infty} \omega(\{u_n^k\}_{n \in \mathbb{N}}) = 0. \tag{3.3}$$

On the other hand, from the proof of Lemma I.I in [36], we have

$$\limsup_{n\to\infty} \int_{\mathbb{R}^3} |u_n^k|^{\frac{10}{3}} d\overrightarrow{x} \leq C \left[\omega(\{u_n^k\}_{n\in\mathbb{N}})\right]^{\frac{2}{3}} \limsup_{n\to\infty} ||u_n^k||^2_{\mathscr{H}^1(\mathbb{R}^3)},$$

where C is a universal constant. Then, since  $\{||u_n^k||_{\mathcal{H}^1(\mathbb{R}^3)}^2\}_{n\in\mathbb{N}}$  is uniformly bounded in k and by (3.3),

$$\lim_{k\to\infty} \limsup_{n\to\infty} \int_{\mathbb{R}^3} |u_n^k|^q d\vec{x} = 0,$$

hence

$$\liminf_{k\to\infty}\mathscr{I}_0^{p,q}\left(M-\sum_{i=0}^k m^i\right)=\liminf_{k\to\infty}\lim_{n\to\infty}\mathscr{E}_0^{p,q}(u_n^k)\geq 0.$$

But then, since  $\mathscr{I}_0^{p,q}$  is strictly negative, equations in (1.12) follow.

All the above prove that statements (1.10) (by the Brezis-Lieb Lemma [10]), (1.11), and (1.12) still hold if the splitting process continues indefinitely, in which case  $N = \infty$ .

Now we show that  $\|\vec{x}_n^k - \vec{x}_n^i\| \xrightarrow[n \to \infty]{} \infty$  for all  $i \neq k$ . Suppose this is not the case, and take the <u>smallest</u> k > i for which  $\{\|\vec{x}_n^k - \vec{x}_n^i\|\}_{n \in \mathbb{N}}$  remains bounded along some subsequence. (And so  $\|\vec{x}_n^i - \vec{x}_n^j\| \xrightarrow[n \to \infty]{} \infty$  for all i < j < k.) Taking a further subsequence if necessary,  $(\vec{x}_n^k - \vec{x}_n^i) \xrightarrow[n \to \infty]{} \vec{\xi}$  for some  $\vec{\xi} \in \mathbb{R}^3$ . Note that

$$u_n^i(\vec{x}) = u_n^k(\vec{x}) + \sum_{j=i+1}^k u^j(\vec{x} + \vec{x}_n^j),$$

and hence

$$u_n^i(\vec{x} - \vec{x}_n^i) = u_n^k(\vec{x} - \vec{x}_n^i) + u^k(\vec{x} - \vec{x}_n^i + \vec{x}_n^i) + \sum_{i=i+1}^k u^j(\vec{x} - \vec{x}_n^i + \vec{x}_n^j). \tag{3.4}$$

Since  $\|\vec{x}_n^j - \vec{x}_n^i\| \xrightarrow[n \to \infty]{} \infty$  for i < j < k,  $u^j(\cdot - \vec{x}_n^i + \vec{x}_n^j) \xrightarrow[n \to \infty]{} 0$ , while  $u^k(\cdot - \vec{x}_n^i + \vec{x}_n^k) \xrightarrow[n \to \infty]{} u^k(\cdot + \vec{\xi})$ . And  $u_n^k(\cdot - \vec{x}_n^i) \xrightarrow[n \to \infty]{} 0$ , and hence we pass to the limit in (3.4) to obtain  $u_n^i(\cdot - \vec{x}_n^i) \xrightarrow[n \to \infty]{} u^k(\cdot + \vec{\xi}) \not\equiv 0$ , which is a contradiction. Hence (1.13) is verified.

Next, we show that each  $u^i$  solves the Euler-Lagrange equation with the same Lagrange multiplier  $\mu$ . By the Ekeland Variational Principle [17] (see also [54, Corollary 5.3],) we may find a minimizing sequence  $\{v_n\}_{n\in\mathbb{N}}$ , with  $\|v_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M$  and  $\|v_n - u_n\| \xrightarrow[n\to\infty]{} 0$ , for which the Euler-Lagrange equation is solved up to an small error in  $\mathscr{H}^{-1}(\mathbb{R}^3)$ . That is,  $\exists \mu_n \in \mathbb{R}$  with

$$D\mathscr{E}_V^{p,q}(v_n) - \mu_n v_n \xrightarrow[n \to \infty]{} 0$$
 in  $\mathscr{H}^{-1}$  norm.

The Lagrange multipliers may be expressed as:

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

as minimizing sequences are bounded. By Propositions 3 10 11,  $\{|\mu_n|\}_{n\in\mathbb{N}}$  is bounded, and hence (up to a sequence) we may assume  $\mu_n \xrightarrow[n\to\infty]{} \mu$  for some  $\mu\in\mathbb{R}$ . As  $u_n(\cdot-\vec{x}_n^i) \xrightarrow[n\to\infty]{} u^i$  weakly in  $\mathscr{H}^1(\mathbb{R}^3)$ , the same

is true for  $\tilde{v}_n := v_n(\cdot - \overrightarrow{x}_n^i) \xrightarrow[n \to \infty]{} u^i$ ,  $i = 0, \dots, N$ . Hence, for every  $\varphi \in C_0^{\infty}(\mathbb{R}^3)$ ,

$$\langle D\mathscr{E}_{V}^{p,q}(u^{0}) - \mu u^{0}, \varphi \rangle = \lim_{n \to \infty} \langle D\mathscr{E}_{V}^{p,q}(\tilde{v}_{n}) - \mu_{n}\tilde{v}_{n}, \varphi \rangle = 0,$$

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

For  $V \equiv 0$ , the functional  $\mathcal{E}_0^{p,q}$  is translation invariant. Hence, we may begin the process at the Step k=1, defining  $\omega(\{u_n\}_{n\in\mathbb{N}})$  and identifying a first set of translates  $\{\vec{x}_n^0\}$  as above. By translation invariance,  $\tilde{u}_n=u_n(\cdot-\vec{x}_n^1)$  is also a minimizing sequence for  $\mathcal{I}_0^{p,q}(M)$ , and the weak limit  $u^0=w-\lim_{n\to\infty}\tilde{u}_n$  is nontrivial. The rest of the proof continues as in the case of nontrivial V.

### 3.2 Potentials that are at least Newtonian

The proof of Theorem 5 relies on the splitting structure given in Theorem 4, and on the idea that, when calculating the interaction energy between fleeing components  $u^i(\vec{x} + \vec{x}_n^i)$ , only the mass  $m^i$  and centers  $\vec{x}_n^i$  enter into the computation at first order. The following Lemma makes this precise for compactly supported components:

**Lemma 6.** (a) Let  $v^1, v^2 \in \mathcal{H}^1(\mathbb{R}^3)$  be functions with compact support, supp  $v^i \subset B_\rho(\overrightarrow{\zeta}^i)$ , i = 1, 2, with  $1 < \rho < \frac{1}{4}R$ ,  $R = \|\overrightarrow{\zeta}^1 - \overrightarrow{\zeta}^2\| > 0$ . Then,

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

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

$$\left| \int_{B_{\rho}(\vec{\zeta})} \frac{|\nu(\vec{x})|^2}{\|\vec{x} - \vec{r}\|^{\nu}} d\vec{x} - \frac{\|\nu\|_{\mathscr{L}^2(\mathbb{R}^3)}^2}{\|\vec{\zeta}\|^{\nu}} \right| \leq C_{\nu} \frac{\rho}{R^{\nu+1}} \|\nu\|_{\mathscr{L}^2(\mathbb{R}^3)}^2.$$

*Proof.* These follow from the pointwise estimates,

$$\left| \frac{1}{\|\overrightarrow{\zeta}^{1} - \overrightarrow{\zeta}^{2}\|} - \frac{1}{\|\overrightarrow{x} - \overrightarrow{y}\|} \right| \leq \frac{2\rho}{(R - \rho)^{2}} \leq \frac{4\rho}{R^{2}},$$

$$\left| \frac{1}{\|\overrightarrow{\zeta}\|^{\theta}} - \frac{1}{\|\overrightarrow{x} - \overrightarrow{r}\|^{\theta}} \right| \leq \frac{\theta\rho}{(\|\overrightarrow{\zeta}\| - \rho - \|r\|)^{\theta + 1}} \leq C_{\theta} \frac{\rho}{R^{1 + \theta}},$$

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

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 proves effective provided we are in a situation where the minimizers  $u^i$  have

exponential decay. To generate localization functions, let us fix any smooth  $\phi: \mathbb{R} \to [0,1]$  for which

$$\phi \mathbb{1}_{(-\infty,0]} \equiv 1, \quad \phi \mathbb{1}_{[1,\infty)} \equiv 0, \quad \|\phi'\|_{\mathscr{L}^{\infty}(\mathbb{R})} \le 2.$$
 (3.5)

Now we prove Theorem 5 and Proposition 1, on the size of the compact part of minimizing sequences. We note that the argument for the first Theorem is similar to Lions' proof of existence of minimizers [37] for TFDW type models in the case  $V = V_{TFDW}$  and  $M \le \mathcal{Z}$ .

Proof of Theorem 5. We rewrite the potential  $V = V_{TFDW} + W$ , where  $W(\vec{x}) \ge 0$  and W satisfies (1.2). To obtain a contradiction, assume  $\{u_n\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_V^{p,q}(M)$  that splits but  $0 < m^0 < \mathscr{Z}$ . We let  $u^i, m^i = \|u^i\|_{\mathscr{L}^2(\mathbb{R}^3)}^2$ , i = 0, ..., N be as given by Theorem 4. Fix unit vectors

$$\vec{v}^i = (0, \cos(2\pi/i), \sin(2\pi/i)) \in \mathbb{R}^3,$$

and for  $\rho > 1$  define  $\overrightarrow{q}_{i=0}^{i^{\infty}}$  by

$$\vec{q}^0 := \vec{0}, \qquad \vec{q}^1 := e^{\sqrt{\rho}} \vec{v}^1, \qquad \vec{q}^i := e^{(i+1)\rho} \vec{v}^i, i = 2, \dots, N.$$

Then we define the truncated components,

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

Each function  $U^i$  has been truncated to have support in the ball  $B_{\rho}(\vec{q}^i)$ .

As  $m^0 < \mathscr{Z}$ , by Proposition 11,  $\mu < 0$  for all Lagrange multipliers corresponding to  $u^i$ , i = 0, ..., N, and hence the exponential decay estimate (2.22) holds for all of them. We choose the constant  $\lambda = \frac{1}{2}\sqrt{-\mu}$  for simplicity. Then,

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

and

$$\mathscr{E}_V^{p,q}(U^0_\rho)=\mathscr{E}_V^{p,q}(u^0)+O(e^{-\lambda\rho}),\qquad \mathscr{E}_0^{p,q}(U^i_\rho)=\mathscr{E}_0^{p,q}(u^i)+O(e^{-\lambda\rho}),\quad i=1,\dots,N.$$

Let

$$w_{\rho} := U_{\rho}^{0} + \sum_{i=1}^{N} U_{\rho}^{i}.$$

As  $\|w_{\rho}\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 < M$ , by monotonicity of  $\mathcal{I}_V^{p,q}(M)$  (see Proposition 7) we have

$$\begin{split} \mathscr{I}_{V}^{p,q}(M) &\leq \mathscr{I}_{V}^{p,q}(\|w_{\rho}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}) \leq \mathscr{E}_{V}^{p,q}(w_{\rho}) \\ &\leq \mathscr{E}_{V}^{p,q}(U_{\rho}^{0}) + \sum_{i=1}^{N} \mathscr{E}_{0}^{p,q}(U_{\rho}^{i}) + \sum_{\stackrel{i,j=0}{i \neq j}}^{N} \int_{B_{\rho}(\vec{q}^{i})} \int_{B_{\rho}(\vec{q}^{j})} \frac{|U_{\rho}^{i}(\vec{x})|^{2} |U_{\rho}^{j}(\vec{y})|^{2}}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y} \\ &- \sum_{i=1}^{N} \int_{B_{\rho}(\vec{q}^{i})} [V_{TFDW}(\vec{x}) + W(\vec{x})] |U_{\rho}^{i}(\vec{x})|^{2} d\vec{x} + O(e^{-\frac{\lambda}{2}\rho}) \end{split}$$

$$= \mathscr{I}_{V}^{p,q}(m^{0}) + \sum_{i=1}^{N} I_{0}(m^{i}) + \sum_{\substack{i,j=0\\i\neq j}}^{N} \int_{B_{\rho}(\vec{q}^{i})} \int_{B_{\rho}(\vec{q}^{j})} \frac{|U_{\rho}^{i}(\vec{x})|^{2} |U_{\rho}^{j}(\vec{y})|^{2}}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y}$$

$$- \sum_{i=1}^{N} \int_{B_{\rho}(\vec{q}^{i})} [V_{TFDW}(\vec{x}) + W(\vec{x})] |U_{\rho}^{i}(\vec{x})|^{2} d\vec{x} + O(e^{-\frac{\lambda}{2}\rho}).$$
(3.6)

Next, we use Lemma 6 to evaluate the interaction terms. Note that  $R^{i,j} = \|\vec{q}^i - \vec{q}^j\|$  is of order  $e^{\sqrt{\rho}}$  when i+j=1, and of order  $e^{3\rho}$  otherwise, and

$$0 < m^i - m^i_\rho < O(e^{-\lambda \rho}).$$

Thus, we have

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

and for i = 1, ..., N, the interaction with  $V_{TFDW}$  gives

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

Substituting into (3.6), and using  $W \ge 0$ , we obtain the strict subadditivity of  $\mathscr{I}_V^{p,q}(M)$ ,

$$\mathscr{I}_{V}^{p,q}(M) - \left[ \mathscr{I}_{V}^{p,q}(m^{0}) + \sum_{i=1}^{N} I_{0}(m^{i}) \right] \leq \frac{m^{0}m^{1} - \mathscr{Z}m^{1}}{e^{\sqrt{\rho}}} + O(e^{-\min\{3/2,\mu/2\}\rho}) < 0,$$

for all  $\rho$  sufficiently large, since we are assuming  $m^0 < \mathcal{Z}$ . However, this contradicts (1.12) in the Concentration Theorem 4. Thus  $m^0 \geq \mathcal{Z}$ , and the Theorem is proved.

The following is stated as part of Proposition 1, but its proof only depends on the bounds stated in Proposition 4, and the result is needed below.

**Proposition 15.** Let  $u_n$  minimize  $\mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M)$ , where  $V_n$  is as in (1.14). Then  $\{u_n\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M)$ .

*Proof.* Let  $u_n$  be a minimizer for  $\mathcal{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M)$ ,  $n \in \mathbb{N}$ . First, note that  $V_1 \geq V_n \geq V_{TFDW}$ , and hence

$$\mathscr{E}_{V_1}^{\frac{10}{3},\frac{8}{3}}(u_n) \leq \mathscr{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}(u_n) = \mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M) \leq \mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M) < 0$$

for all n. Applying Proposition 4 with  $V = V_1$ , the sequence  $\{u_n\}_{n \in \mathbb{N}}$  satisfies the bounds in Lemma 4 uniformly in  $n \in \mathbb{N}$ . Next, we observe that  $\|\vec{x}\|^{-\nu} \in \mathcal{L}^{\frac{3}{2}}_{loc}(\mathbb{R}^3)$  for  $0 < \nu < 1$ , and thus

$$Z_n \int_{\mathbb{R}^3} \frac{u_n^2(\overrightarrow{x})}{\|\overrightarrow{x}\|^{\nu}} d\overrightarrow{x} \leq Z_n \int_{B_1(\overrightarrow{0})} \frac{u_n^2(\overrightarrow{x})}{\|\overrightarrow{x}\|^{\nu}} d\overrightarrow{x} + Z_n \int_{\mathbb{R}^3 \setminus B_1(\overrightarrow{0})} u_n^2(\overrightarrow{x}) d\overrightarrow{x}$$

$$\leq Z_n \|u_n\|_{\mathscr{L}^6(\mathbb{R}^3)}^2 \|\|\overrightarrow{x}\|^{-\nu}\|_{\mathscr{L}^{\frac{3}{2}}(B_1(\overrightarrow{0}))} + Z_n M$$
  
$$\leq c Z_n \|\nabla u_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 + Z_n M \xrightarrow[n \to \infty]{} 0.$$

In particular,

$$\mathscr{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}(u_n) = \mathscr{E}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(u_n) + o(1),$$

and therefore we may conclude,

$$\begin{split} \mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M) & \leq \liminf_{n \to \infty} \mathscr{E}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(u_n) = \liminf_{n \to \infty} \mathscr{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}(u_n) \\ & = \liminf_{n \to \infty} \mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M) \\ & \leq \limsup_{n \to \infty} \mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M) \leq \mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M). \end{split}$$

*Proof of Proposition 1.* In Proposition 15 we have already shown that any sequence of minimizers  $u_n$  of  $\mathcal{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}$  forms a minimizing sequence for  $\mathcal{I}_{V_nFDW}^{\frac{10}{3},\frac{8}{3}}(M)$ . Part (ii) then follows from Theorem 5.

**Lemma 7.** Under all hypotheses of Theorem 6, we have that, up to a subsequence, for all  $0 < t < \sqrt{-\mu/c_W}$ , there exists a constant C independent of n with

$$0 < |u_n(\vec{x})| + ||\nabla u_n(\vec{x})|| \le Ce^{-t\sigma_n(\vec{x})}, \text{ pointwise almost everywhere in } \mathbb{R}^3, \tag{3.7}$$

where

$$\sigma_n(\overrightarrow{x}) := \min_{0 \le i \le N} \|\overrightarrow{x} - \overrightarrow{x}_n^i\|_{\underline{x}}$$

and  $\vec{x}_n^i$  are as in the Concentration Theorem 4.

*Proof.* By Proposition 11, we may take  $u_n > 0$  in  $\mathbb{R}^3$ . Alama *et al.* [3] proved that

$$-c_W \Delta u_n = \left(\mu_n - \frac{5}{3}c_{TF}u_n^{\frac{4}{3}} + \frac{4}{3}c_D u_n^{\frac{2}{3}} + V_n - u_n^2 \star \|\cdot\|^{-1}\right) u_n, \tag{3.8}$$

for some  $\mu_n < 0$ . Additionally, by the final step in the proof of the Concentration Theorem 4,  $\mu_n \xrightarrow[n \to \infty]{} \mu$ . Fix  $t \in (0, \sqrt{-\mu/c_W})$ ; then, for n sufficiently large, we have

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

Furthermore, by Lemma 4 and equation (3.8), 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 apply Theorem 8.17 by Gilbarg and Trudinger [26] to obtain:

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

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

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

On the other hand, by Proposition 15,  $\{u_n\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M)$ , and hence the conclusions of Concentration Theorem 4 hold. In particular, this implies that given  $\varepsilon > 0$ , there exists  $R_0 = R_0(\varepsilon) \ge 1$  such that

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

and (1.10), (1.13), the Rellich-Kondrakov compactness Theorem, and the decay of all  $u^i$  (2.22) ensure that, up to a subsequence,

$$u_n(\cdot + \overrightarrow{x}_n^i) \xrightarrow[n \to \infty]{} u^i \text{ in } \mathscr{L}^2(B_{R/2}(\overrightarrow{0})), \quad i = 0, ...N, R \ge R_0.$$

Consequently,

$$\begin{split} \lim_{n \to \infty} \|u_n\|_{\mathscr{L}^2(\mathbb{R}^3 \setminus B_{R/2}(\vec{x}_n^i))}^2 &= M - \lim_{n \to \infty} \|u_n\|_{\mathscr{L}^2(\cup B_{R/2}(\vec{x}_n^i))}^2 \\ &= M - \lim_{n \to \infty} \sum_{i=0}^N \|u_n(\vec{x} + \vec{x}_n^i)\|_{\mathscr{L}^2(B_{R/2}(\vec{0}))}^2 \\ &= M - \sum_{i=0}^N \|u^i\|_{\mathscr{L}^2(B_{R/2}(\vec{0}))}^2 \\ &= \sum_{i=0}^N \|u^i\|_{\mathscr{L}^2(\mathbb{R}^3 \setminus B_{R/2}(\vec{0}))}^2 < \varepsilon. \end{split}$$

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

$$\limsup_{n\to\infty} \|u_n\|_{\mathscr{L}^{\infty}(\mathbb{R}^3\setminus \cup B_R(\vec{x}_n^i)))} \leq \varepsilon, \quad R\geq R_0,$$

and hence for large enough n and R,

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

Next, we can check that

$$-\Delta e^{-t\sigma_n} + t^2 e^{-t\sigma_n} > 0$$
, pointwise almost everywhere in  $\mathbb{R}^3 \setminus \cup B_R(\overrightarrow{x}_n^i)$ ,

and that there exists C > 0 so that

$$|u_n|_{\partial \cup B_R(\vec{x}_n^i)} \le Ce^{-tR} = Ce^{-t\sigma_n(\vec{x})}|_{\partial \cup B_R(\vec{x}_n^i)}$$

Thus,

$$-\Delta[u_n(\vec{x}) - Ce^{-t\sigma_n(\vec{x})}] + t^2[u_n(\vec{x}) - Ce^{-t\sigma_n(\vec{x})}] < 0, \text{ pointwise almost everywhere in } \mathbb{R}^3 \setminus \cup B_R(\vec{x}_n^i).$$

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

$$0 < u_n(\vec{x}) \le v(\vec{x}) = Ce^{-t\sigma_n(\vec{x})}, \qquad \vec{x} \in \Omega_n.$$

The estimate on  $\|\nabla u_n\|$  then follows from standard elliptic estimates; see for instance Theorems 8.22 and 8.32 of [26].

**Proposition 16.** Let  $F_{N,(m^0,m^1,...,m^N)}$  and  $\bar{F}_{N,(m^1,m^2,...,m^N)}$  be as in Theorem 6. Then,

$$\inf_{\Sigma_N} F_{N,(m^0,m^1,\dots,m^N)} + \inf_{\bar{\Sigma_N}} \bar{F}_{N,(m^1,m^2,\dots,m^N)} > -\infty$$

and for each infimum, minimizing sequences are compact.

*Proof.* With no loss of generality, assume we are studying a functional of the form

$$G_N(\vec{w}^1, \dots, \vec{w}^N) := \sum_{1 \le i < j \le N} \frac{m^i m^j}{|||\vec{w}^i - \vec{w}^j||} + b \sum_{i=1}^N \frac{m^i}{||\vec{w}^i||} - \sum_{i=1}^N \frac{m^i}{||\vec{w}^i||^V},$$

over

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

with  $m^1, \ldots, m^N, b > 0$  fixed.  $-\infty < \inf_{\Sigma_N} G_N < 0$  as

$$\lim_{t \to 0^+} (at^{-1} - bt^{-v}) = \infty, \quad a > 0,$$

and

$$\lim_{t \to \infty} (at^{-1} - bt^{-v}) = 0, \quad at^{-1} - bt^{-v} < 0 \text{ for } t \gg 1.$$
(3.9)

Next, suppose, by contradiction, that

$$\inf_{\Sigma_N} G_N = \lim_{n \in \mathbb{N}} G_N(\overrightarrow{\xi}_n^1, \dots, \overrightarrow{\xi}_n^N)$$

but  $\{\overrightarrow{\xi}_n^i\}_{n\in\mathbb{N}}$  is not compact for some  $i\in\{1,\ldots,N\}\setminus I^*=:I^{**}\neq\emptyset$ .

First, we observe that  $I^* \neq \emptyset$  because of (3.9) and  $\inf_{\Sigma_N} G_N < 0$ . Then, up to (not relabeled) subsequences,

$$\overrightarrow{\xi}_{n}^{i} \xrightarrow[n \to \infty]{} \overrightarrow{\xi}^{i}, i \in I^{*} \text{ and } \|\overrightarrow{\xi}_{n}^{i}\| \xrightarrow[n \to \infty]{} \infty, i \in I^{**}$$

Therefore,

$$\inf_{\Sigma_{N}} G_{N} = \sum_{i,j \in I^{*}} \frac{m^{i} m^{j}}{|||\vec{\xi}^{i} - \vec{\xi}^{j}||} + b \sum_{i \in I^{*}} \frac{m^{i}}{||\vec{\xi}^{i}||} - \sum_{i \in I^{*}} \frac{m^{i}}{||\vec{\xi}^{i}||^{v}} + \lim_{n \in \mathbb{N}} \sum_{i < j \in I^{**}} \frac{m^{i} m^{j}}{|||\vec{\xi}^{i}_{n} - \vec{\xi}^{j}_{n}||}.$$

On the other hand, we can check that for each  $j \in I^{**}$ ,

$$-\infty < \inf_{\overrightarrow{w} \neq 0} \left( \sum_{i \in I^*} \frac{m^i m^j}{\|\overrightarrow{w} - \overrightarrow{\xi}^i\|} + b \frac{m^j}{\|\overrightarrow{w}\|} - \frac{m^j}{\|\overrightarrow{w}\|^{\mathsf{V}}} \right) < 0$$

is attained at a vector  $\overrightarrow{\xi}^j$ . Then, we replace one of the sequences  $\{\overrightarrow{\xi}_n^j\}_{n\in\mathbb{N}}$ ,  $j\in I^{**}$ , by the constant sequence  $\{\overrightarrow{\xi}_n^j\}_{n\in\mathbb{N}}$ , and then evaluate  $G_n$  at the new vector of sequences. By doing so, we obtain

$$\sum_{i < j \in I^* \cup \{j_0\}} \frac{m^i m^j}{|||\overrightarrow{\xi}^i - \overrightarrow{\xi}^j||} + b \sum_{i \in I^* \cup \{j_0\}} \frac{m^i}{||\overrightarrow{\xi}^i||} - \sum_{i \in I^* \cup \{j_0\}} \frac{m^i}{||\overrightarrow{\xi}^i||^{\nu}} + \lim_{n \in \mathbb{N}} \sum_{i < j \in I^{**} \setminus \{j_0\}} \frac{m^i m^j}{|||\overrightarrow{\xi}^i_n - \overrightarrow{\xi}^j_n||} < \inf_{\Sigma_N} G_N$$

in the limit. However, the equation above contradicts the fact that the original sequence was a minimizing sequence. Hence we cannot have  $I^{**} \neq \emptyset$ .

## 3.3 Potentials approaching a Newtonian potential

The proof of Theorem 6 is more intricate than that of Theorem 5, as it requires us to make a finer estimate of the smaller order terms in the expansion of the energy.

By (i) of Proposition 1,  $\{u_n\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $\mathscr{I}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(M)$ , and hence the conclusions of Concentration Theorem 4 hold with  $N<\infty$ . We assume there is splitting, that is,  $N\geq 1$ , and let  $u^i$ ,  $m^i=\|u^i\|_{\mathscr{L}^2(\mathbb{R}^3)}^2$ , and  $\vec{x}_n^i$  (with  $\vec{x}_n^0=\vec{0}$ ,) 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 5 we construct comparison functions by localization to balls with centers  $q^i$  spreading to infinity. However, we have limited control on the errors introduced by the passage of  $u_n(\cdot - \vec{x}_n^i) \xrightarrow[n \to \infty]{} u^i$ , and thus we use truncations of the minimizers themselves to make these constructions.

Let us set

$$R_n := \min_{0 \le i < j} \|\vec{x}_n^i - \vec{x}_n^j\|. \tag{3.10}$$

Consider also a sequence  $\rho_n \xrightarrow[n \to \infty]{} \infty$  and translations  $\{\vec{q}_n^0 = \vec{0}\}_{n \in \mathbb{N}}, \dots, \{\vec{q}_n^N\}_{n \in \mathbb{N}} \subset \mathbb{R}^3$  (all to be chosen later,) satisfying

$$1 \le \rho_n \le \frac{1}{4} \min\{R_n, Q_n\} \quad \text{where } Q_n := \min_{i < j} \| \vec{q}_n^i - \vec{q}_n^j \|. \tag{3.11}$$

Using the same cutoff functions  $\phi$  defined in (3.5), we then set

$$\chi_{\rho_n}(\cdot) := \phi(\|\cdot\| - \rho_n + 1),$$

$$G_n^i(\cdot) := \chi_{\rho_n}(\cdot - \overrightarrow{x}_n^i)u_n(\cdot), \quad and \quad H_n^i(\cdot) := G_n^i(\cdot + \overrightarrow{x}_n^i - \overrightarrow{q}_n^i). \tag{3.12}$$

Thus, each  $G_n^i$  is compactly supported in a ball  $B_{\rho_n}(\vec{x}_n^i)$ , while  $H_n^i$  is the same function but translated to have centers at  $\vec{q}_n^i$ , which we choose later to create appropriate comparison functions. Set

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

The following Lemma states that truncations we just defined provide a good approximation to the limit profiles.

**Lemma 8.** For any  $\rho_n$  satisfying (3.11),

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

*Proof.* First, we have that  $G_n^i(\cdot + \vec{x}_n^i) \xrightarrow[n \to \infty]{} u^i$ , i = 0, ..., N weakly in  $\mathscr{H}^1(\mathbb{R}^3)$  by construction, and in the norm on  $\mathscr{L}^2_{loc}(\mathbb{R}^3)$  by the Rellich-Kondrakov compactness Theorem. As a consequence,

$$m^{i} = \|u_{i}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} \leq \liminf_{n \to \infty} m_{n}^{i}. \tag{3.13}$$

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

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

In particular, the limit

$$M = \lim_{n \to \infty} \sum_{i=0}^{N} m_n^i$$

exists. Since individually the terms are bounded below via (3.13), we claim that each of the terms  $m_n^i \xrightarrow[n \to \infty]{} m^i$ ,  $i = 0, \dots, N$ . Indeed, given  $\varepsilon > 0$  there exists K > 0 for which  $\sum_{i=0}^N m_n^i < M + \varepsilon$  and for any  $i, m_n^i \ge m^i - \varepsilon/N$ , whenever  $n \ge K$ . Thus, for each j we have

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

and so  $m_n^j < m^j + 2\varepsilon$ , for all  $n \ge K$ , that is,  $\limsup_{n \to \infty} m_n^i \le m^i$ , for each i, and the claim is proved.

Since we assume  $\mu < 0$ , the exponential decay of each  $u_n$  away from balls  $B_{\rho_n}(\vec{x}_n^i)$  (see Lemma 7) allows us to localize the energy  $\mathscr{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}(u_n)$  with an exponentially small error as stated in the following:

**Lemma 9.** Let  $\rho_n \xrightarrow[n \to \infty]{} \infty$  with  $\rho_n \leq \frac{1}{4}R_n$ . Then,

$$\begin{split} \mathscr{E}_{V_{n}}^{\frac{10}{3} \cdot \frac{8}{3}}(u_{n}) & \geq \mathscr{E}_{V_{TFDW}}^{\frac{10}{3} \cdot \frac{8}{3}}\left(G_{n}^{0}\right) + \sum_{i=1}^{N} \mathscr{E}_{0}\left(G_{n}^{i}\right) - Z_{n} \int_{\mathbb{R}^{3}} \frac{|G_{n}^{0}(\vec{x})|^{2}}{\|\vec{x}\|^{V}} d\vec{x} \\ & + \sum_{1 \leq i < j} \frac{m_{n}^{i} m_{n}^{j}}{\|\vec{x}_{n}^{i} - \vec{x}_{n}^{j}\|} + \left(m_{n}^{0} - \mathscr{Z}\right) \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{x}_{n}^{i}\|} - Z_{n} \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{x}_{n}^{i}\|^{V}} - \varepsilon_{1,n}, \end{split}$$

where

$$|\varepsilon_{1,n}| \le C \left( \frac{\rho_n}{R_n^2} + \frac{Z_n \rho_n}{R_n^{1+\nu}} + e^{-\frac{\sqrt{-\mu}}{2}\rho_n} \right), \tag{3.14}$$

as  $n \to \infty$ , with C depending on  $\{m^i\}_{i=0}^N$  and  $\mathscr{Z}$  but independent of translations  $\{\vec{x}_n^i\}, \{\vec{x}_n^1\}, \dots, \{\vec{x}_n^N\}$ .

*Proof.* By Lemma 7, for sufficiently large n,

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

where  $\sigma_n(\vec{x})$  is as in Lemma 7. This together with (3.7), (3.8),  $\mu_n \xrightarrow[n \to \infty]{} \mu$ , Lemma 4,  $\|\nabla \chi_{n,\rho_n}\|_{\mathscr{L}^{\infty}(\mathbb{R}^3)} \le 2$ , and Hölder estimates for first derivatives imply

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

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

$$\mathcal{E}_{V_{n}}^{\frac{10}{3},\frac{8}{3}}(u_{n}) = \sum_{i=0}^{N} \mathcal{E}_{V_{n}}(G_{n}^{i}) + \sum_{i < j} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \frac{|G_{n}^{i}(\vec{x})|^{2} |G_{n}^{j}(\vec{y})|^{2}}{\|\vec{x} - \vec{y}\|} d\vec{x} dy + \varepsilon_{1,n}$$

$$= \mathcal{E}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(G_{n}^{0}) - Z_{n} \int_{B_{\rho_{n}}(\vec{0})} \frac{|G_{n}^{0}(\vec{x})|^{2}}{\|\vec{x}\|^{V}} d\vec{x}$$

$$+ \sum_{i=1}^{N} \left[ \mathcal{E}_{0}(G_{n}^{i}) - \int_{\mathbb{R}^{3}} V(\vec{x}) |G_{n}^{i}(\vec{x})|^{2} d\vec{x} - Z_{n} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \frac{|G_{n}^{i}(\vec{x})|^{2}}{\|\vec{x}\|^{V}} d\vec{x} \right]$$

$$+ \sum_{i < j} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \frac{|G_{n}^{i}(\vec{x})|^{2} |G_{n}^{j}(\vec{y})|^{2}}{\|\vec{x} - \vec{y}\|} d\vec{x} dy + \varepsilon_{1,n}$$

$$= \mathcal{E}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}(G_{n}^{0}) + \sum_{i=1}^{N} \mathcal{E}_{0}(G_{n}^{i}) - Z_{n} \int_{B_{\rho_{n}}(\vec{0})} \frac{|G_{n}^{0}(\vec{x})|^{2}}{\|\vec{x}\|^{V}} d\vec{x}$$

$$+ \sum_{i < j} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \frac{|G_{n}^{i}(\vec{x})|^{2} |G_{n}^{j}(\vec{y})|^{2}}{\|\vec{x} - \vec{y}\|} d\vec{x} d\vec{y}$$

$$- \sum_{i=1}^{N} \sum_{k=1}^{K} \alpha_{k} \int_{\mathbb{R}^{3}} \frac{|G_{n}^{i}(\vec{x})|^{2}}{|x - r_{k}|} d\vec{x} - Z_{n} \sum_{i=1}^{N} \int_{B_{\rho_{n}}(\vec{x}_{n}^{i})} \frac{|G_{n}^{i}(\vec{x})|^{2}}{\|\vec{x}\|^{V}} d\vec{x} + \varepsilon_{1,n}.$$
(3.15)

Now, we apply Lemma 6 to evaluate the interaction terms. In this way we have:

$$\begin{split} \int_{B\rho_{n}(\overrightarrow{x}_{n}^{i})} \int_{B\rho_{n}(\overrightarrow{x}_{n}^{j})} \frac{|G_{n}^{i}(\overrightarrow{x})|^{2} |G_{n}^{j}(\overrightarrow{y})|^{2}}{\|\overrightarrow{x} - \overrightarrow{y}\|} d\overrightarrow{x} d\overrightarrow{y} &\geq \frac{m_{n}^{i} m_{n}^{j}}{\|\overrightarrow{x}_{n}^{i} - \overrightarrow{x}_{n}^{j}\|} - 4m_{n}^{i} m_{n}^{j} \frac{\rho_{n}}{R_{n}^{2}}, \\ \int_{\mathbb{R}^{3}} \frac{|G_{n}^{i}(\overrightarrow{x})|^{2}}{|x - r_{k}|} d\overrightarrow{x} &\leq \frac{m_{n}^{i}}{\|\overrightarrow{x}_{n}^{i}\|} + C_{1} m_{n}^{i} \frac{\rho_{n}}{R_{n}^{2}}, \end{split}$$

$$\int_{B\rho_n(\vec{x}_n^i)} \frac{|G_n^i(\vec{x})|^2}{\|\vec{x}\|^{\nu}} d\vec{x} \leq \frac{m_n^i}{\|\vec{x}_n^i\|^{\nu}} + C_{\nu} m_n^i \frac{\rho_n}{R_n^{\nu+1}}.$$

By substituting these estimates into (3.15) we arrive at the desired lower bound.

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  $\vec{x}_n^i$ . 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  $\vec{q}_n^i$ . The advantage of this over the upper bound constructed for the proof of Theorem 5 is that the terms of order O(1) exactly match those in the lower bound given by Lemma 9.

**Lemma 10.** Let  $\{\rho_n\}_{n\in\mathbb{N}}\subset (1,\infty)$  and  $\{\overrightarrow{q}_n^0=\overrightarrow{0}\}_{n\in\mathbb{N}},\ldots,\{\overrightarrow{q}_n^N\}_{n\in\mathbb{N}}\subset\mathbb{R}^3$  satisfy (3.11). Then,

$$\begin{split} \mathscr{E}_{V_{n}}^{\frac{10}{3},\frac{8}{3}}(u_{n}) < \mathscr{E}_{V_{TFDW}}^{\frac{10}{3},\frac{8}{3}}\left(G_{n}^{0}\right) + \sum_{i=1}^{N} \mathscr{E}_{0}\left(G_{n}^{i}\right) - Z_{n} \int_{\mathbb{R}^{3}} \frac{|G_{n}^{0}(\overrightarrow{x})|^{2}}{\|\overrightarrow{x}\|^{V}} d\overrightarrow{x} \\ + \sum_{1 \leq i < j < N} \frac{m_{n}^{i} m_{n}^{j}}{\|\overrightarrow{q}_{n}^{i} - \overrightarrow{q}_{n}^{j}\|} + \left(m_{n}^{0} - \mathscr{Z}\right) \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\overrightarrow{q}_{n}^{i}\|} - Z_{n} \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\overrightarrow{q}_{n}^{i}\|^{V}} + \varepsilon_{2,n}, \end{split}$$

where

$$|\varepsilon_{2,n}| \le C\left(\frac{\rho_n}{Q_n^2} + \frac{Z_n \rho_n}{Q_n^{1+\nu}} + e^{-\frac{\sqrt{-\mu}}{2}\rho_n}\right),\tag{3.16}$$

as  $n \to \infty$ , with C depending on  $\{m^i\}_{i=0}^N$  and  $\mathscr{Z}$  but independent of  $\{\overrightarrow{q}_n^i\}_{i=0}^N$ 

Proof. Set

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

As  $0 \le w_n(\vec{x}) \le u_n(\vec{x})$  for all  $\vec{x} \in \mathbb{R}^3$ ,  $||w_n||^2_{\mathscr{L}^2(\mathbb{R}^3)} < ||u_n||^2_{\mathscr{L}^2(\mathbb{R}^3)}$ . By the monotonicity of  $\mathscr{I}_{V_n}^{\frac{10}{3}, \frac{8}{3}}(M)$  (Proposition 7,)

$$\mathscr{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}(u_n) = \mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M) < \mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}\left(\|w_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2\right) \leq \mathscr{E}_{V_n}^{\frac{10}{3},\frac{8}{3}}(w_n).$$

Using the support properties of  $H_n^i$  and recognizing

$$\mathscr{E}^{rac{10}{3},rac{8}{3}}_{V_{TFDW}}(H_n^0) = \mathscr{E}^{rac{10}{3},rac{8}{3}}_{V_{TFDW}}(G_n^0), \quad \mathscr{E}_0(H_n^i) = \mathscr{E}_0(G_n^i),$$

we expand as in the proof of Lemma 9 to obtain the desired upper bound.

By matching the lower bound from Lemma 9 with the upper bound from Lemma 10, we conclude for any choice of  $\rho_n$ ,  $\{\vec{q}_n^i\}$  satisfying (3.11), we have the following bound satisfied by the translations  $\{\vec{x}_n^i\}$ :

$$\sum_{1 \leq i < j \leq N} \frac{m_n^i m_n^j}{\|\overrightarrow{x}_n^i - \overrightarrow{x}_n^j\|} + \left(m_n^0 - \mathcal{Z}\right) \sum_{i=1}^N \frac{m_n^i}{\|\overrightarrow{x}_n^i\|} - Z_n \sum_{i=1}^N \frac{m_n^i}{\|\overrightarrow{x}_n^i\|^{\mathsf{V}}}$$

$$\leq \sum_{1\leq i < j < N} \frac{m_n^i m_n^j}{\|\vec{q}_n^i - \vec{q}_n^j\|} + \left(m_n^0 - \mathcal{Z}\right) \sum_{i=1}^N \frac{m_n^i}{\|\vec{q}_n^i\|} - Z_n \sum_{i=1}^N \frac{m_n^i}{\|\vec{q}_n^i\|^{\mathsf{V}}} + \varepsilon_{1,n} + \varepsilon_{2,n}, \quad (3.17)$$

where  $\varepsilon_{1,n}, \varepsilon_{2,n}$  are defined in the statements of the Lemmas 9 and 10.

In what follows we exploit the freedom we have of choosing vectors  $\vec{q}_n^i$  and radii  $\rho_n$  to prove Theorem 6. First we must find the correct scale for the diverging centers  $\{\vec{x}_n^i\}$ . We define

$$R_n^0 := \min_{1 \le i \le N} \| \overrightarrow{x}_n^i \|,$$

and for  $N \ge 2$ ,

$$\overline{R}_n := \min_{1 \le i < j \le N} \| \overrightarrow{x}_n^i - \overrightarrow{x}_n^j \|.$$

By Concentration Theorem 4, each diverges to infinity; furthermore,  $R_n = \min\{\overline{R}_n, R_n^0\}$  (see (3.10).) By passing to a subsequence and reordering the components if necessary, we may assume that the first diverging center is the closest:

$$\|\overrightarrow{x}_n^1\| = R_n^0, \quad n \in \mathbb{N}.$$

**Lemma 11.** (a) If  $m^0 > \mathcal{Z}$ , then

$$\liminf_{n \to \infty} R_n Z_n^{\frac{1}{1-\nu}} > 0.$$
(3.18)

(b) If  $N \ge 2$  and

$$\limsup_{n\to\infty}\frac{R_n^0}{\overline{R}_n}>0,$$

then there exists a subsequence for which (3.18) holds.

(c) If  $N \ge 2$  and

$$\frac{R_n^0}{\overline{R}_n} \xrightarrow[n \to \infty]{} 0,$$

then

$$\liminf_{n \to \infty} \overline{R}_n Z_n^{\frac{1}{1-\nu}} > 0.$$

*Proof.* First assume  $m^0 > \mathcal{Z}$ . By contradiction, assume that along some subsequence

$$R_n Z_n^{\frac{1}{1-\nu}} \xrightarrow[n \to \infty]{0}$$
.

Choose vectors  $\vec{q}_n^i = R_n \vec{p}^i$ , for distinct fixed vectors  $\vec{p}^i$ , i = 1, ..., N, and  $\vec{p}^0 = \vec{0}$ . We denote by  $\vec{y}_n^i = R_n^{-1} \vec{x}_n^i$ . By the definition of  $R_n$ , we have  $||\vec{y}_n^i|| \ge 1$  for all i = 1, ..., N, and  $||\vec{y}_n^i - \vec{y}_n^j|| \ge 1$  for all  $0 \le i < j \le N$ . Extracting a further subsequence if necessary, we may assume that either

$$\|\vec{y}_{n}^{1}\| = 1$$
, or, there exists  $i_{0}, j_{0} \neq 0$  for which  $\|\vec{y}_{n}^{i_{0}} - \vec{y}_{n}^{j_{0}}\| = 1, n \in \mathbb{N}$ . (3.19)

Set  $\rho_n = \sqrt{R_n}$ , and so (3.11) is satisfied for these choices, and in fact  $R_n \varepsilon_{1,n}$ ,  $R_n \varepsilon_{2,n} \xrightarrow[n \to \infty]{} 0$ , where  $\varepsilon_{1,n}$ ,  $\varepsilon_{2,n}$  are the remainder terms defined in Lemmas 9 and 10.

Then, we multiply (3.17) by  $R_n$  to obtain:

$$\sum_{1 \leq i < j \leq N} \frac{m_{n}^{i} m_{n}^{j}}{\|\vec{y}_{n}^{i} - \vec{y}_{n}^{j}\|} + (m_{n}^{0} - \mathcal{Z}) \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{y}_{n}^{i}\|} \leq \sum_{1 \leq i < j \leq N} \frac{m_{n}^{i} m_{n}^{j}}{\|\vec{p}^{i} - \vec{p}^{j}\|} + (m_{n}^{0} - \mathcal{Z}) \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{p}^{i}\|} 
- Z_{n} R_{n}^{1-\nu} \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{p}^{i}\|^{\nu}} + Z_{n} R_{n}^{1-\nu} \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{y}_{n}^{i}\|^{\nu}} 
+ R_{n} \varepsilon_{1,n} + R_{n} \varepsilon_{2,n} 
\leq \sum_{1 \leq i < j \leq N} \frac{m_{n}^{i} m_{n}^{j}}{\|\vec{p}^{i} - \vec{p}^{j}\|} + (m_{n}^{0} - \mathcal{Z}) \sum_{i=1}^{N} \frac{m_{n}^{i}}{\|\vec{p}^{i}\|} + o(1),$$
(3.20)

as  $Z_n R_n^{1-\nu} \xrightarrow[n \to \infty]{} 0$  by the contradiction hypothesis. Assuming that  $||y_n^{i_0} - y_n^{j_0}|| = 1$  is chosen in (3.19), we then obtain

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

which holds for all  $n \in \mathbb{N}$  and any choice of vectors  $\{\vec{p}^i\}_{i=0}^N$ . Since  $m_n^i \xrightarrow[n \to \infty]{} m^i > 0$ ,  $i = 0, \dots, N$ , we obtain a contradiction by choosing  $\|\vec{p}^i - \vec{p}^j\|$  (with  $0 \le i < j \le N$ ) sufficiently large. If the choice in (3.19) gives  $\|\vec{y}_n^1\| = 1$ , we instead have

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

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

In order to prove (b), we assume  $N \ge 2$  and there exists a subsequence and r > 0 for which  $R_n^0 \ge r\overline{R}_n$ , but

$$R_n Z_n^{\frac{1}{1-\nu}} \xrightarrow[n\to\infty]{} 0.$$

Recall that  $R_n = \min\{R_n^0, \overline{R}_n\}$ , and so

$$\min\{r,1\}\overline{R}_n < R_n < \overline{R}_n$$

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

$$\|\vec{y}_{n}^{i_{0}} - \vec{y}_{n}^{j_{0}}\|^{-1} = \frac{R_{n}}{\overline{R}_{n}} \ge \min\{1, r\}.$$

Again, multiply (3.17) by  $R_n$ , and pass to the limit as in (3.20) to obtain:

$$\min\{1,r\}m_n^{i_0}m_n^{j_0} + \left(m_n^0 - \mathscr{Z}\right)\sum_{i=1}^N \frac{m_n^i}{\|\overrightarrow{\mathcal{Y}}_n^i\|} \leq \sum_{0 \leq i \leq j} \frac{m_n^i m_n^j}{\|\overrightarrow{\mathcal{P}}^i - \overrightarrow{\mathcal{P}}^j\|} + \left(m_n^0 - \mathscr{Z}\right)\sum_{i=1}^N \frac{m_n^i}{\|\overrightarrow{\mathcal{P}}^i\|} + o(1),$$

for all n and any choice of vectors  $\vec{p}^i$ . Since  $m_n^i \xrightarrow[n \to \infty]{} m^i > 0$  and  $m^0 \ge \mathscr{Z}$  by Theorem 5, we obtain a contradiction by choosing vectors  $\vec{p}^i$  with  $\|\vec{p}^i - \vec{p}^j\|$  sufficiently large.

Finally, to prove (c) we assume

$$\frac{R_n^0}{\overline{R}_n} \xrightarrow[n \to \infty]{} 0,$$

and suppose that  $\overline{R}_n Z_n^{\frac{1}{1-\nu}} \xrightarrow[n \to \infty]{} 0$  instead. First, we note that

$$\|\vec{x}_{n}^{i}\| = \|\vec{x}_{n}^{i} - \vec{x}_{n}^{1} + \vec{x}_{n}^{1}\| \ge \|\vec{x}_{n}^{i} - \vec{x}_{n}^{1}\| - \|\vec{x}_{n}^{1}\| \ge \overline{R}_{n} - R_{n}^{0} \ge \frac{1}{2}\overline{R}_{n} \gg \|\vec{x}_{n}^{1}\|, \quad i \ge 2, n \gg 1.$$

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

Choose cut-off radii  $\rho_n$  in Lemmas 9 and 10 with  $R_n^0 \ll \rho_n \ll \overline{R}_n$ ; for instance,  $\overline{\rho}_n = \sqrt{R_n^0 \overline{R}_n}$ . Notice that the ball  $B_{\rho_n}(\overrightarrow{0})$  now includes both  $\overrightarrow{x}_n^0 = 0$  and  $\overrightarrow{x}_n^1$ . In particular, when defining the disjoint components  $G_n^i, H_n^i$  with  $\overline{R}_n$  and  $\overline{\rho}_n$ , 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  $\overrightarrow{x}_n^1$ . In particular, we have,

$$||G_n^0||_{\mathscr{L}^2(\mathbb{R}^3)}^2 = ||H_n^0||_{\mathscr{L}^2(\mathbb{R}^3)}^2 = m^0 + m^1 + o(1) > \mathscr{Z}. \tag{3.21}$$

In this way, we return to the same situation as in part (a), but where  $\overline{R}_n$  replaces  $R_n$  as the decisive length scale. As in (a), we choose distinct vectors  $\overrightarrow{q}^0 = \overrightarrow{0}$  and  $\overrightarrow{q}^i$ , i = 2, ..., N, and set  $\overrightarrow{p}_n^i := \overline{R}_n \overrightarrow{q}^i$ , and (as before)  $\overrightarrow{y}_n^i = \overrightarrow{x}_n^i/\overline{R}_n$ . Modulo a subsequence, either there is a pair with

$$\|\vec{y}_{n}^{i_{0}} - \vec{y}_{n}^{j_{0}}\| = 1, i_{0}, j_{0} \ge 2,$$

or  $i_0 \ge 2$  with  $\|\vec{y}_n^{i_0}\| = 1, n \in \mathbb{N}$ . Then we multiply (3.17) by  $\overline{R}_n$ , to obtain:

$$\begin{split} \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{\|\overrightarrow{y}_n^i - \overrightarrow{y}_n^j\|} + \left(m^0 + m^1 - \mathscr{Z} + o(1)\right) \sum_{i=2}^N \frac{m_n^i}{\|\overrightarrow{y}_n^i\|} - Z_n \overline{R}_n^{1-\nu} \sum_{i=2}^N \frac{m_n^i}{\|\overrightarrow{y}_n^i\|^{\nu}} \\ \leq \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{\|\overrightarrow{p}^i - \overrightarrow{p}^j\|} + \left(m^0 + m^1 - \mathscr{Z} + o(1)\right) \sum_{i=2}^N \frac{m_n^i}{\|\overrightarrow{p}^i\|} - Z_n \overline{R}_n^{1-\nu} \sum_{i=2}^N \frac{m_n^i}{\|\overrightarrow{p}^i\|^{\nu}} + \overline{R}_n \overline{\varepsilon}_{1,n} + \overline{R}_n \overline{\varepsilon}_{2,n}, \end{split}$$

where  $\overline{\varepsilon}_{1,n}$  and  $\overline{\varepsilon}_{2,n}$  satisfy (3.14) and (3.16), for  $\overline{R}_n, \overline{\rho}_n$  replacing  $R_n, \rho_n$ . In particular,  $\overline{R}_n \overline{\varepsilon}_{1,n}, \overline{R}_n \overline{\varepsilon}_{2,n} \xrightarrow[n \to \infty]{} 0$ . Employing the contradiction hypothesis  $\overline{R}_n Z_n^{\frac{1}{1-\nu}} \xrightarrow[n \to \infty]{} 0$ , and the choice of  $\overline{R}_n, \overline{\rho}_n$  we deduce that (in the case  $\|\vec{y}_n^{i_0} - \vec{y}_n^{j_0}\| = 1$ ,)

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

or (in the case  $\|\overrightarrow{y}_n^{i_0}\| = 1$ ,)

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

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

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

Proof of Theorem 6. Let  $u_n$  attain the minimum in  $\mathscr{I}_{V_n}^{\frac{10}{3},\frac{8}{3}}(M)$ ,  $n \in \mathbb{N}$ . Applying the Concentration Theorem 4, we obtain a value of  $N \in \mathbb{N}$ , masses  $\{m^i\}_{i=0}^N$ , and translations  $\{\vec{x}_n^i\}$ .

For part (i), we assume  $m^0 \in \mathcal{M}_{V_{TFDW}}^*$  and  $m^0 > \mathcal{Z}$ . For any choice of N and masses  $m^0, \ldots, m^N$  with  $m^0 > \mathcal{Z}$ , all minimizing sequences for  $F_{N,(m^0,\ldots,m^N)}(\overrightarrow{w}^1,\ldots,\overrightarrow{w}^N)$  on  $\Sigma_N$  are convergent by Propositon 16. Let  $(\overrightarrow{a}^1,\ldots,a^N) \in \Sigma_N$  be such a minimizer,

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

We define the vectors

$$\vec{\xi}_n^i := Z_n^{\frac{1}{1-\nu}} \vec{x}_n^i.$$

By Lemma 11,  $\|\overrightarrow{\xi}_n^i\|$ ,  $\|\overrightarrow{\xi}_n^i - \overrightarrow{\xi}_n^j\| \ge c > 0$  are bounded below, for each  $i = 1, \dots, N$  and  $j \ne i$ . Set

$$\rho_n := Z_n^{-\frac{1}{2(1-\nu)}}, \text{ and } \overrightarrow{q}_n^i := Z_n^{-\frac{1}{1-\nu}} \overrightarrow{a}^i.$$

Then, by the previous Lemma, up to a subsequence,

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

so that equation (3.17) holds, and

$$\sum_{1 \leq i < j} \frac{m_n^i m_n^j}{\|\vec{\xi}_n^i - \vec{\xi}_n^j\|} + (m_n^0 - \mathscr{Z}) \sum_{i=1}^N \frac{m_n^i}{\|\vec{\xi}_n^i\|} - \sum_{i=1}^N \frac{m_n^i}{\|\vec{\xi}_n^i\|^V} \\
\leq \sum_{1 \leq i < j} \frac{m_n^i m_n^j}{\|\vec{a}^i - \vec{a}^j\|} + (m_n^0 - \mathscr{Z}) \sum_{i=1}^N \frac{m_n^i}{\|\vec{a}^i\|} - \sum_{i=1}^N \frac{m_n^i}{\|\vec{a}^i\|^V} + Z_n^{-\frac{1}{1-V}} (\varepsilon_n + \hat{\varepsilon}_n), \quad (3.22)$$

where  $\varepsilon_n$  and  $\hat{\varepsilon}_n$  satisfy (3.14) and (3.16), correspondingly. In particular,  $Z_n^{-\frac{1}{1-\nu}}\varepsilon_n, Z_n^{-\frac{1}{1-\nu}}\hat{\varepsilon}_n \xrightarrow[n \to \infty]{} 0$ . In addition to this, by Lemma 11.

$$\liminf_{n\to\infty} \|\vec{\xi}_n^i - \vec{\xi}_n^j\| \ge \liminf_{n\to\infty} Z_n^{\frac{1}{1-\nu}} R_n > 0. \tag{3.23}$$

By Lemma 8,  $\lim_{n\to\infty} m_n^i = m^i$ , and hence applying (3.22) and (3.23) we obtain:

$$\begin{split} \limsup_{n \to \infty} F_{N,(m^0, \dots, m^N)}(\overrightarrow{\xi}_n^1, \dots, \overrightarrow{\xi}_n^N) \\ &= \limsup_{n \to \infty} \left[ \sum_{1 \le i < j \le N} \frac{m_n^i m_n^j}{\|\overrightarrow{\xi}_n^i - \overrightarrow{\xi}_n^j\|} + \left( m_n^0 - \mathscr{Z} \right) \sum_{i=1}^N \frac{m_n^i}{\|\overrightarrow{\xi}_n^i\|} - \sum_{i=1}^N \frac{m_n^i}{\|\overrightarrow{\xi}_n^i\|^V} \right] \\ &\leq \limsup_{n \to \infty} \left[ \sum_{1 \le i < j \le N} \frac{m_n^i m_n^j}{\|a^i - a^j\|} + \left( m_n^0 - \mathscr{Z} \right) \sum_{i=1}^N \frac{m_n^i}{\|a^i\|} - \sum_{i=1}^N \frac{m_n^i}{\|a^i\|^V} \right] \\ &= F_{N,(m^0, \dots, m^N)}(a^1, \dots, a^N) \\ &= \min_{(w^1, \dots, w^N) \in \Sigma_N} F_{N,(m^0, \dots, m^N)}(w^1, \dots, w^N). \end{split}$$
(3.24)

Therefore,  $\{(\overrightarrow{\xi}_n^1,\ldots,\overrightarrow{\xi}_n^N)\}_{n\in\mathbb{N}}$  is a minimizing sequence for  $F_{N,(m^0,\ldots,m^N)}$  in  $\Sigma_N$ , and by Proposition 16,

$$\overrightarrow{\xi}_{n}^{i} = \overrightarrow{x}_{n}^{i} Z^{\frac{1}{1-\nu}} \xrightarrow[n \to \infty]{} \overrightarrow{y}^{i}, i = 0, \dots, N,$$

with  $(\vec{y}^1, \dots, \vec{y}^N)$  a minimizing configuration for  $F_{N,(m^0,\dots,m^N)}$ . This completes the proof in case  $m^0 > \mathcal{Z}$ .

Now consider (ii), for which  $m^0 = \mathscr{Z}$ . We first show that  $\|\vec{x}_n^1\| \ll Z_n^{\frac{1}{\nu-1}}$ . Indeed, assume the contrary that, up to a subsequence,  $\|\vec{x}_n^1\|Z_n^{\frac{1}{1-\nu}} \ge c > 0$  for all n. In case  $N \ge 2$ , by part (b) of Lemma 11, then  $R_n Z_n^{\frac{1}{\nu-1}} \ge c' > 0$ . As in the proof of (i), define

$$\overrightarrow{\xi}_{n}^{i} := \overrightarrow{x}_{n}^{i} Z_{n}^{\frac{1}{1-\nu}};$$

then  $\|\vec{\xi}_n^i\| \ge c$ , i = 1, ..., N, is bounded below. We also fix any distinct points  $p^1, ..., p^N \in \mathbb{R}^3 \setminus \{0\}$  and  $\vec{q}_n^i = p^i Z_n^{i-1}$ .

We now proceed as above, arriving at (3.22). Note that the inequality (3.22) holds for any  $N \ge 1$ . 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 (3.24), and recalling  $m_n^0 \xrightarrow[n \to \infty]{} \mathscr{Z}$ , we then have

$$\limsup_{n\to\infty} F_{N,(\mathscr{Z},m^1,\ldots,m^N)}(\overrightarrow{\xi}_n^1,\ldots,\overrightarrow{\xi}_n^N) \leq F_{N,(\mathscr{Z},m^1,\ldots,m^N)}(\overrightarrow{p}^1,\ldots,\overrightarrow{p}^N),$$

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

Lastly, for  $m^0 = \mathscr{Z}$  and  $N \geq 2$  we prove the asymptotic distribution of the concentration centers. For this, we return to the definitions of  $\overline{R}_n, \overline{\rho}_n$  in the proof of Lemma 11 (c) above, in which we proved that  $\overline{R}_n \geq c Z_n^{\frac{1}{\nu-1}}$ . We recall that the components  $G_n^0, H_n^0$  defined in (3.12) (but using  $\overline{\rho}_n$  in the cut-off  $\chi_{\overline{\rho}_n}$ ,) enclose neighborhoods of both  $\overrightarrow{x}_n^0 = \overrightarrow{0}$  and  $\overrightarrow{x}_n^1$ , and hence their masses combine in  $G_n^0, H_n^0$ , as in (3.21). By the same arguments as in [3, Proposition 8], all minimizing sequences of the interaction energy  $\overline{F}_{N,(m^1,m^2,\dots,m^N)}$ 

converge to a minimizer  $(\vec{y}^2, \dots, \vec{y}^N) \in \overline{\Sigma}_N$ . Define  $q_n^0 = 0$  and  $\vec{q}_n^i = \vec{y}^i Z_n^{\frac{1}{\nu-1}}$ ,  $i = 2, \dots, N$ . Applying (3.17) with these choices, we have:

$$\begin{split} \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{\|\vec{x}_n^i - \vec{x}_n^j\|} + \left( m^0 + m^1 - \mathscr{Z} + o(1) \right) \sum_{i=2}^N \frac{m_n^i}{\|\vec{x}_n^i\|} - Z_n \sum_{i=2}^N \frac{m_n^i}{\|\vec{x}_n^i\|^V} \\ \leq \sum_{2 \leq i < j} \frac{m_n^i m_n^j}{\|\vec{q}_n^i - \vec{q}_n^j\|} + \left( m^0 + m^1 - \mathscr{Z} + o(1) \right) \sum_{i=2}^N \frac{m_n^i}{\|\vec{q}_n^i\|} - Z_n \sum_{i=2}^N \frac{m_n^i}{\|\vec{q}_n^i\|^V} + \overline{\varepsilon}_{1,n} + \overline{\varepsilon}_{2,n}, \end{split}$$

with (as in part (i))

$$Z_n^{\frac{1}{\nu-1}}\overline{\varepsilon}_{1,n}, Z_n^{\frac{1}{\nu-1}}\overline{\varepsilon}_{2,n} \xrightarrow[n \to \infty]{} 0.$$

Multiplying the above inequality by  $Z_n^{\frac{1}{\nu-1}}$ , we pass to the limit and obtain an inequality for  $\overline{F}_{N,(m^1,m^2,...,m^N)}$ ,

$$\limsup_{n\to\infty} \overline{F}_{N,(m^1,m^2,\ldots,m^N)}(\overrightarrow{\xi}_n^2,\cdots,\overrightarrow{\xi}_n^N) \leq \overline{F}_{N,(m^1,m^2,\ldots,m^N)}(\overrightarrow{y}^2,\cdots,\overrightarrow{y}^N).$$

Again, the renormalized centers  $(\overrightarrow{\xi}_n^2, \dots, \overrightarrow{\xi}_n^N)$  give a minimizing sequence for  $\overline{F}_{N,(m^1,m^2,\dots,m^N)}$  and must converge to a minimizer. This completes the proof of Theorem 6.

#### 3.4 Infimum over the class of radial functions

In this section we consider the minimization problem in a radial class. We set

$$\mathscr{I}_{V}^{p,q,radial}(M):=\inf\left\{\mathscr{E}_{V}^{p,q}(u)\;;\;u\in H^{1}_{radial}(\mathbb{R}^{3}),\|u\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}=M\right\}.$$

**Remark 5.** 1. If the binding inequality holds, its proof is not the same we showed for the general case.

2. Corollary 2 does not necessarily hold because the proof used the binding inequality.

**Proposition 17.**  $\mathscr{I}_{V}^{p,q,radial} \leq 0$ ; moreover, if q < 8/3 or  $c \ll 1$ , the inequality is strict.

*Proof.* The transformation (2.1) does not only keep the  $\mathcal{L}^2$  norm, but it is also invariant under rotations. Then, just as in the proof of part (i) of Proposition 7, and since

$$\int_{\mathbb{R}^3} Vu^2 d\vec{x} = \int_{\mathbb{R}^3} Z \frac{|\sigma^{3/2} u(\sigma \vec{x})|^2}{\|\vec{x}\|^{\nu}} d\vec{x} = \sigma^3 \sigma^{\nu} \int_{\mathbb{R}^3} Z \frac{u^2(\sigma \vec{x})}{\|\sigma \vec{x}\|^{\nu}} d\vec{x} = \sigma^{\nu} \int_{\mathbb{R}^3} Vu^2 d\vec{x},$$

$$\mathscr{E}_{V}^{p,q}(u_{\sigma}) = \int_{\mathbb{R}^{3}} \left( c_{W} \sigma^{2} \|\nabla u\|^{2} + c_{TF} \sigma^{3p/2-3} |u|^{p} - c_{D} \sigma^{3q/2-3} |u|^{q} \sigma^{v} V u^{2} \right) d\vec{x} + \frac{1}{2} \sigma D(u^{2}, u^{2}). \quad (3.25)$$

As a result, the nonpositivity follows from (3.25) by taking  $\sigma \to 0^+$ , while the strict negativity follows from the fact that when q < 8/3 or  $c \ll 1$ , the dominant term as  $\sigma \to 0$  is negative.

**Theorem 10.** Let q < 2.4 and M be any positive real number. If

$$V \equiv 0 \text{ or } \mathbf{v} \in \left[\frac{2q-4}{4-q}, \frac{3q-6}{q}\right] (\subseteq (0,1)),$$

then  $\mathcal{I}_{V}^{p,q,radial}(M)$  is attained.

**Remark 6.** If q < 2.4 the interval for v is well defined.

**Remark 7.** In particular, if q < 2.4, then  $\mathscr{I}_{V}^{p,q,radial}(M) < \mathscr{I}_{0}^{p,q,radial}(M)$ .

*Proof.* Let  $\{u_n\}_{n\in\mathbb{N}}$  be a minimizing sequence for  $\mathscr{I}_V^{p,q,radial}(M)$ . Up to a subsequence (not relabelled),  $u_n \xrightarrow[n \to \infty]{} u$  in  $H^1_{radial}(\mathbb{R}^3)$  for some u because (2.6) ensures  $\{u_n\}_{\mathbb{N}}$  is bounded in  $\mathscr{H}^1(\mathbb{R}^3)$ . Then,

$$u_n \to u \in \mathcal{L}^r(\mathbb{R}^3), 2 < r < 6, \tag{3.26}$$

by compactness of the embedding  $H^1_{radial}(\mathbb{R}^3) \hookrightarrow \mathcal{L}^r(\mathbb{R}^3)$  for  $2 < r < 2^* = 6$ ,

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} V u_n^2 d\vec{x} = \int_{\mathbb{R}^3} V u^2 d\vec{x}$$

by Proposition 5, and

$$m := \int_{\mathbb{R}^3} u^2 d\vec{x} \le M. \tag{3.27}$$

Furthermore,  $u_n \xrightarrow[n \to \infty]{} u$  in  $\mathscr{H}^1(\mathbb{R}^3)$ , (3.26), q < 8/3 and Proposition 17 combined imply

$$\mathscr{E}_{V}^{p,q,radial}(u) \leq \liminf_{n \to \infty} \mathscr{E}_{V}^{p,q,radial}(u_n) = \mathscr{I}_{V}^{p,q,radial}(M) < 0,$$

so that m = 0 cannot happen, while  $\mathcal{I}_V^{p,q} < 0$  and (3.26)-(3.27) yield

$$\frac{\mathscr{I}_{V}^{p,q}(m)}{m^{\gamma}} \leq \frac{\mathscr{E}_{V}^{p,q}(u)}{m^{\gamma}} \leq \frac{\mathscr{E}_{V}^{p,q}(u)}{M^{\gamma}} \leq \frac{\liminf_{n \to \infty} \mathscr{E}_{V}^{p,q}(u_n)}{M^{\gamma}} = \frac{\mathscr{I}_{V}^{p,q}(M)}{M^{\gamma}}, \gamma \geq 0. \tag{3.28}$$

Therefore, part 3 of Lemma 4, which is also valid in the radial case, ensures M = m, otherwise  $\mathcal{E}_V^{p,q,radial}(u) < 0$  and (3.28) would give

$$\frac{\mathscr{I}_{V}^{p,q}(M)}{m^{\gamma}} < \frac{\mathscr{I}_{V}^{p,q}(M)}{M^{\gamma}}.$$

As a result, *u* is a minimizer.

## **Chapter 4**

# Convergence to the Liquid Drop model

In this chapter we prove Theorem 7. From now on, we assume V satisfies (1.17). Recall

$$\begin{split} \mathscr{E}^{V}_{\varepsilon}(u) &:= \int_{\mathbb{R}^{3}} \left[ \frac{\varepsilon}{2} \|\nabla u\|^{2} + \frac{1}{2\varepsilon} W(u) - Vu^{2} \right] dx + D(u^{2}, u^{2}), \quad W(u) := u^{2} \left( |u|^{\frac{2}{3}} - 1 \right)^{2}, \\ \mathscr{E}^{V}_{0}(u) &:= \frac{1}{8} \int_{\mathbb{R}^{3}} \|\nabla u\| - \int_{\mathbb{R}^{3}} Vu^{2} d\overrightarrow{x} + D(u^{2}, u^{2}), \\ \mathscr{H}^{M} &:= \left\{ u \in \mathscr{H}^{1}(\mathbb{R}^{3}) \, ; \, \|u\|^{2}_{\mathscr{L}^{2}(\mathbb{R}^{3})} = M \right\}, \\ \mathscr{X}^{M} &:= \left\{ u \in BV(\mathbb{R}^{3}, \{0, \pm 1\}) \, ; \, \|u\|^{2}_{\mathscr{L}^{2}(\mathbb{R}^{3})} = M \right\}, \\ e^{V}_{\varepsilon}(M) &:= \inf \left\{ \mathscr{E}^{V}_{\varepsilon}(u) \, ; \, u \in \mathscr{H}^{M} \right\}, \qquad e^{V}_{0}(M) &:= \inf \left\{ \mathscr{E}^{V}_{0}(u) \, ; \, u \in \mathscr{X}^{M} \right\}, \\ \mathscr{F}^{V}_{0}(\{u^{i}\}_{i=0}^{\infty}) &:= \begin{cases} \mathscr{E}^{V}_{0}(u^{0}) + \sum_{i=1}^{\infty} \mathscr{E}^{0}_{0}(u^{i}), \quad \{u^{i}\}_{i=0}^{\infty} \in \mathscr{H}^{M}_{0}, \\ \infty, & otherwise, \end{cases} \end{split}$$

and

$$\mathscr{H}_0^M := \left\{ \{u^i\}_{i=0}^{\infty} \subset BV(\mathbb{R}^3, \{0, \pm 1\}); \ \sum_{i=0}^{\infty} \int_{\mathbb{R}^3} \|\nabla u^i\| < \infty, \ \sum_{i=0}^{\infty} \|u^i\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M \right\}.$$

### 4.1 Compactness and Lower Bound

In this section we prove part (i) of Theorem 7. This involves combining lower bounds on singularly perturbed problems of Cahn-Hilliard type with concentration-compactness methods, to deal with possible loss of compactness via splitting.

We begin with some preliminary estimates.

**Lemma 12.** Let  $\{v_{\varepsilon}\}_{{\varepsilon}>0} \subset \mathcal{H}^1(\mathbb{R}^3)$ , with  $\|v_{\varepsilon}\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \leq M$  and  $\mathcal{E}_{\varepsilon}^V(v_{\varepsilon}) \leq K_0$ , where  $K_0 > 0$  is a constant independent of  $\varepsilon$ . Then there exists a constant  $C_0 = C_0(K_0, M, V)$  such that for all  $0 < \varepsilon < \frac{1}{4}$ , we have

$$\int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \| \nabla v_{\varepsilon} \|^2 + \frac{1}{2\varepsilon} W(v_{\varepsilon}) \right] d\vec{x} + D(|v_{\varepsilon}|^2, |v_{\varepsilon}|^2) \le C_0.$$

*Proof.* First by (1.17), we write  $V = V_{5/2} + V_{\infty}$ , where  $V_{5/2} \in \mathcal{L}^{\frac{5}{2}}(\mathbb{R}^3)$  and  $V_{\infty} \in \mathcal{L}^{\infty}(\mathbb{R}^3)$ , and fix K > 0 large enough so that

$$|t|^{\frac{10}{3}} \le \frac{5}{3}W(t), \quad |t| > K.$$

Then, by Young's inequality, for any  $u \in \mathcal{H}^1(\mathbb{R}^3)$ ,

$$\begin{split} \int_{\mathbb{R}^{3}} V u^{2} d\vec{x} &\leq \int_{\mathbb{R}^{3}} V_{5/2} u^{2} d\vec{x} + \|V_{\infty}\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})} \int_{\mathbb{R}^{3}} u^{2} d\vec{x} \\ &\leq \frac{2}{5} \int_{\mathbb{R}^{3}} |V_{5/2}|^{\frac{5}{2}} d\vec{x} + \frac{3}{5} \int_{\mathbb{R}^{3}} |u|^{\frac{10}{3}} d\vec{x} + \|V_{\infty}\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})} \int_{\mathbb{R}^{3}} u^{2} d\vec{x} \\ &\leq C \left(1 + \int_{\{|u| < K\}} |u|^{2} d\vec{x}\right) + \int_{\{|u| > K\}} W(u) d\vec{x} + \|V_{\infty}\|_{\mathscr{L}^{\infty}(\mathbb{R}^{3})} \int_{\mathbb{R}^{3}} u^{2} d\vec{x} \\ &\leq C_{2} + C_{1} \int_{\mathbb{R}^{3}} u^{2} d\vec{x} + \frac{1}{2\varepsilon} \int_{\mathbb{R}^{3}} W(u) d\vec{x}. \end{split}$$

Hence, there exist constants  $C_1, C_2 > 0$  for which

$$2\mathscr{E}_{\varepsilon}^{V}(u) + C_1 \int_{\mathbb{R}^3} u^2 d\overrightarrow{x} + C_2 \ge \int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \|\nabla u\|^2 + \frac{1}{2\varepsilon} W(u) \right] d\overrightarrow{x} + D(u^2, u^2),$$

and the desired estimate follows.

**Remark 8.** Under the hypotheses of Lemma 12,  $\{v_{\varepsilon}\}_{{\varepsilon}>0}$  is bounded in  $\mathscr{L}^{\frac{10}{3}}(\mathbb{R}^3)$  and

$$\int_{\mathbb{R}^3} W(v_{\varepsilon}) d\overrightarrow{x} \xrightarrow[\varepsilon \to 0^+]{} 0.$$

Next, we prepare the way for the proof of the compactness part of Theorem 7 by establishing that sequences  $\{u_{\varepsilon}\}_{{\varepsilon}>0}$  with bounded energy must have centers of concentration, even if they are divergent. The following Lemma is used to rule out vanishing of  $\{u_{\varepsilon}\}_{{\varepsilon}>0}$  as long as the BV norm is bounded and the  $\mathscr{L}^{\frac{4}{3}}$  norm of  $u_{\varepsilon}$  is not vanishing:

**Lemma 13.** There exists a universal constant C > 0 such that for all  $\psi \in \mathcal{BV}(\mathbb{R}^3)$ ,

$$\|\psi\|_{\mathscr{B}\mathscr{V}(\mathbb{R}^3)} \left[ \sup_{\overrightarrow{a} \in \mathbb{R}^3} \int_{B_1(\overrightarrow{a})} |\psi| d\overrightarrow{x} \right]^{\frac{1}{3}} \ge C \int_{\mathbb{R}^3} |\psi|^{\frac{4}{3}} d\overrightarrow{x}. \tag{4.1}$$

*Proof.* It suffices to prove (4.1) holds for  $\psi \in W^{1,1}(\mathbb{R}^3)$ , as we can extend it to  $\psi \in \mathscr{BV}(\mathbb{R}^3)$  by using a density argument [5, Theorem 3.9.].

Let  $\psi \in W^{1,1}(\mathbb{R}^3)$ , and define  $\chi_{\overrightarrow{a}} := \chi(\overrightarrow{x} - \overrightarrow{a})$ , where  $\chi \in C_0^{\infty}(\mathbb{R}^3) \setminus \{0\}$  is any nonnegative function that is compactly supported in  $B_1(\overrightarrow{0})$ .

Then, by Hölder's inequality and Sobolev's inequality,

$$\begin{split} \int_{B_{1}(\overrightarrow{a})} |\chi_{\overrightarrow{a}}\psi|^{\frac{4}{3}} d\overrightarrow{x} &= \int_{B_{1}(\overrightarrow{a})} |\chi_{\overrightarrow{a}}\psi|^{\frac{1}{3}} |\chi_{\overrightarrow{a}}\psi| d\overrightarrow{x} \\ &\leq \left[ \int_{B_{1}(\overrightarrow{a})} |\chi_{\overrightarrow{a}}\psi| d\overrightarrow{x} \right]^{\frac{1}{3}} \left( \int_{\mathbb{R}^{3}} |\chi_{\overrightarrow{a}}\psi|^{\frac{3}{2}} d\overrightarrow{x} \right)^{\frac{2}{3}} \\ &\leq C \left[ \sup_{\overrightarrow{a} \in \mathbb{R}^{3}} \int_{B_{1}(\overrightarrow{a})} |\psi| d\overrightarrow{x} \right]^{\frac{1}{3}} \int_{\mathbb{R}^{3}} ||\nabla(\chi_{\overrightarrow{a}}\psi)|| d\overrightarrow{x} \\ &\leq C \left[ \sup_{\overrightarrow{a} \in \mathbb{R}^{3}} \int_{B_{1}(\overrightarrow{a})} |\psi| d\overrightarrow{x} \right]^{\frac{1}{3}} \int_{\mathbb{R}^{3}} (\chi_{\overrightarrow{a}} ||\nabla\psi|| + ||\nabla\chi_{\overrightarrow{a}}||\psi|| d\overrightarrow{x}. \end{split}$$

We conclude the proof of this Lemma by integrating with respect to  $\vec{a} \in \mathbb{R}^3$ .

From this Lemma we may then conclude that noncompactness of sequences with bounded  $\mathscr{BV}(\mathbb{R}^3)$  norm is due to splitting and translation. The following is an adaptation of [21, Proposition 2.1], which is proved for characteristic functions of finite perimeter sets.

**Proposition 18.** Assume  $\{\psi_n\}_{n\in\mathbb{N}}$  is a bounded sequence in  $\mathscr{BV}(\mathbb{R}^3)$ , for which  $\liminf_{n\to\infty} \|\psi_n\|_{\mathscr{L}^{\frac{4}{3}}(\mathbb{R}^3)} > 0$ . Then, there exists translations  $\{a_n\}_{n\in\mathbb{N}}\subset\mathbb{R}^3$ , and  $\psi^0\in\mathscr{BV}(\mathbb{R}^3)\setminus\{0\}$ , such that for some (not relabeled) subsequence we have:

(a) 
$$\psi_n(\cdot - a_n) \xrightarrow[n \to \infty]{} \psi^0 \text{ in } \mathscr{L}^1_{loc}(\mathbb{R}^3),$$

$$(b) \| \boldsymbol{\psi}^0 \|_{\mathscr{B}\mathscr{V}(\mathbb{R}^3)} \leq \liminf_{n \to \infty} \| \boldsymbol{\psi}_n \|_{\mathscr{B}\mathscr{V}(\mathbb{R}^3)}.$$

Proof. By Lemma 13, we have

$$\sup_{\vec{a}\in\mathbb{R}^3}\int_{B_1(\vec{a})}|\psi_n|d\vec{x}\geq \left[C\frac{\int_{\mathbb{R}^3}|\psi|^{\frac{4}{3}}d\vec{x}}{\|\psi_n\|_{\mathscr{B}^{\mathscr{V}}(\mathbb{R}^3)}}\right]^3\geq 2c,$$

for some c > 0 independent of n. Hence, for each  $n \in \mathbb{N}$  we may choose vectors  $\vec{a}_n \in \mathbb{R}^3$  for which

$$\int_{B_1(\overrightarrow{a}_n)} |\psi_n| d\overrightarrow{x} \ge c > 0. \tag{4.2}$$

As  $\{\psi_n(\cdot - \vec{a}_n)\}_{n \in \mathbb{N}}$  is bounded in  $\mathscr{BV}(\mathbb{R}^3)$ , there exists a subsequence and  $\psi^0 \in \mathscr{BV}(\mathbb{R}^3)$  for which (a) and (b) hold. By (4.2) and  $\mathscr{L}^1_{loc}$  convergence, the limit  $\psi^0 \not\equiv 0$ .

Once we have localized a piece of our  $\mathscr{BV}(\mathbb{R}^3)$ -bounded sequence  $\{\psi_n\}_{n\in\mathbb{N}}$  as an  $\mathscr{L}^1_{loc}$ -converging part, we need to separate the compact piece from the rest, which converges locally to zero but may carry nontrivial

 $\mathscr{L}^1$ -mass to infinity. To do this, we first define a smooth cut-off function  $\omega:\mathbb{R}\to[0,1]$ , with

$$\omega \equiv 1 \text{ for } x < 0, \quad \omega \equiv 0 \text{ for } x > 1, \text{ and } \|\omega'\|_{\mathscr{L}^{\infty}(\mathbb{R}^3)} \leq 2,$$

and for any  $\rho > 0$ ,

$$\omega_{\rho}(\vec{x}) = \omega(\|\vec{x}\| - \rho). \tag{4.3}$$

The next Proposition is based on [21, Lemma 2.2.]:

**Proposition 19.** Let  $\{\psi_n\}_{n\in\mathbb{N}}$  be bounded in  $\mathscr{BV}(\mathbb{R}^3)$  with  $\psi_n \xrightarrow[n\to\infty]{} \psi^0$  in  $\mathscr{L}^1_{loc}(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ , for some function  $\psi^0 \in \mathscr{BV}(\mathbb{R}^3)$ . If  $0 < \|\psi^0\|_{\mathscr{L}^1(\mathbb{R}^3)} < \liminf_{n\to\infty} \|\psi_n\|_{\mathscr{L}^1(\mathbb{R}^3)}$ , then there exist radii  $\{\rho_n\}_{n\in\mathbb{N}} \subset (0,\infty)$  such that, up to a subsequence,

$$\int_{\mathbb{R}^3} [\|\nabla \psi_n\| - \|\nabla (\psi_n \omega_{\rho_n})\| - \|\nabla (\psi_n - \psi_n \omega_{\rho_n})\|] \xrightarrow[n \to \infty]{} 0. \tag{4.4}$$

Furthermore,

$$\psi_n \omega_{\rho_n} \xrightarrow[n \to \infty]{} \psi^0 \text{ in } \mathscr{L}^1(\mathbb{R}^3) \text{ and } \psi_n(1 - \omega_{\rho_n}) \xrightarrow[n \to \infty]{} 0 \text{ in } \mathscr{L}^1_{loc}(\mathbb{R}^3),$$
(4.5)

with each converging pointwise almost everywhere in  $\mathbb{R}^3$ .

Proof. Note that

$$\begin{split} \int_{\mathbb{R}^{3}} \|\nabla \psi_{n}\| &\leq \int_{\mathbb{R}^{3}} \|\nabla (\psi_{n} \omega_{\rho_{n}})\| + \int_{\mathbb{R}^{3}} \|\nabla \left[\psi_{n} (1 - \omega_{\rho_{n}})\right]\| \\ &\leq \int_{\mathbb{R}^{3}} \|\nabla \psi_{n}\| + 2 \int_{\mathbb{R}^{3}} \|\psi_{n} \nabla \omega (\|\overrightarrow{x}\| - \rho_{n})\| d\overrightarrow{x} \\ &\leq \int_{\mathbb{R}^{3}} \|\nabla \psi_{n}\| + 4 \int_{B_{Q_{n+1}}(\overrightarrow{0}) \setminus B_{Q_{n}}(\overrightarrow{0})} |\psi_{n}| d\overrightarrow{x}. \end{split}$$

Therefore, (4.4) holds if we find  $\{\rho_n\}_{n\in\mathbb{N}}\subset(0,\infty)$  such that

$$\int_{B_{2n+1}(\overrightarrow{0})\setminus B_{2n}(\overrightarrow{0})} |\psi_n| d\overrightarrow{x} \xrightarrow[n\to\infty]{} 0. \tag{4.6}$$

We consider two different cases.

First, suppose that supp  $\psi^0 \subset B_R(\overrightarrow{0})$ , for some R > 0. In this case, we claim that it suffices to choose radii  $\rho_n = R$  for all  $n \in \mathbb{N}$ . Indeed, by  $\mathcal{L}^1_{loc}(\mathbb{R}^3)$  convergence and the compact support of  $\psi^0$ ,

$$||\psi_n\omega_{\rho_n}||_{\mathscr{L}^1(\mathbb{R}^3)}=||\psi_n\omega_{\rho_n}||_{\mathscr{L}^1(B_{R+1}(\overrightarrow{0}))}\xrightarrow[n\to\infty]{}||\psi^0||_{\mathscr{L}^1(\mathbb{R}^3)},$$

and therefore (4.5) holds by the Brezis-Lieb Lemma [10] with each sequence converging pointwise almost everywhere in  $\mathbb{R}^3$ . Also, since  $\psi^0 \mathbb{1}_{B_{R+1}(\vec{0}) \setminus B_R(\vec{0})} \equiv 0$  and  $\psi_n \xrightarrow[n \to \infty]{} \psi^0$  in  $\mathscr{L}^1(B_{R+1}(\vec{0}))$ , we conclude that (4.6) is also verified in case supp  $(\psi^0)$  is compact.

In the second case, if supp  $\psi^0$  is essentially unbounded, note that  $\|\psi^0\|_{\mathscr{L}^1(\mathbb{R}^3)} < \liminf_{n \to \infty} \|\psi_n\|_{\mathscr{L}^1(\mathbb{R}^3)}$  implies that along some subsequence (not relabeled) we may choose radii  $R_n$  such that

$$\int_{B_{R_n}(\vec{0})} |\psi_n| d\vec{x} = \|\psi^0\|_{\mathscr{L}^1(\mathbb{R}^3)}. \tag{4.7}$$

We claim that, chosen this way,  $R_n \xrightarrow[n \to \infty]{} \infty$ . Indeed, assume that (taking a further subsequence if necessary),  $R_n \xrightarrow[n \to \infty]{} R_0 := \sup_{n \in \mathbb{N}} R_n$ . Then,

$$\|\psi^{0}\|_{\mathscr{L}^{1}(\mathbb{R}^{3})} = \liminf_{n \to \infty} \|\psi_{n} \mathbb{1}_{B_{R_{n}}}\|_{\mathscr{L}^{1}(\mathbb{R}^{3})} \leq \liminf_{n \to \infty} \|\psi_{n} \mathbb{1}_{B_{R_{0}}}\|_{\mathscr{L}^{1}(\mathbb{R}^{3})} = \|\psi^{0} \mathbb{1}_{B_{R_{0}}}\|_{\mathscr{L}^{1}(\mathbb{R}^{3})} < \|\psi^{0}\|_{\mathscr{L}^{1}(\mathbb{R}^{3})},$$

since we are assuming that supp  $\psi^0$  is essentially unbounded. Thus,  $R_n \xrightarrow[n \to \infty]{} \infty$ .

Next, fix R > 1 such that

$$\int_{B_R(\overrightarrow{0})} |\psi^0| d\overrightarrow{x} \ge \frac{1}{2} \|\psi^0\|_{\mathscr{L}^1(\mathbb{R}^3)}.$$

By  $\mathcal{L}^1_{loc}(\mathbb{R}^3)$  convergence, for all sufficiently large n we have

$$\int_{B_{R}(\vec{0})} |\psi_{n}| d\vec{x} \ge \frac{1}{4} \|\psi^{0}\|_{\mathcal{L}^{1}(\mathbb{R}^{3})}. \tag{4.8}$$

We now claim that for *n* large enough such that  $R_n > R$ , there exists  $\rho_n \in \left[\frac{R+R_n}{2}, R_n\right]$  for which

$$\int_{B_{\rho_n+1}(\overrightarrow{0})\setminus B_{\rho_n}(\overrightarrow{0})} |\psi_n| d\overrightarrow{x} \le \frac{3}{R_n - R} \|\psi^0\|_{\mathscr{L}^1(\mathbb{R}^3)}. \tag{4.9}$$

If so, then (4.6) is satisfied with this choice of  $\rho_n \ge r_n := \frac{R+R_n}{2} \xrightarrow[n\to\infty]{} \infty$ . To verify the claim, suppose the contrary, and so for every  $\rho \in [r_n, R_n]$  we have the opposite inequality to (4.9). For fixed n, choose a constant  $K \in \mathbb{N}$  with  $R_n - 1 \le r_n + K < R_n$ , so there are K intervals of unit length lying in  $[r_n, R_n]$ . Then, by (4.7), (4.8),

$$\begin{split} \frac{3}{4} \| \psi^{0} \|_{\mathscr{L}^{1}(\mathbb{R}^{3})} &\geq \int_{B_{R_{n}}(\overrightarrow{0})} |\psi_{n}| d\overrightarrow{x} - \int_{B_{R}(\overrightarrow{0})} |\psi_{n}| d\overrightarrow{x} \\ &\geq \int_{B_{r_{n}+K}(\overrightarrow{0}) \setminus B_{r_{n}}(\overrightarrow{0})} |\psi_{n}| d\overrightarrow{x} \\ &> K \frac{3}{R_{n}-R} \| \psi^{0} \|_{\mathscr{L}^{1}(\mathbb{R}^{3})} \\ &\geq 3 \frac{R_{n}-r_{n}-1}{R_{n}-R} \| \psi^{0} \|_{\mathscr{L}^{1}(\mathbb{R}^{3})} \\ &= \frac{3}{2} \frac{R_{n}-R-2}{R_{n}-R} \| \psi^{0} \|_{\mathscr{L}^{1}(\mathbb{R}^{3})}, \end{split}$$

for all sufficiently large n, a contradiction. This completes the proof of (4.4). Finally, note that  $\psi_n \omega_{\rho_n} \xrightarrow[n \to \infty]{} \psi^0$  pointwise almost everywhere in  $\mathbb{R}^3$ , Fatou's Lemma, (4.6),  $\rho_n \leq R_n$ , and (4.7) imply that

$$\|\psi^0\|_{\mathscr{L}^1(\mathbb{R}^3)} \leq \liminf_{n \to \infty} \int_{\mathbb{R}^3} |\psi_n \omega_{\rho_n}| d\overrightarrow{x}$$

$$\begin{split} &= \liminf_{n \to \infty} \left[ \int_{B_{\rho_n}(\vec{0})} |\psi_n \omega_{\rho_n}| d\vec{x} + \int_{B_{\rho_{n+1}}(\vec{0}) \setminus B_{\rho_n}(\vec{0})} |\psi_n \omega_{\rho_n}| d\vec{x} \right] \\ &= \liminf_{n \to \infty} \int_{B_{\rho_n}(\vec{0})} |\psi_n| d\vec{x} \le \|\psi^0\|_{\mathcal{L}^1(\mathbb{R}^3)}. \end{split}$$

Then, (4.5) follows from the Brezis-Lieb Lemma [10], with each sequence converging pointwise almost everywhere in  $\mathbb{R}^3$ .

**Remark 9.** By lower semicontinuity of the total variation with respect to the  $\mathcal{L}^1$  convergence, up to a subsequence,

$$\int_{\mathbb{R}^3} \|\nabla \psi^0\| \leq \lim_{n \to \infty} \int_{\mathbb{R}^3} \left( \|\nabla \psi_n\| - \|\nabla (\psi_n - \psi_n \omega_{\rho_n})\| \right)$$

We are now ready to prove the compactness and  $\Gamma$ -liminf part of the theorem:

*Proof of Theorem 7 (i).* Let  $\{u_{\varepsilon}\}_{{\varepsilon}>0}$  be a family in  $\mathscr{H}^M$  with  $\mathscr{E}^V_{\varepsilon}(u_{\varepsilon}) \leq K_0$ ,  ${\varepsilon}>0$ .

#### Step 1: Truncation.

First, we show that when proving (i) it suffices to restrict to  $u_{\varepsilon}$  satisfying the pointwise bounds  $-1 \le u_{\varepsilon} \le 1$  pointwise almost everywhere in  $\mathbb{R}^3$ . Indeed, we define the truncations

$$u_{\varepsilon}^* := \begin{cases} -1, & u_{\varepsilon} < -1, \\ u_{\varepsilon}, & |u_{\varepsilon}| \le 1, \\ 1, & u_{\varepsilon} > 1. \end{cases}$$

We show that  $\|u_{\varepsilon} - u_{\varepsilon}^*\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 \xrightarrow[\varepsilon \to 0^+]{} 0$ , and

$$\liminf_{\varepsilon \to 0^+} \mathscr{E}_{\varepsilon}^{V}(u_{\varepsilon}^*) \le \liminf_{\varepsilon \to 0^+} \mathscr{E}_{\varepsilon}^{V}(u_{\varepsilon}). \tag{4.10}$$

To accomplish this, we first note that by Remark 8, we have that

$$0 \le \int_{\mathbb{R}^3} |u_{\varepsilon} - u_{\varepsilon}^*|^2 d\vec{x} = \int_{\{|u_{\varepsilon}| > 1\}} (|u_{\varepsilon}| - 1)^2 d\vec{x} \le C \int_{\mathbb{R}^3} W(u_{\varepsilon}) d\vec{x} \xrightarrow{\varepsilon \to 0^+} 0,$$

where C is a constant independent of  $\varepsilon$ . Also by Remark 8,  $\{u_{\varepsilon}\}_{{\varepsilon}>0}$  is bounded in  $\mathscr{L}^2(\mathbb{R}^3)\cap \mathscr{L}^{\frac{10}{3}}(\mathbb{R}^3)$ , and hence the sequence of truncation s  $\{u_{\varepsilon}^*\}_{{\varepsilon}>0}$  is as well. By Proposition 6, we conclude that the local potential terms are close,

$$\int_{\mathbb{R}^3} V\left(|u_{\varepsilon}|^2 - |u_{\varepsilon}^*|^2\right) d\overrightarrow{x} \xrightarrow[\varepsilon \to 0^+]{} 0.$$

Finally, each of the other terms decreases under truncation,

$$\|\nabla u_{\varepsilon}^*\| \leq \|\nabla u_{\varepsilon}\|, \quad W(u_{\varepsilon}^*) \leq W(u_{\varepsilon}), \quad D(|u_{\varepsilon}^*|^2, |u_{\varepsilon}^*|^2) \leq D(|u_{\varepsilon}|^2, |u_{\varepsilon}|^2),$$

and so (4.10) is verified.

In the following we therefore assume, without loss of generality, that  $-1 \le u_{\varepsilon} \le 1$ ,  $\varepsilon > 0$ , pointwise almost everywhere in  $\mathbb{R}^3$ .

**Step 2:** Passing to the first limit.

Let  $\phi_{\varepsilon} := \Phi(u_{\varepsilon})$ , where  $\Phi : \mathbb{R} \to \mathbb{R}$  is defined by

$$\Phi(t) := \int_0^t \sqrt{W(\tau)} d\tau.$$

Then,

$$\phi_{\varepsilon} = \int_0^{u_{\varepsilon}} |t| (1 - |t|^{\frac{2}{3}}) dt = sign(u_{\varepsilon}) \left( \frac{1}{2} |u_{\varepsilon}|^2 - \frac{3}{8} |u_{\varepsilon}|^{\frac{8}{3}} \right),$$

and since  $||u_{\varepsilon}||_{\mathscr{L}^{\infty}(\mathbb{R}^3)} \leq 1$ ,

$$\frac{1}{8}|u_{\varepsilon}|^2 \le |\phi_{\varepsilon}| \le \frac{1}{2}|u_{\varepsilon}|^2 \quad \text{and} \quad |\phi_{\varepsilon}| \le \phi_{\varepsilon}(1) = \frac{1}{8}. \tag{4.11}$$

In particular,

$$\|\phi_{\varepsilon}\|_{\mathscr{L}^1(\mathbb{R}^3)} \leq \frac{1}{2} \|u_{\varepsilon}\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 \leq \frac{M}{2}.$$

Furthermore,  $\{\phi_{\varepsilon}\}_{0<\varepsilon<\frac{1}{4}}$  is bounded in  $BV(\mathbb{R}^3)$ . Indeed, by Young's inequality and Lemma 12 with  $v_{\varepsilon}=u_{\varepsilon}$ ,

$$\int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon}\| d\vec{x} = \int_{\mathbb{R}^3} \sqrt{W(u_{\varepsilon})} \|\nabla u_{\varepsilon}\| d\vec{x} \le \int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \|\nabla u_{\varepsilon}\|^2 + \frac{1}{2\varepsilon} W(u_{\varepsilon}) \right] d\vec{x} \le K_1, \tag{4.12}$$

with constant  $K_1 = K_1(K_0, M, V)$ . Consequently,  $\{\|\phi_{\varepsilon}\|_{\mathscr{BV}(\mathbb{R}^3)}\}_{0<\varepsilon<\frac{1}{4}}$  is bounded.

Now let  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$  be any sequence. By the compact embedding of  $\mathscr{BV}(\mathbb{R}^3)$  in  $\mathscr{L}^1_{loc}(\mathbb{R}^3)$  there exist a subsequence, which we continue to denote by  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$ , and a function  $\phi^0 \in \mathscr{BV}(\mathbb{R}^3)$  so that  $\phi_{\varepsilon_k} \xrightarrow[k \to \infty]{} \phi^0$  in  $\mathscr{L}^1_{loc}(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ . What is more, by lower semicontinuity of the total variation with respect to the  $\mathscr{L}^1$  convergence,

$$\int_{\mathbb{R}^3} \|\nabla \phi^0\| \le \liminf_{k \to \infty} \int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon_k}\| d\overrightarrow{x}. \tag{4.13}$$

Now we can use the invertibility of  $\Phi$  and the local uniform continuity of  $\Phi^{-1}$  to obtain that  $u_{\varepsilon_k} \xrightarrow[k \to \infty]{} u^0 := \Phi^{-1}(\phi^0)$  pointwise almost everywhere in  $\mathbb{R}^3$ . Then, by Fatou's Lemma and Remark 8, we have

$$0 \le \int_{\mathbb{R}^3} W(u^0) d\overrightarrow{x} \le \liminf_{k \to \infty} \int_{\mathbb{R}^3} W(u_{\varepsilon_k}) d\overrightarrow{x} = 0$$

hence  $W(u^0) \equiv 0$ ,  $u^0(\vec{x}) \in \{0, \pm 1\}$  pointwise almost everywhere, and

$$\phi^0 = \frac{1}{8}u^0 \text{ pointwise almost everywhere in } \mathbb{R}^3.$$
 (4.14)

As a result, by Fatou's Lemma and (4.11), for any compact  $K \subset \mathbb{R}^3$ ,

$$\int_{K} |\phi^{0}| d\overrightarrow{x} = \frac{1}{8} \int_{K} |u^{0}|^{2} d\overrightarrow{x} \le \frac{1}{8} \liminf_{k \to \infty} \int_{K} |u_{\varepsilon_{k}}|^{2} d\overrightarrow{x} \le \lim_{k \to \infty} \int_{K} |\phi_{\varepsilon_{k}}| d\overrightarrow{x} = \int_{K} |\phi^{0}| d\overrightarrow{x}. \tag{4.15}$$

Thus,  $u_{\mathcal{E}_k} \xrightarrow[k \to \infty]{} u^0$  pointwise almost everywhere in  $\mathbb{R}^3$  and , by Brezis-Lieb Lemma [10], in  $\mathscr{L}^2_{loc}(\mathbb{R}^3)$ , while by Fatou's Lemma  $\|u^0\|^2_{\mathscr{L}^2(\mathbb{R}^3)} \leq M$ .

For the nonlocal term, as  $u_{\varepsilon_k} \xrightarrow[k \to \infty]{} u^0$  locally, along a further subsequence it converges pointwise almost everywhere in  $\mathbb{R}^3$ , and hence by Fatou's Lemma,

$$D(|u^{0}|^{2},|u^{0}|^{2}) \leq \liminf_{k \to \infty} D(|u_{\varepsilon_{k}}|^{2},|u_{\varepsilon_{k}}|^{2}), \tag{4.16}$$

and by Proposition 6 with  $u_n = u_{\varepsilon_k}$  and  $v_n = u^0$ , (4.13), (4.12), and (4.14) we have

$$\mathscr{E}_0^V(u^0) \leq \liminf_{k \to \infty} \mathscr{E}_{\varepsilon_k}^V(u_{\varepsilon_k}).$$

If  $\phi_{\mathcal{E}_k} \xrightarrow[k \to \infty]{} \phi^0$  in  $\mathscr{L}^1(\mathbb{R}^3)$ , then by the same argument as (4.15) we may conclude that  $u_{\mathcal{E}_k} \xrightarrow[k \to \infty]{} u^0$  converges in  $\mathscr{L}^2(\mathbb{R}^3)$ , and so  $m^0 := \|u^0\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M$ , and setting  $u^i \equiv 0$  for all  $i \geq 1$ , the proof is complete.

**Step 3:** Splitting off the remainder sequence. If  $m^0 = M$ , then  $u_{\mathcal{E}_k} \xrightarrow[k \to \infty]{} u^0$  in  $\mathcal{L}^2(\mathbb{R}^3)$  by the Brezis-Lieb Lemma [10], and setting  $u^i \equiv 0$  for all  $i \geq 1$ , the proof is complete. To continue we assume that  $m^0 := \|u^0\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 < M$ , so the first limit does not capture all of the mass in the sequence  $u_{\mathcal{E}_k}$ . In this case, both  $u_{\mathcal{E}_k}$  and  $\phi_{\mathcal{E}_k}$  converge only locally (and not in norm), that is,

$$\|\phi^0\|_{\mathscr{L}^1(\mathbb{R}^3)} < \liminf_{k \to \infty} \|\phi_{\varepsilon_k}\|_{\mathscr{L}^1(\mathbb{R}^3)},$$

and similarly for  $u_{\varepsilon_k}$ , by the Brezis-Lieb Lemma [10].

Applying Proposition 19 and Remark 9 to  $\phi_{\epsilon_k}$ , and the fact that we do not have global convergence, there exists a sequence of radii  $\{\rho_k\}_{k\in\mathbb{N}}\subset (0,\infty)$  with  $\rho_k\xrightarrow[k\to\infty]{}\infty$  so that, for

$$\phi_{arepsilon_k}^0 := \omega_{
ho_k} \phi_{arepsilon_k}, \quad \phi_{arepsilon_k}^1 := (1 - \omega_{
ho_k}) \phi_{arepsilon_k},$$

where  $\omega_p$  is defined in (4.3), and for a subsequence (which we continue to write as  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$ ),

$$\phi_{\varepsilon_k}^0 \xrightarrow[k \to \infty]{} \phi^0 \quad \text{in } \mathscr{L}^1(\mathbb{R}^3), \quad \phi_{\varepsilon_k}^1 \xrightarrow[k \to \infty]{} 0 \text{ in } \mathscr{L}^1_{loc}(\mathbb{R}^3),$$
 (4.17)

 $\phi_{\varepsilon_k}^0 \xrightarrow[k \to \infty]{} \phi^0$  and  $\phi_{\varepsilon_k}^1 \xrightarrow[k \to \infty]{} 0$  pointwise almost everywhere in  $\mathbb{R}^3$ , and

$$\int_{\mathbb{R}^3} \|\nabla \phi^0\| + \int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon_k}^1\| d\vec{x} \le \int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon_k}\| d\vec{x} + o(1). \tag{4.18}$$

Moreover, from (4.6) and (4.11) the mass contained in the cut-off region is negligible:

$$\lim_{k \to \infty} \int_{B_{\rho_k+1}(\vec{0}) \setminus B_{\rho_k}(\vec{0})} |\phi_{\varepsilon_k}| d\vec{x} = 0 = \lim_{k \to \infty} \int_{B_{\rho_k+1}(\vec{0}) \setminus B_{\rho_k}(\vec{0})} |u_{\varepsilon_k}|^2 d\vec{x}. \tag{4.19}$$

We also decompose  $u_{\varepsilon_k}$  into two pieces,

$$u_{\varepsilon_k}^0 = u_{\varepsilon_k} \sqrt{\omega_{\rho_k}}, \text{ and } u_{\varepsilon_k}^1 = u_{\varepsilon_k} \sqrt{1 - \omega_{\rho_k}},$$
 (4.20)

so that  $(u_{\varepsilon_k})^2 = (u_{\varepsilon_k}^0)^2 + (u_{\varepsilon_k}^1)^2$  and  $u_{\varepsilon_k}^1 \xrightarrow[k \to \infty]{} 0$  pointwise almost everywhere in  $\mathbb{R}^3$ . Note that  $\phi_{\varepsilon_k}^i = \Phi(u_{\varepsilon_k}^i)$  holds in  $\mathbb{R}^3 \setminus \{\rho_k < \|\vec{x}\| < \rho_k + 1\}$ , and by (4.19) the region where they are no longer explicitly related carries a negligible amount of the mass of  $u_{\varepsilon_k}$ .

Equations (4.18), (4.14) and (4.12) give

$$\frac{1}{8} \int_{\mathbb{R}^3} \|\nabla u^0\| + \lim_{k \to \infty} \int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon_k}^1\| d\vec{x} \le \liminf_{k \to \infty} \int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \|\nabla u_{\varepsilon}\|^2 + \frac{1}{2\varepsilon} W(u_{\varepsilon}) \right] d\vec{x} \le K_0, \tag{4.21}$$

and in particular,  $\{\phi_{\mathcal{E}_k}^1\}_{k\in\mathbb{N}}$  is bounded in  $\mathscr{BV}(\mathbb{R}^3)$ . The nonlocal term also splits in the same way. Indeed, by (4.20),  $u_{\mathcal{E}_k}^0 \xrightarrow[k \to \infty]{} u^0$  pointwise almost everywhere in  $\mathbb{R}^3$ , the positivity of D(f,g) for  $f,g \geq 0$ , and (4.16)

$$\lim_{k \to \infty} \inf D(|u_{\varepsilon_{k}}|^{2}, |u_{\varepsilon_{k}}|^{2}) = \lim_{k \to \infty} \inf D(|u_{\varepsilon_{k}}^{0}|^{2} + |u_{\varepsilon_{k}}^{1}|^{2}, |u_{\varepsilon_{k}}^{0}|^{2} + |u_{\varepsilon_{k}}^{1}|^{2})$$

$$\geq \lim_{k \to \infty} \inf D(|u_{\varepsilon_{k}}^{0}|^{2}, |u_{\varepsilon_{k}}^{0}|^{2}) + D(|u_{\varepsilon_{k}}^{1}|^{2}, |u_{\varepsilon_{k}}^{1}|^{2})$$

$$\geq D(|u^{0}|^{2}, |u^{0}|^{2}) + \liminf_{k \to \infty} D(|u_{\varepsilon_{k}}^{1}|^{2}, |u_{\varepsilon_{k}}^{1}|^{2}).$$
(4.22)

Additionally, (4.14), Fatou's Lemma, (4.11), and (4.17) give

$$\int_{\mathbb{R}^3} |\phi^0| d\overrightarrow{x} = \frac{1}{8} \int_{\mathbb{R}^3} |u^0|^2 d\overrightarrow{x} \le \frac{1}{8} \liminf_{k \to \infty} \int_{\mathbb{R}^3} |u_{\varepsilon_k}^0|^2 d\overrightarrow{x} \le \lim_{k \to \infty} \int_{\mathbb{R}^3} |\phi_{\varepsilon_k}^0| d\overrightarrow{x} = \int_{\mathbb{R}^3} |\phi^0| d\overrightarrow{x}.$$

thus  $u^0_{\mathcal{E}_k} \xrightarrow[k \to \infty]{} u^0$  in  $\mathscr{L}^2(\mathbb{R}^3)$ . As a result,

$$M = m^0 + \lim_{k \to \infty} M_{\varepsilon_k}^1, \quad \text{where} \quad M_{\varepsilon_k}^1 := \|u_{\varepsilon_k}^1\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = \|u_{\varepsilon_k} - u^0\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 + o(1). \tag{4.23}$$

Lastly, as  $u_{\varepsilon_k} \xrightarrow[k \to \infty]{} u^0$  in  $\mathscr{L}^2_{loc}(\mathbb{R}^3)$ , by Proposition 6 we have

$$\int_{\mathbb{R}^3} V |u_{\varepsilon_k}|^2 d\vec{x} = \int_{\mathbb{R}^3} V |u^0|^2 d\vec{x} + o(1),$$

and hence we conclude by (4.14) and (4.21),

$$\mathscr{E}_0^V(u^0) + \liminf_{k \to \infty} \left[ \int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon_k}^1\| d\overrightarrow{x} + D\left(|u_{\varepsilon_k}^1|^2, |u_{\varepsilon_k}^1|^2\right) \right] \leq \liminf_{\varepsilon \to 0^+} \mathscr{E}_\varepsilon^V(u_\varepsilon).$$

**Step 4:** Concentration in the remainder sequence.

For any bounded sequence  $\{\psi_k\}_{k\in\mathbb{N}}$  in  $\mathcal{L}^1(\mathbb{R}^3)$  we define

$$\mathscr{M}(\{\psi_k\}) := \sup\{\|\psi\|_{\mathscr{L}^1(\mathbb{R}^3)} : \exists x_k \in \mathbb{R}^3, \psi_k(\cdot + x_k) \xrightarrow[k \to \infty]{} \psi \text{ in } \mathscr{L}^1_{loc}(\mathbb{R}^3)\},$$

So  $\mathcal{M}(\{\psi_k\})$  identifies the largest possible  $\mathcal{L}^1_{loc}$  limiting mass of the sequence, up to translation.

We claim that for our remainder sequence,  $\mathcal{M}(\{\phi_{\varepsilon_k}^1\}) > 0$ . Indeed, this follows from Proposition 18 once we have established the hypotheses. We first note that by (4.21),  $\{\phi_{\varepsilon_k}^1\}_{k\in\mathbb{N}}$  is bounded in  $\mathscr{BV}(\mathbb{R}^3)$ . Next, we must show that the  $\mathscr{L}^{\frac{4}{3}}$  norm of  $\phi_{\varepsilon_k}^1$  is bounded below. As  $u_{\varepsilon_k}^1 = u_{\varepsilon_k}$  pointwise almost everywhere in  $\mathbb{R}^3 \setminus B_{\rho_k+1}(\overrightarrow{0})$ , from Lemma 12 we have

$$2C_0\varepsilon_k \geq \int_{\mathbb{R}^3 \setminus B_{\rho_k+1}(\overrightarrow{0})} W(u_{\varepsilon_k}) d\overrightarrow{x} = \int_{\mathbb{R}^3 \setminus B_{\rho_k+1}(\overrightarrow{0})} W(u_{\varepsilon_k}^1) d\overrightarrow{x},$$

and thus, from (4.11), (4.6), (4.23), and  $t^{\frac{8}{3}} = (t^{\frac{10}{3}} + t^2)/2 - W(t)/2$ , we have:

$$\int_{\mathbb{R}^{3}\backslash B_{\rho_{k}+1}(\vec{0})} |\phi_{\varepsilon_{k}}^{1}|^{\frac{4}{3}} d\vec{x} \geq \frac{1}{16} \int_{\mathbb{R}^{3}\backslash B_{\rho_{k}+1}(\vec{0})} |u_{\varepsilon_{k}}^{1}|^{\frac{8}{3}} d\vec{x} 
\geq \frac{1}{32} \int_{\mathbb{R}^{3}\backslash B_{\rho_{k}+1}(\vec{0})} \left( |u_{\varepsilon_{k}}|^{\frac{10}{3}} + |u_{\varepsilon_{k}}|^{2} \right) d\vec{x} - C_{0} \varepsilon_{k} 
> \frac{1}{32} \int_{\mathbb{R}^{3}\backslash B_{\rho_{k}}(\vec{0})} |u_{\varepsilon_{k}}|^{2} d\vec{x} - o(1) 
\geq \frac{1}{32} \int_{\mathbb{R}^{3}} |u_{\varepsilon_{k}}^{1}|^{2} d\vec{x} + o(1) 
= \frac{M_{\varepsilon_{k}}^{1}}{32} + o(1) = \frac{1}{32} (M - m^{0}) + o(1) > 0.$$
(4.24)

Applying Proposition 18 the claim follows.

By the claim and Proposition 18, we may choose a subsequence, translations  $\{\vec{x}_k^1\}_{k\in\mathbb{N}}$ , and  $\phi^1 \in \mathscr{BV}(\mathbb{R}^3)$  with

$$\phi_{\varepsilon_k}^1(\cdot - \overrightarrow{x}_k^1) \xrightarrow[k \to \infty]{} \phi^1 \text{ in } \mathscr{L}^1_{loc}(\mathbb{R}^3), \text{ and } \|\phi^1\|_{\mathscr{L}^1(\mathbb{R}^3)} \ge \frac{1}{2}\mathscr{M}(\{\phi_{\varepsilon_k}^1\}).$$

Note that since  $\phi_{\mathcal{E}_k}^1 \xrightarrow[k \to \infty]{} 0$  in  $\mathscr{L}^1_{loc}(\mathbb{R}^3)$ , the sequence  $\|\vec{x}_k^1\| \xrightarrow[k \to \infty]{} \infty$ . By the same arguments as in Step 1 we may conclude that  $u^1_{\mathcal{E}_k}(\cdot - \vec{x}_k^1) \xrightarrow[k \to \infty]{} u^1 = 8\phi^1$  in  $\mathscr{L}^2_{loc}(\mathbb{R}^3)$  and pointwise almost everywhere in  $\mathbb{R}^3$ , with  $W(u^1) \equiv 0$  pointwise almost everywhere in  $\mathbb{R}^3$ , and hence  $u^1 \in BV(\mathbb{R}^3, \{0, \pm 1\})$  with  $\|u^1\|^2_{\mathscr{L}^2(\mathbb{R}^3)} =: m^1 \leq (M-m^0)$ .

Finally, the nonlocal term, which splits as in (4.22), passes to the limit using Fatou's Lemma,

$$\begin{split} D(|u^{0}|^{2},(|u^{0}|^{2})+D(|u^{1}|^{2},|u^{1}|^{2}) &\leq D(|u^{0}|^{2},|u^{0}|^{2}) + \liminf_{k \to \infty} D\left(|u_{\varepsilon_{k}}^{1}|^{2},|u_{\varepsilon_{k}}^{1}|^{2}\right) \\ &\leq \liminf_{k \to \infty} D(|u_{\varepsilon_{k}}|^{2},|u_{\varepsilon_{k}}|^{2}). \end{split}$$

In conclusion, using the previous inequality and (4.21) we have

$$\mathscr{E}_0^V(u^0) + \mathscr{E}_0^0(u^1) \leq \mathscr{E}_0^V(u^0) + \liminf_{k \to \infty} \left[ \int_{\mathbb{R}^3} \|\nabla \phi_{\varepsilon_k}^1\| d\, \overrightarrow{x} + D\left(|u_{\varepsilon_k}^1|^2, |u_{\varepsilon_k}^1|^2\right) \right] \leq \liminf_{\varepsilon \to 0^+} \mathscr{E}_\varepsilon^V(u_\varepsilon),$$

with  $m^0 + m^1 \le M$ . If  $m^1 = \|u^1\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M - m^0$ , then  $u^1_{\varepsilon_k}(\cdot - \overrightarrow{x}_k^1) \xrightarrow[k \to \infty]{} u^1$  in  $\mathscr{L}^2(\mathbb{R}^3)$  by the Brezis-Lieb Lemma [10], and the proof terminates, with  $u^i \equiv 0$  for all  $i \ge 2$ .

**Step 5:** *Iterating the argument.* 

If  $m^0+m^1 < M$ , then as in Step 3, the convergence of  $\phi^1_{\varepsilon_k}(\cdot - \overrightarrow{x}^1_k) \xrightarrow[k \to \infty]{} \phi^1$  is only local and not in the norm of  $\mathscr{L}^1(\mathbb{R}^3)$  (and similarly for  $u^1_{\varepsilon_k}(\cdot - \overrightarrow{x}^1_k) \xrightarrow[k \to \infty]{} u^1$  in  $\mathscr{L}^2(\mathbb{R}^3)$ ), and so there is again a remainder part to be separated via Proposition 19. That is, we may choose radii  $\{\rho^1_k\}_{k \in \mathbb{N}}$  going to infinity and further decompose  $\phi^1_{\varepsilon_k}(\cdot - \overrightarrow{x}^1_k)$ ,

$$\phi^1_{\varepsilon_k}(\cdot - \overrightarrow{x}_k^1)\omega_{\rho_k^1} \xrightarrow[k \to \infty]{} \phi^1 \text{ in } \mathscr{L}^1 \text{ norm}, \quad \phi^2_{\varepsilon_k} := \phi^1_{\varepsilon_k}(\cdot - \overrightarrow{x}_k^1)(1 - \omega_{\rho_k^1}) \xrightarrow[k \to \infty]{} 0 \text{ in } \mathscr{L}^1_{loc}(\mathbb{R}^3),$$

with the same consequences as in Step 4, identifying a mass center for  $\phi_{\mathcal{E}_k}^2$  via Proposition 18, translating and passing to a local  $\mathcal{L}^1$  limit to find  $\phi^2 = \frac{1}{8}u^2$ , and creating a refined lower bound.

Assuming the procedure has been done for the first n steps, we would have  $u^0, \dots u^n \in BV(\mathbb{R}^3, \{0, \pm 1\})$  with masses  $\|u^i\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = m^i$ , and translations  $\{\overrightarrow{x}_k^i\}_{k \in \mathbb{N}}$  for each  $i = 1, \dots, n$ , such that:

$$u_{\varepsilon_{k}} = u^{0} + \sum_{i=1}^{n} u^{i}(\cdot - \vec{x}_{k}^{i}) + u_{\varepsilon_{k}}^{n+1}(\cdot - \vec{x}_{k}^{n}), \text{ and } u_{\varepsilon_{k}}^{n+1}(\cdot - \vec{x}_{k}^{n}) \xrightarrow[k \to \infty]{} 0 \text{ in } \mathcal{L}_{loc}^{2}(\mathbb{R}^{3});$$

$$m^{i} = \|u^{i}\|_{\mathcal{L}^{2}(\mathbb{R}^{3})}^{2}, \quad i = 0, \dots, n;$$

$$\|\vec{x}_{k}^{i}\| \xrightarrow[k \to \infty]{} \infty, \quad \|\vec{x}_{k}^{i} - \vec{x}_{k}^{j}\| \xrightarrow[k \to \infty]{} \infty, \quad 1 \le i \ne j;$$

$$M = \sum_{i=0}^{n} m^{i} + \lim_{k \to \infty} \|u_{\varepsilon_{k}}^{n+1}\|_{\mathcal{L}^{2}(\mathbb{R}^{3})}^{2};$$

$$\mathcal{L}_{0}^{V}(u^{0}) + \sum_{i=1}^{n} \mathcal{L}_{0}^{0}(u^{i}) \le \liminf_{\varepsilon \to 0^{+}} \mathcal{L}_{0}^{V}(u_{\varepsilon}).$$

$$(4.25)$$

If for some  $n \in \mathbb{N}$ , the remainder  $\phi_{\mathcal{E}_k}^i \xrightarrow[k \to \infty]{} 0$  in  $\mathscr{L}^1(\mathbb{R}^3)$ , then the iteration terminates at that n, and the proof (i) of Theorem 7 is completed by choosing  $u^i = 0$  for all  $i \ge n+1$ . If the iteration continues indefinitely, we must verify that the entire mass corresponding to  $\{u_{\mathcal{E}_k}\}_{k \in \mathbb{N}}$  is exhausted by the  $\{u^i\}_{i=0}^{\infty}$ . It is here that we use  $\mathscr{M}(\{\phi_{\mathcal{E}_k}^i\})$ . When localizing mass in the remainder term  $\phi_{\mathcal{E}_k}^i$ , the translations  $\{\vec{x}_k^i\}$  and limit  $\phi^i = \frac{1}{8}u^i$  are chosen via Proposition 18 in such a way that

$$\|\phi^i\|_{\mathscr{L}^1(\mathbb{R}^3)} \geq \frac{1}{2} \mathscr{M}\left(\{\phi_{\varepsilon_k}^i\}\right), \quad i = 1, \dots, n.$$

In this way, the boundedness of the partial sums  $\sum_{i=0}^n m^i \leq M$  implies that, should the process continue indefinitely, the residual mass  $\mathscr{M}\left(\left\{\phi_{\varepsilon_k}^i\right\}\right) \leq 2m^i \xrightarrow[i \to \infty]{} 0$ . We claim that this implies that

$$M = \sum_{i=0}^{\infty} m^{i} = \sum_{i=0}^{\infty} \|u^{i}\|_{\mathcal{L}^{2}(\mathbb{R}^{3})}^{2}, \tag{4.26}$$

and that the entire mass corresponding to  $\{u_{\varepsilon_k}\}_{k\in\mathbb{N}}$  is exhausted by the  $\{u^i\}_{i=0}^{\infty}$ . Indeed, if  $\sum_{i=0}^{\infty} m^i = M' < M$ , then each remainder sequence satisfies

$$\|\phi_{\varepsilon_k}^i\|_{\mathscr{L}^1(\mathbb{R}^3)} \geq \frac{M-M'}{8}.$$

Returning to Step 4, and calculating as in (4.24), we obtain a lower bound up to a subsequence

$$\int_{\mathbb{D}^3} |\phi_{\varepsilon_k}^i|^{\frac{4}{3}} d\overrightarrow{x} \ge C(M - M'),$$

for a constant C independent of k, i. Using Lemma 13 we then have a uniform lower bound,

$$\mathscr{M}(\{\phi_{\varepsilon_k}^i\}) \ge \sup_{\overrightarrow{a} \in \mathbb{R}^3} \int_{B_1(\overrightarrow{a})} |\phi_{\varepsilon_k}^i| d\overrightarrow{x} \ge C'(M - M')^3,$$

for each  $i \in \mathbb{N}$ , with C' depending on the upper energy bound  $K_0$ , but independent of k,i. This contradicts  $\mathscr{M}(\{\phi_{\varepsilon_k}^i\}) < 2m^i \longrightarrow 0$ . Hence (4.26) is established, and passing to the limit  $n \to \infty$  in (4.25) we conclude the proof of (i) of Theorem 7.

#### 4.2 Upper bound

In this section we prove part (ii) of Theorem 7, the construction of recovery sequences in the  $\Gamma$ -convergence of  $\mathscr{E}^V_{\varepsilon}$ . As the space  $\mathscr{H}^M_0$  consists of a collection of functions in  $BV(\mathbb{R}^3, \{0, \pm 1\})$ , we build the recovery sequence by superposition of each, using the following lemma:

**Lemma 14.** Given  $v^0 \in BV(\mathbb{R}^3, \{0, \pm 1\})$  with  $||v^0||^2_{\mathscr{L}^2(\mathbb{R}^3)} = M$ , there exists  $\varepsilon_0 = \varepsilon_0(v^0) > 0$  and functions  $\{v_{\varepsilon}\}_{0 < \varepsilon < \varepsilon_0} \subset \mathscr{H}^M$  of compact support, such that

$$\|v_{\varepsilon}-v^{0}\|_{\mathscr{L}^{r}(\mathbb{R}^{3})}\xrightarrow[\varepsilon\to 0^{+}]{}0,\ 1\leq r<\infty,\quad \ \ \text{and}\quad \ \mathscr{E}^{V}_{\varepsilon}(v_{\varepsilon})\xrightarrow[\varepsilon\to 0^{+}]{}\mathscr{E}^{V}_{0}(v^{0}).$$

*Proof.* The basic construction is familiar, based on that of Sternberg [52, Proof of inequalities (1.12) and (1.13)], so we highlight the modifications necessary for our case.

The first step is to regularize  $v^0$ . As compactly supported functions are dense in the  $\mathscr{BV}(\mathbb{R}^3)$  norm, we may assume that supp  $v^0$  is bounded. Next, define a smooth mollifier, using  $\varphi \in C_0^{\infty}(B_1(\vec{0}))$ ,  $\varphi(\vec{x}) \geq 0$ ,  $\int_{B_1(\vec{0})} \varphi d\vec{x} = 1$  to generate

$$\varphi_n(\vec{x}) = n^3 \varphi(n\vec{x}) \in C_0^{\infty}(B_{\perp}(\vec{0})).$$

Following the proof of regularization of BV functions (see [5, Theorem 3.42.]), we create a sequence  $w_n = \varphi_n * v^0$  which is smooth and supported in a  $\frac{1}{n}$ -neighborhood of the support of  $v^0$ . As in [5], the regularization is obtained as a level surface of  $w_n$ . Here, we have two components, corresponding to the regularizations of  $v_+^0$  and  $v_-^0$ , in case  $v_-^0$  takes on both values  $\pm 1$ . By Sard's Theorem [18, 3.4.3.], there exist values  $t_+ \in (0,1)$  and  $t_- \in (-1,0)$  for which the boundaries of the sets

$$F_n^+ := \{ \vec{x} \in \mathbb{R}^3 | w_n(\vec{x}) > t_+ > 0 \}, \quad F_n^- := \{ \vec{x} \in \mathbb{R}^3 | w_n(\vec{x}) < t_- < 0 \}$$

are smooth for each  $n \in \mathbb{N}$ ,  $v_n^{\pm} := \mathbb{1}_{F_n^{\pm}} \xrightarrow[n \to \infty]{} v_{\pm}^0$  in  $\mathscr{L}^1(\mathbb{R}^3)$ , and

$$\int_{\mathbb{R}^3} \|\nabla v_n^{\pm}\| \xrightarrow[n \to \infty]{} \int_{\mathbb{R}^3} \|\nabla v_{\pm}^0\|.$$

Note by this construction that the sets  $F_n^{\pm}$  are smooth and disjoint for each n. Hence, the construction in [52] may be done separately for the components  $F_n^{\pm}$ , for any  $0 < \varepsilon < \eta_n$ , with  $\eta_n > 0$  being chosen so that the neighborhoods of radius  $\sqrt{\varepsilon}$  of the boundaries  $F_n^{\pm}$  are disjoint. Thus, applying the result of Sternberg [52]<sup>1</sup> for each  $n \in \mathbb{N}$ , and each  $0 < \varepsilon < \eta_n$ , there exists  $\tilde{v}_{n,\varepsilon}^{\pm}(\vec{x}) \in \mathscr{H}^1(\mathbb{R}^3)$  with  $\tilde{v}_{n,\varepsilon}^{+}, \tilde{v}_{n,\varepsilon}^{-}$  disjointly supported,  $0 \le \tilde{v}_{n,\varepsilon}^{\pm} \le 1$ , and

$$\|\tilde{v}_{n,\varepsilon}^{\pm} - v_n^{\pm}\|_{\mathcal{L}^1(\mathbb{R}^3)} \xrightarrow[\varepsilon \to 0^+]{} 0, \quad \text{and} \int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \|\nabla \tilde{v}_{n,\varepsilon}^{\pm}\|^2 + \frac{1}{2\varepsilon} W(\tilde{v}_{n,\varepsilon}^{\pm}) \right] \xrightarrow[\varepsilon \to 0^+]{} \frac{1}{8} \int_{\mathbb{R}^3} \|\nabla v_n^{\pm}\|. \tag{4.27}$$

Writing  $\tilde{v}_{n,\varepsilon} = \tilde{v}_{n,\varepsilon}^+ - \tilde{v}_{n,\varepsilon}^-$  (again, a disjoint sum for all  $0 < \varepsilon < \eta_n$ ), the same properties (4.27) hold for  $\tilde{v}_{n,\varepsilon}$  and  $v_n^0 = v_n^+ - v_n^-$ .

Next, we adjust the  $\tilde{v}_{n,\varepsilon}$  so that for each  $n,\varepsilon$ , each has  $\mathcal{L}^2$  norm equal to M, and hence defines a function in  $\mathcal{H}^M$ . For this we use dilation: let

$$\lambda_{oldsymbol{arepsilon}} := rac{\left\| ilde{v}_{n, oldsymbol{arepsilon}}
ight\|_{\mathscr{L}^2(\mathbb{R}^3)}^2}{M} \stackrel{rac{1}{3}}{\longrightarrow} 1.$$

We define the rescaled functions  $\hat{v}_{n,\varepsilon}: \mathbb{R}^3 \to \mathbb{R}$  by:

$$\hat{v}_{n,\varepsilon}(\overrightarrow{x}) := \tilde{v}_{n,\varepsilon}(\lambda_{\varepsilon}x), \text{ and } \hat{v}_n^{\pm}(\overrightarrow{x}) := v_n^{\pm}(\lambda_{\varepsilon}\overrightarrow{x}).$$

First, by rescaling we have  $\|\hat{v}_{n,\varepsilon}\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M$ , and so  $\hat{v}_{n,\varepsilon} \in \mathscr{H}^M$  for all  $n,\varepsilon$ . Next, we observe that, since the supports  $F_n^{\pm}$  of the components of  $v_n^0$  are smooth, for  $|\lambda_{\varepsilon} - 1|$  sufficiently small, we may estimate

$$\|\hat{v}_{n}^{0} - v_{n}^{0}\|_{\mathscr{L}^{1}(\mathbb{R}^{3})} \le c|\lambda_{\varepsilon}^{\frac{1}{3}} - 1|\int_{\mathbb{R}^{3}} \|\nabla v_{n}^{0}\|.$$

Hence, we have convergence in the  $\mathcal{L}^1$  norm,

$$0 \leq \|\hat{v}_{n,\varepsilon} - v_n^0\|_{\mathscr{L}^1(\mathbb{R}^3)} \leq \|\hat{v}_{n,\varepsilon} - \hat{v}_n^0\|_{\mathscr{L}^1(\mathbb{R}^3)} + \|\hat{v}_n^0 - v_n^0\|_{\mathscr{L}^1(\mathbb{R}^3)} \\ \leq \lambda_{\varepsilon}^{-1} \|\tilde{v}_{n,\varepsilon} - v_n^0\|_{\mathscr{L}^1(\mathbb{R}^3)} + c|\lambda_{\varepsilon}^{\frac{1}{3}} - 1|\int_{\mathbb{R}^3} \|\nabla v_n^0\| \xrightarrow[\varepsilon \to 0^+]{} 0.$$

As each of  $|\hat{v}_{n,\varepsilon}| \leq 1$  pointwise almost everywhere in  $\mathbb{R}^3$ , and for fixed n each is of uniformly bounded support, the convergence extends to any  $\mathcal{L}^r(\mathbb{R}^3)$ ,  $r \geq 1$ . Moreover,

$$\begin{split} \int_{\mathbb{R}^3} \left[ \frac{\varepsilon}{2} \|\nabla \hat{v}_{n,\varepsilon}^{\pm}\|^2 + \frac{1}{2\varepsilon} W(\hat{v}_{n,\varepsilon}^{\pm}) \right] d\vec{x} \\ &= \left[ \lambda_{\varepsilon}^{-\frac{1}{3}} \int_{\mathbb{R}^3} \frac{\varepsilon}{2} \|\nabla \tilde{v}_{n,\varepsilon}^{\pm}\|^2 d\vec{x} + \lambda_{\varepsilon}^{-1} \int_{\mathbb{R}^3} \frac{1}{2\varepsilon} W(\tilde{v}_{n,\varepsilon}^{\pm}) d\vec{x} \right] \xrightarrow[\varepsilon \to 0^+]{} \frac{1}{8} \int_{\mathbb{R}^3} \|\nabla v_n^0\|, \end{split}$$

<sup>&</sup>lt;sup>1</sup>We note that the potential in [52] has two wells at  $u = \pm 1$ , whereas our transitions connect v = 0 to  $v = \pm 1$ , and so our  $\tilde{v}_{n,\varepsilon}^{\pm} = \frac{1}{2}(\rho_{\varepsilon} + 1)$  for  $\rho_{\varepsilon}$  as constructed in [52].

which holds for each  $n \in \mathbb{N}$ . As in [52], by a diagonal argument, there exists  $\varepsilon_0 = \varepsilon_0(v^0) > 0$  so that for any sequence  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$  with  $\varepsilon_k < \varepsilon_0$ , we obtain a sequence  $\{v_{\varepsilon_k}\}_{k \in \mathbb{N}}$  with

$$\|v_{\varepsilon_k} - v^0\|_{\mathscr{L}^r(\mathbb{R}^3)} \xrightarrow[k \to \infty]{} 0, r \ge 1, \quad \text{and} \ \int_{\mathbb{R}^3} \left[ \frac{\varepsilon_k}{2} \|\nabla v_{\varepsilon_k}\|^2 + \frac{1}{2\varepsilon_k} W(v_{\varepsilon_k}) \right] d\overrightarrow{x} \xrightarrow[k \to \infty]{} \frac{1}{8} \int_{\mathbb{R}^3} \|\nabla v_{\pm}^0\|.$$

The local potential terms also converge by Proposition 6. Furthermore, by the Hardy-Littlewood-Sobolev inequality [34, Theorem 4.3] (with p = 6/5 = r),

$$\begin{split} 0 &\leq \left| D(|v_{\varepsilon_{k}}|^{2}, |v_{\varepsilon_{k}}|^{2}) - D(|v^{0}|^{2}, |v^{0}|^{2}) \right| \\ &= \left| D(|v_{\varepsilon_{k}}|^{2} - |v^{0}|^{2}, |v_{\varepsilon_{k}}|^{2} + |v^{0}|^{2}) \right| \\ &\leq \left\| |v_{\varepsilon_{k}}|^{2} - |v^{0}|^{2} \right\|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \left\| |v_{\varepsilon_{k}}|^{2} + |v^{0}|^{2} \right\|_{\mathscr{L}^{\frac{6}{5}}(\mathbb{R}^{3})} \xrightarrow[k \to \infty]{} 0. \end{split}$$

This completes the proof of Lemma 14.

Proof of (ii) of Theorem 7. If  $\{u^i\}_{i=0}^{\infty}$  is a finite collection with N nontrivial components, this follows easily from Lemma 14. Indeed, for any sequence  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$  with

$$0 < \varepsilon_k < \min_{i=0,\ldots,N} \{\varepsilon_0(u^i)\}_{i=0,\ldots,N},$$

we apply the lemma to find  $u_{\varepsilon}^{i} \xrightarrow[\varepsilon \to 0^{+}]{} u^{i}$ ,  $i = 0, \dots, N$ , and form the disjoint sum,

$$u_{\varepsilon_k}(\vec{x}) = u_{\varepsilon_k}^0(\vec{x}) + \sum_{i=1}^N u_{\varepsilon_k}^i(\vec{x} - \vec{x}_k^i),$$

by choosing translations  $\{\vec{x}_k^i\}_{k\in\mathbb{N}}$  which tend to infinity and far from each other quickly enough in k.

If  $\{u^i\}_{i=0}^{\infty}$  has an infinite number of nontrivial elements, we must be more careful. In particular, as we go down the list of the  $\{u^i\}_{i=0}^{\infty}$ , the characteristic length scale of each  $u^i$  gets smaller, and for any particular  $\varepsilon > 0$  there can only be a finite number of i with  $0 < \varepsilon < \varepsilon_0(u^i)$ , for which the trial functions  $u^i_{\varepsilon}$  can be constructed via Lemma 14. Take any decreasing sequence  $\varepsilon_k \xrightarrow[k \to \infty]{} 0^+$ . By Lemma 14 and part (i) of Theorem 7, for each  $i = 0, 1, 2, \ldots$  there exist  $\varepsilon^i = \varepsilon_0(u^i) > 0$  and a sequence  $\{u^i_{\varepsilon_k}\}_{k \in \mathbb{N}}$ , for which

$$\left| \mathcal{E}_{\varepsilon_{k}}^{V}(u_{\varepsilon_{k}}^{0}) - \mathcal{E}_{0}^{V}(u^{0}) \right| < \frac{\mathcal{E}_{0}^{V}(u^{0})}{10k} \text{ and } \|u_{\varepsilon_{k}}^{0} - u^{0}\|_{\mathcal{L}^{2}(\mathbb{R}^{3})}^{2} < \frac{m^{0}}{10k}, \quad 0 < \varepsilon_{k} < \varepsilon^{0}, \\
\left| \mathcal{E}_{\varepsilon_{k}}^{0}(u_{\varepsilon_{k}}^{i}) - \mathcal{E}_{0}^{0}(u^{i}) \right| < \frac{\mathcal{E}_{0}^{0}(u^{i})}{10k}, \text{ and } \|u_{\varepsilon_{k}}^{i} - u^{i}\|_{\mathcal{L}^{2}(\mathbb{R}^{3})}^{2} < \frac{m^{i}}{10k}, \quad 0 < \varepsilon_{k} < \varepsilon^{i}, \ i = 1, 2, 3, \dots \right\}$$
(4.28)

By taking  $\varepsilon^i$  smaller if necessary we may assume  $0 < \varepsilon^i < \varepsilon^{i-1}$ . We now construct  $U_{\varepsilon_k}$  as follows: for each  $k \in \mathbb{N}$ , choose the largest integer  $n_k \in \mathbb{N} \cup \{0\}$  such that  $0 < \varepsilon_k < \varepsilon^i$  for all  $i \le n_k$ . Note that  $n_k \xrightarrow[k \to \infty]{} \infty$ . As the  $u^i_{\varepsilon_k}$  are all compactly supported, say  $\sup u^i_{\varepsilon_k} \subset B_{R^i_{\varepsilon_k}}(\overrightarrow{0})$ , we may choose vectors  $\overrightarrow{x}^i_k \in \mathbb{R}^3$ ,  $i = 1, \ldots, n_k$ , so that

$$\|\overrightarrow{x}_k^i - \overrightarrow{x}_k^j\| > 2^{i+j+k+2} (R_{\varepsilon_k}^i + R_{\varepsilon_k}^j + 1) \xrightarrow[k \to \infty]{} \infty.$$

In particular, this implies that the functions  $u_{\varepsilon_k}^i(\vec{x}-\vec{x}_k^i)$  are disjointly supported.

Then, we set

$$U_{\varepsilon_k}(\vec{x}) := u_{\varepsilon_k}^0(\vec{x}) + \sum_{i=1}^{n_k} u_{\varepsilon_k}^i(\vec{x} - \vec{x}_k^i).$$

Note that by the choice of the  $\overrightarrow{x}_k^i$  and  $V \ge 0$ , we have

$$\mathscr{E}^{V}_{\varepsilon_{k}}(U_{\varepsilon_{k}}) \leq \mathscr{E}^{V}_{\varepsilon_{k}}(u^{0}_{\varepsilon_{k}}) + \sum_{i=1}^{n_{k}} \mathscr{E}^{0}_{\varepsilon_{k}}(u^{i}_{\varepsilon_{k}}) + \sum_{i,j=1}^{n_{k}} D(|u^{i}_{\varepsilon_{k}}(\cdot - \overrightarrow{x}^{i}_{\varepsilon_{k}})|^{2}, |u^{j}_{\varepsilon_{k}}(\cdot - \overrightarrow{x}^{j}_{\varepsilon_{k}})|^{2}).$$

Further, since  $supp\ u^i_{\varepsilon_k}(\cdot - \overrightarrow{x}^i_{\varepsilon_k}) \subset B_{R^i_{\varepsilon_k}}(\overrightarrow{x}^i_{\varepsilon_k})$  and

$$\left| \frac{1}{\|\psi^1 - \psi^2\|} - \frac{1}{\|\vec{x} - \vec{y}\|} \right| \le \frac{4\rho}{\|\psi^1 - \psi^2\|^2} \le \frac{1}{\|\psi^1 - \psi^2\|}$$

for  $\vec{x} \in B_{\rho}(\psi^1)$ ,  $\vec{x} \in B_{\rho}(\psi^2)$ ,  $\rho < \frac{1}{4} \|\psi^1 - \psi^2\|$ , we estimate

$$\begin{split} D(|u_{\varepsilon_{k}}^{i}(\cdot-\vec{x}_{\varepsilon_{k}}^{i})|^{2},|u_{\varepsilon_{k}}^{j}(\cdot-\vec{x}_{\varepsilon_{k}}^{j})|^{2}) &= \int_{B_{R_{\varepsilon_{k}}^{i}}(\vec{x}_{\varepsilon_{k}}^{i})} \int_{B_{R_{\varepsilon_{k}}^{j}}(\vec{x}_{\varepsilon_{k}}^{j})} \frac{|u_{\varepsilon_{k}}^{i}(\vec{x}-\vec{x}_{\varepsilon_{k}}^{i})|^{2}|u_{\varepsilon_{k}}^{j}(y-\vec{x}_{\varepsilon_{k}}^{i})|^{2}}{\|\vec{x}-\vec{y}\|} d\vec{x} dy \\ &\leq \frac{2\|u_{\varepsilon_{k}}^{i}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}\|u_{\varepsilon_{k}}^{j}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2}}{\|\vec{x}_{k}^{i}-\vec{x}_{k}^{j}\|} \\ &\leq 2\frac{M^{2}}{\|\vec{x}_{k}^{i}-\vec{x}_{k}^{j}\|} = o(1) \text{ as } k \to \infty. \end{split}$$

As a result,

$$\mathscr{E}_{\varepsilon_k}^V(U_{\varepsilon_k}) \le \mathscr{E}_{\varepsilon_k}^V(u_{\varepsilon_k}^0) + \sum_{i=1}^{n_k} \mathscr{E}_{\varepsilon_k}^0(u_{\varepsilon_k}^i) + o(1) \text{ as } k \to \infty.$$
 (4.29)

On the other hand, the mass  $\|U_{\mathcal{E}_k}\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = \sum_{i=0}^{n_k} m^i = :M^{(k)} \xrightarrow[k \to \infty]{} M^-$  as more components are added to the sum.

We next show that  $\limsup_{k\to\infty} \mathscr{E}^V_{\varepsilon_k}(U_{\varepsilon_k}) \leq \mathscr{F}^V_0(\{u^i\}_{i=0}^\infty)$ . If  $\mathscr{F}^V_0(\{u^i\}_{i=0}^\infty) = \infty$ , then there is nothing to prove. Otherwise, let  $\delta > 0$  be given, and choose a number  $N \in \mathbb{N}$  for which

$$\sum_{i=N+1}^{\infty} \mathcal{E}_0^0(u^i) < \frac{\delta}{5}.\tag{4.30}$$

From Lemma 14, there exists  $K \in \mathbb{N}$  such that for all  $k \ge K$ ,

$$\left| \mathcal{E}_{\varepsilon_k}^V(u_{\varepsilon_k}^0) - \mathcal{E}_0^V(u^0) \right| + \sum_{i=1}^N \left| \mathcal{E}_{\varepsilon_k}^0(u_{\varepsilon_k}^i) - \mathcal{E}_0^0(u^i) \right| < \frac{\delta}{5}. \tag{4.31}$$

Then, for all  $k \ge K$ , using (4.29), (4.31), (4.28), and (4.30), we estimate

$$\mathscr{E}^{V}_{\varepsilon_{k}}(U_{\varepsilon_{k}}) - \mathscr{F}^{V}_{0}(\{u^{i}\}_{i=0}^{\infty}) \leq \mathscr{E}^{V}_{\varepsilon_{k}}(U_{\varepsilon_{k}}) - \mathscr{E}^{V}_{0}(u^{0}) - \sum_{i=0}^{N} \mathscr{E}^{0}_{0}(u^{i})$$

$$\leq \mathcal{E}_{\varepsilon_k}^V(u_{\varepsilon_k}^0) - \mathcal{E}_0^V(u^0) + \sum_{i=1}^N \left[ \mathcal{E}_{\varepsilon_k}^0(u_{\varepsilon_k}^i) - \mathcal{E}_0^0(u^i) \right] + \sum_{i=N+1}^{n_k} \mathcal{E}_{\varepsilon_k}^0(u_{\varepsilon_k}^i) + o(1)$$

$$< \frac{\delta}{5} + \frac{11}{10} \sum_{i=N+1}^{n_k} \mathcal{E}_0^0(u^i) < \frac{\delta}{2}.$$

Then,

$$\limsup_{k\to\infty} \mathscr{E}^{V}_{\varepsilon_k}(U_{\varepsilon_k}) \leq \mathscr{F}^{V}_{0}(\{u^i\}_{i=0}^{\infty}).$$

Now we prove that

$$\left\| U_{\varepsilon_k} - \left( u^0 + \sum_{i=0}^{\infty} u^i (\vec{x} - \vec{x}_k^i) \right) \right\|_{\mathscr{L}^2(\mathbb{R}^3)} \xrightarrow[k \to \infty]{} 0.$$

Let  $\delta > 0$  be given, and choose a number  $N \in \mathbb{N}$  for which

$$\sum_{i=N+1}^{\infty} m^i < \frac{\delta}{5} \tag{4.32}$$

From Lemma 14, there exists  $K \in \mathbb{N}$  such that for all  $k \geq K$ ,

$$\sum_{i=0}^{N} \|u_{\varepsilon_k}^i - u^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 < \frac{\delta}{5}. \tag{4.33}$$

Then, for all  $k \ge K$ , using (4.33), (4.28), and (4.32), we estimate

$$\begin{split} \left\| U_{\mathcal{E}_{k}} - \left( u^{0} + \sum_{i=0}^{\infty} u^{i}(\vec{x} - \vec{x}_{k}^{i}) \right) \right\|_{\mathscr{L}^{2}(\mathbb{R}^{3})} &\leq \sum_{i=0}^{N} \| u_{\mathcal{E}_{k}}^{i} - u^{i} \|_{\mathscr{L}^{2}(\mathbb{R}^{3})} + \sum_{i=N+1}^{n_{k}} \| u_{\mathcal{E}_{k}}^{i} - u^{i} \|_{\mathscr{L}^{2}(\mathbb{R}^{3})} + \sum_{i=n_{k}+1}^{\infty} \| u^{i} \|_{\mathscr{L}^{2}(\mathbb{R}^{3})} \\ &\leq \frac{\delta}{5} + \sum_{i=N+1}^{n_{k}} \frac{m^{i}}{10} + \frac{\delta}{5} < \delta, \end{split}$$

Then,

$$\left|\left|U_{\varepsilon_k}-\left(u^0+\sum_{i=0}^\infty u^i(\overrightarrow{x}-\overrightarrow{x}_k^i)\right)\right|\right|_{\mathscr{L}^2(\mathbb{R}^3)}\xrightarrow[k\to\infty]{}0.$$

It remains to correct the mass of  $U_{\varepsilon_k}$ , so that each  $||U_{\varepsilon_k}||^2_{\mathscr{L}^2(\mathbb{R}^3)} = M$ . This is done as in Lemma 14, dilating each component  $u^i_{\varepsilon_k}$  by the scaling factor

$$\lambda_k = \left(rac{M^{(k)}}{M}
ight)^rac{1}{3} \xrightarrow[k o \infty]{} 1,$$

that is, by setting

$$u_{\varepsilon_k}(\vec{x}) := u_{\varepsilon_k}^0(\lambda_k \vec{x}) + \sum_{i=1}^{n_k} u_{\varepsilon_k}^i(\lambda_k(\vec{x} - x_k)).$$

Then

$$\|u_{\varepsilon_k}\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M, k \in \mathbb{N}, \quad \|u_{\varepsilon_k} - U_{\varepsilon_k}\|_{\mathscr{L}^2(\mathbb{R}^3)} \xrightarrow[k \to \infty]{} 0, \text{ and } |\mathscr{E}^V_{\varepsilon_k}(u_{\varepsilon_k}) - \mathscr{E}^V_{\varepsilon_k}(U_{\varepsilon_k})| \xrightarrow[k \to \infty]{} 0,$$

since 
$$\lambda_k \xrightarrow[k \to \infty]{} 1$$
. This concludes the proof of Theorem 7.

## **Chapter 5**

# Minimizers of the Liquid Drop and TFDW functionals

In this chapter we examine the connection between minimizers of the liquid drop and TDFW functionals. More precisely, we prove Theorems 8 and 9, and Corollary 1. Throughout this chapter, we assume V satisfies (1.17).

Recall  $\mathscr{E}^Z_{\varepsilon}$ ,  $\mathscr{E}^Z_0$  are the energies (1.15) and (1.16), respectively, with the atomic choice  $V = V_Z = Z/\|\overrightarrow{x}\|$ , and

$$e^Z_{\varepsilon}(M) \colon= \inf \left\{ \mathscr{E}^Z_{\varepsilon}(u) \, : \, u \in \mathscr{H}^M_+ \right\}, \quad e^Z_0(M) \colon= \inf \left\{ \mathscr{E}_0(u) \, : \, u \in \mathscr{X}^M_+ \right\}.$$

The compactness of minimizing sequences being a delicate issue which is shared by the two models. First, whether the minimum in  $e_{\varepsilon}^{V}(M)$  is attained or not, the infimum values converge as  $\varepsilon \to 0^+$ :

**Lemma 15.** Assume V satisfies (1.17). Then, for all M > 0,

$$e_{\varepsilon}^{V}(M) \xrightarrow[\varepsilon \to 0^{+}]{} e_{0}^{V}(M).$$

*Proof.* The proof is standard. First, for each  $\varepsilon > 0$ , there is a function  $u_{\varepsilon} \in \mathscr{H}^{M}$  with  $\|u_{\varepsilon}\|_{\mathscr{L}^{2}(\mathbb{R}^{3})}^{2} = M$  and

$$\mathscr{E}_{\varepsilon}^{V}(u_{\varepsilon}) \leq e_{\varepsilon}^{V}(M) + \varepsilon.$$

It suffices to prove that for any sequence  $\varepsilon_n \xrightarrow[n \to \infty]{} 0^+$ , the is a (not relabeled) subsequence for which  $e_{\varepsilon_n}^V(M) \xrightarrow[n \to \infty]{} e_0^V(M)$ . By Theorem 7 (i), there exists a sequence  $\{u^i\}_{i=0}^\infty \in \mathscr{H}_0^M$  and a subsequence  $\varepsilon_n \xrightarrow[n \to \infty]{} 0^+$  with

$$e_0^V(M) \leq \mathscr{F}_0^V(\{u^i\}_{i=0}^\infty) \leq \liminf_{n \to \infty} \mathscr{E}_{\varepsilon_n}^V(u_{\varepsilon_n}) = \liminf_{n \to \infty} e_{\varepsilon_n}^V(M).$$

For the complementary inequality, for any  $\delta > 0$ , there exists a sequence  $\{v^i\}_{i=0}^{\infty} \in \mathcal{H}_0^M$  with

$$\mathscr{F}_0^V(\{v^i\}_{i=0}^{\infty}) < e_0^V(M) + \delta.$$

Then, by (ii) in Theorem 7, for any  $\varepsilon > 0$ ,  $\exists v_{\varepsilon} \in \mathscr{H}^{M}$  with

$$e_0^V(M) + \delta > \mathscr{F}_0^V(\{v^i\}_{i=0}^\infty) \geq \limsup_{\varepsilon \to 0^+} \mathscr{E}_\varepsilon^V(v_\varepsilon) \geq \limsup_{\varepsilon \to 0^+} e_\varepsilon^V(M).$$

Putting the above inequalities together, and letting  $\delta \to 0^+$ , we obtain the desired conclusion.

Proof of Corollary 1. In [3, Theorems 1 and 2] it is proved that for V satisfying (1.7), the minimum for both  $\mathscr{E}_0^V$  and  $\mathscr{E}_{\varepsilon}^V$  are attained, correspondingly. Indeed, the proof of these results in [3] actually yields the stronger conclusion that  $\underline{\mathrm{all}}$  minimizing sequences for either the TDFW or liquid drop functionals are convergent. Thus, for all  $\varepsilon > 0$ , there exists a function  $u_{\varepsilon} \in \mathscr{H}^M$  which attains the minimum,  $e_{\varepsilon}^V(M) = \mathscr{E}_{\varepsilon}^V(u_{\varepsilon})$ . By Lemma 15,  $\mathscr{E}_{\varepsilon}^V(u_{\varepsilon}) \xrightarrow[\varepsilon \to 0^+]{} e_0^V(M)$ , so for any sequence  $\varepsilon_n \xrightarrow[n \to \infty]{} 0^+$ , by Theorem 7 (i), there exists a sequence of functions  $\{u^i\}_{i=0}^{\infty} \in \mathscr{H}_0^M$  with

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^{\infty}) \leq \liminf_{n \to \infty} \mathscr{E}_{\varepsilon_n}^V(u_{\varepsilon_n}) = e_0^V(M).$$

Defining  $m^i := ||u^i||_{\mathscr{L}^2(\mathbb{R}^3)}^2$ , we have

$$e_0^V(M) = e_0^V(m^0) + \sum_{i=1}^{\infty} e_0^0(m^i),$$
 (5.1)

We then obtain a contradiction by using Step 6 in the proof of Theorem 1 of [3]. Indeed, by choosing compactly supported  $v^0, v^1 \in \mathscr{H}^M$  whose energies are close to the infima  $e_0^V(m^0), e_0^0(m^1)$  as in Step 6, we obtain the strict subadditivity condition,

$$e_0^V(M) < e_0^V(m^0) + e_0^0(m^1) + e_0^0(M - m^0 - m^1) \le e_0^V(m^0) + \sum_{i=1}^{\infty} e_0^0(m^i),$$

and the desired contradiction to (5.1).

Analyzing the possible loss of compactness in minimizing sequences for  $e_{\varepsilon}^{Z}(M)$ ,  $\varepsilon \geq 0$  and  $Z \geq 0$ , requires the use of concentration-compactness methods [36]. The following are standard results for problems where loss of compactness entails splitting of mass to infinity:

**Lemma 16.** Assume V satisfies (1.17). Then, for any  $\varepsilon \geq 0$  and M > 0,

(i) If 
$$\forall m^0 \in (0, M)$$
, 
$$e_{\varepsilon}^V(M) < e_{\varepsilon}^V(m^0) + e_{\varepsilon}^0(M - m^0), \tag{5.2}$$

then all minimizing sequences for  $e_{\varepsilon}^{V}(M)$  are precompact.

(ii) If there exist non-precompact minimizing sequences for  $e_{\varepsilon}^{V}(M)$ , then  $\exists m^{0} \in (0,M)$  such that  $e_{\varepsilon}^{V}(m^{0})$  attains a minimizer and

$$e_{\varepsilon}^{V}(M) = e_{\varepsilon}^{V}(m^{0}) + e_{\varepsilon}^{0}(M - m^{0}).$$

Statement (ii) is a useful precision of the contrapositive of (i). The proof for the TFDW functional was done in [37], and for Liquid Drop Models it may be derived from the more detailed concentration lemma in [2]; although it is stated there for V of a special form, in fact it is true for a much larger class including those satisfying (1.17).

Next, we specialize to the atomic case,

$$V(\vec{x}) = \frac{Z}{\|\vec{x}\|},$$

and present the following refinement of the existence result of [40] for the Liquid Drop Model with atomic potential:

**Proposition 20.** There exists a constant  $\mu_0 > 0$  such that for all  $Z \ge 0$  and for all  $M \in (0, Z + \mu_0)$ :

- (i) All minimizing sequences for  $e_0^Z(M)$  are precompact.
- (ii) The unique minimizer (up to translations if Z=0) of  $e_0^Z(M)$  is the ball  $\mathbb{B}_M(\overrightarrow{0})$  of radius

$$r_M = \left(\frac{3M}{4\pi}\right)^{1/3}.$$

*Proof.* Statement (ii) is proved in Theorem 2 of [40], using Theorem 2.1 in [27]. The case Z = 0 was proved in [28].

We sketch the proof of (i), since we need certain definitions and estimates for (ii). As in Julin [27], we define an asymmetry function corresponding to a fixed set  $\Omega$  of finite perimeter,

$$\gamma(\Omega) := \min_{y \in \mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\mathbb{1}_B(\overrightarrow{x}) - \mathbb{1}_{\Omega}(\overrightarrow{x} + \overrightarrow{y})}{\|\overrightarrow{x}\|} d\overrightarrow{x},$$

where  $B = \mathbb{B}_M(\overrightarrow{0})$  is the ball of mass M centered at the origin. The quantitative isoperimetric inequality (see (2.3) of [27] or [24]) then asserts the existence of a universal constant  $\mu_0 > 0$ , such that

$$\int_{\mathbb{R}^3} \|\nabla \mathbb{1}_{\Omega}\| - \int_{\mathbb{R}^3} \|\nabla \mathbb{1}_{B}\| \ge \mu_0 \gamma(\Omega),$$

with equality if and only if  $\Omega$  is a translate of B. Then, as in the proof of Theorem 1.1 of [27] in the three-dimensional case, we may estimate the difference in the nonlocal terms by the asymmetry,

$$D(\mathbb{1}_B, \mathbb{1}_B) - D(\mathbb{1}_\Omega, \mathbb{1}_\Omega) \le |B|\gamma(\Omega).$$

The optimality of the ball  $B = \mathbb{B}_M$  follows easily from this: assume  $\Omega$  is of finite perimeter, with  $|\Omega| = M$ . Then, provided  $\Omega$  is not a translate of the ball  $B = \mathbb{B}_M$ ,

$$\mathscr{E}_{0}^{Z}(\mathbb{1}_{\Omega}) - \mathscr{E}_{0}^{Z}(\mathbb{1}_{B}) > (\mu_{0} - M)\gamma(\Omega) + Z\left(\int_{\mathbb{R}^{3}} \frac{\mathbb{1}_{B}(\overrightarrow{x}) - \mathbb{1}_{\Omega}(\overrightarrow{x})}{\|\overrightarrow{x}\|} d\overrightarrow{x}\right) \ge (Z + \mu_{0} - M)\gamma(\Omega) > 0, \quad (5.3)$$

for all  $M < Z + \mu_0$ .

To obtain (i), the precompactness of all minimizing sequences, we use the above to establish strict subadditivity of  $e_0^Z(M)$ , as in Lions [36]. Let  $M = m^0 + m^1$  with  $m^0, m^1 > 0$ ; we show that (5.2) holds, and then by Lemma 16 all minimizing sequences for  $e_0^Z(M)$  are precompact.

Since  $0 < m^0 < M < Z + \mu_0$ , both  $e_0^Z(M)$ ,  $e_0^Z(m^0)$  are attained by balls  $B = \mathbb{B}_M(\vec{0})$ ,  $B^0 = B_{r_{m^0}}(\vec{0})$ . For any  $\delta > 0$  (to be chosen later ), we may choose a bounded open set  $\omega$  with  $\vec{0} \in \omega$ ,  $|\omega| = m^1$ , and

$$\mathscr{E}_0(\mathbb{1}_{\omega}) < e_0^0(m^1) + \delta.$$

Note that if  $m^0 \ge Z$ , then  $0 < m^1 < \mu_0$  and we may choose the set  $\omega = B^1 = B_{r_{m^1}}$  which attains  $e_0^0(m^1)$ . Define

$$\omega_{\overrightarrow{\xi}} := \omega + \overrightarrow{\xi}$$
, and  $\Omega = \Omega_{\overrightarrow{\xi}} = B^0 \cup \omega_{\overrightarrow{\xi}}$ ,

with  $\|\vec{\xi}\|$  sufficiently large that the union is disjoint. We first claim that  $\exists R > 1$  such that  $\gamma(\Omega_{\vec{\xi}}) \geq C > 0$  is bounded away from zero for all  $\vec{\xi}$  with  $\|\vec{\xi}\| > R$ , with constant  $C = C(m^0, m^1)$ . Indeed, for  $\vec{y} \in \mathbb{R}^3$  define

$$v = v^0 + v^1, \quad v^0(\overrightarrow{y}) = \int_{B^0} \frac{d\overrightarrow{x}}{\|\overrightarrow{x} - \overrightarrow{y}\|}, \quad v^1(\overrightarrow{y}) = \int_{\omega_{\overrightarrow{\xi}}} \frac{d\overrightarrow{x}}{\|\overrightarrow{x} - \overrightarrow{y}\|},$$

so that

$$\gamma(\Omega_{\overrightarrow{\xi}}) = \int_{B} \frac{d\overrightarrow{x}}{\|\overrightarrow{x}\|} - \max_{\mathbf{y} \in \mathbb{R}^{3}} v(\overrightarrow{y}).$$

Hence, to bound  $\gamma(\Omega_{\vec{\xi}})$  from below we must bound  $v(\vec{y})$  uniformly from above. As  $-\Delta v = 4\pi(\mathbbm{1}_{B^0}(\vec{y}) + \mathbbm{1}_{\omega_{\vec{\xi}}}(\vec{y}))$  in  $\mathbb{R}^3$ , it attains its maximum at  $y \in \Omega_{\vec{\xi}} = B^0 \cup \omega_{\vec{\xi}}$ . Thus, there are two possibilities: if the maximum occurs at  $y \in B^0$ , then  $v(\vec{y}) = v^0(\vec{y}) + O(\|\vec{\xi}\|^{-1})$ . Since  $v^0$  is maximized at y = 0, there exists  $C_0 = C_0(M, m^0)$  and R > 1 with

$$\gamma(\Omega_{\overrightarrow{\xi}}) \ge \int_{B \setminus B^0} \frac{d\overrightarrow{x}}{\|\overrightarrow{x}\|} - O(\|\overrightarrow{\xi}\|^{-1}) \ge C_0 > 0,$$

for all  $\|\overrightarrow{\xi}\| > R$ .

In case the maximum of v occurs at  $y \in \omega_{\vec{\xi}}$ , then  $v(\vec{y}) = v^1(\vec{y}) + O(\|\vec{\xi}\|^{-1})$ . For any domain D with  $|D| = m^1$  we have

$$\int_{D} \frac{d\overrightarrow{x}}{\|\overrightarrow{x}\|} \le \int_{B^{1}} \frac{d\overrightarrow{x}}{\|\overrightarrow{x}\|},$$

where  $B^1 = B_{r_{m,1}}(\vec{0})$  is the ball with mass  $m^1$ . It follows that

$$v^{1}(\overrightarrow{y}) = \int_{\omega_{\overrightarrow{\xi}}} \frac{d\overrightarrow{x}}{\|\overrightarrow{x} - \overrightarrow{y}\|} \le \int_{B^{1}} \frac{d\overrightarrow{x}}{\|\overrightarrow{x}\|}.$$

Therefore, as in the previous case, there exist  $C_1 = C_1(M, m^1)$  and R > 1 with  $\gamma(\Omega_{\vec{\xi}}) \ge C_1 > 0$ , for all  $\|\vec{\xi}\| > R$ , and the claim is established, with  $C = \min\{C_0, C_1\}$ .

To conclude, we choose a constant

$$0<\delta<\frac{1}{2}\left(Z+\mu_0-M\right)C\leq\frac{1}{2}\left(Z+\mu_0-M\right)\gamma(\Omega_{\overrightarrow{\xi}}),$$

for any  $\|\overrightarrow{\xi}\| > R$ , and using (5.3),

$$\begin{split} e^Z_0(M) &= \mathcal{E}^Z_0(\mathbbm{1}_B) < \mathcal{E}^Z_0(\mathbbm{1}_{\Omega_{\overrightarrow{\xi}}}) - (Z + \mu_0 - M) \, \gamma(\Omega_{\overrightarrow{\xi}}) \\ &\leq \mathcal{E}^Z_0(\mathbbm{1}_{B^0}) + \mathcal{E}^Z_0(\mathbbm{1}_{\omega_{\overrightarrow{\xi}}}) - (Z + \mu_0 - M) \, \gamma(\Omega_{\overrightarrow{\xi}}) + 2 \int_{B^0} \int_{\omega_{\overrightarrow{\xi}}} \frac{d \, \overrightarrow{x} \, d \, \overrightarrow{y}}{\| \, \overrightarrow{x} - \overrightarrow{y} \|} \\ &\leq \mathcal{E}^Z_0(\mathbbm{1}_{B^0}) + \mathcal{E}^0_0(\mathbbm{1}_\omega) - (Z + \mu_0 - M) \, \gamma(\Omega_{\overrightarrow{\xi}}) + O(\| \, \overrightarrow{\xi} \, \|^{-1}) \\ &\leq e^Z_0(m^0) + e^0_0(m^1) + \delta - (Z + \mu_0 - M) \, \gamma(\Omega_{\overrightarrow{\xi}}) + O(\| \, \overrightarrow{\xi} \, \|^{-1}). \end{split}$$

Taking  $\|\vec{\xi}\|$  sufficiently large, (5.2) holds for all  $M \in (0, Z + \mu_0)$ .

Remark 10. Thanks to Proposition 20, we may conclude that for the Liquid Drop Model with

$$V(\overrightarrow{x}) = \frac{Z}{\|\overrightarrow{x}\|}$$

with  $0 < M < Z + \mu_0$ , the <u>unique</u> generalized minimizer (see Definition 1) is the singleton  $\{u^0 = \mathbb{1}_{\mathbb{B}_M}\}$ . Indeed, this is true for any functional which satisfies the strict subadditivity condition (5.2).

Next, we prove Theorem 8. In fact, we prove the following slightly more general version, which is also a step towards the proof of Theorem 9.

**Lemma 17.** Let M > 0 and  $\delta_n, \varepsilon_n \xrightarrow[n \to \infty]{} 0^+$ . Assume  $u_n \in \mathcal{H}^M$  for which

$$\mathscr{E}^{V}_{\varepsilon_n}(u_n) \leq e^{V}_{\varepsilon_n}(M) + \delta_n, \quad n \in \mathbb{N}.$$

Then, there exists a subsequence and a generalized minimizer  $\{u^0, \dots, u^N\}$  of  $\mathcal{E}_0^V$  for which (1.19) and (1.20) hold for  $i = 0, \dots, N$ , and

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^N) = e_0^V(M) = \lim_{n \to \infty} e_{\varepsilon_n}^V(M).$$

*Proof.* By (i) of Theorem 7, there exists a subsequence along which  $u_n$  decomposes as in (1.19), with  $\{u^i\}_{i=0}^{\infty} \in \mathcal{H}_0^M$  satisfying (1.21). By (ii) of Theorem 7 we have

$$\mathscr{F}_0^V(\{u^i\}_{i=0}^{\infty}) = \lim_{n \to \infty} \mathscr{E}_{\varepsilon_n}^V(u_n) = \lim_{n \to \infty} e_{\varepsilon_n}^V(M) = e_0^V(M).$$

Let  $m^i = \|u^i\|_{\mathcal{L}^2(\mathbb{R}^3)}^2$ . It suffices to show that  $u^0$  minimizes  $e_0^V(m^0)$  and  $u^i$  minimizes  $e_0^0(m^i)$ , for each  $i \ge 1$ , and that all but a finite number of the  $u^i \equiv 0$ . First, by (1.18) we have

$$e_0^V(m^0) + \sum_{i=1}^\infty e_0^0(m^i) \leq \mathscr{E}_0^V(u^0) + \sum_{i=1}^\infty \mathscr{E}_0^0(u^i) = \mathscr{F}_0^V(\{u^i\}_{i=0}^\infty) = e_0^V(M) \leq e_0^V(m^0) + \sum_{i=1}^\infty e_0^0(m^i),$$

the last step by the Binding Inequality (subadditivity) of  $e_0$  see e.g. [2].) As each term is non-negative, equality holds in each relation. Furthermore, as  $e_0^V(m^0) \le \mathcal{E}_0^V(u^0)$  and each  $e_0^0(m^i) \le \mathcal{E}_0^0(u^i)$ , we must have equality in these as well. This proves that each  $u^i$ ,  $i \ge 0$ , is minimizing.

Finally, suppose infinitely many  $u^i \not\equiv 0$ . Then, by the convergence of the series,  $0 < m^i < \mu_0$  for all but finitely many i; assume  $0 < m^j, m^{j+1} < \mu_0$ . Then by the strict subadditivity, proved in the proof of Proposition 20,

$$e_0^0(m^j) + e_0^0(m^{j+1}) > e_0^0(m^j + m^{j+1}).$$

But then,

$$e_0^V(M) = e_0^V(m^0) + \sum_{i=1}^\infty e_0^0(m^i) > e_0^V(m^0) + \sum_{i \neq j, j+1} e_0^0(m^i) + e_0^0(m^j + m^{j+1}) \geq e_0^V(M),$$

a contradiction.

We finish with the proof of Theorem 9.

*Proof.* Recall that we assume  $V(\vec{x}) = Z/\|\vec{x}\|$ , Z > 0. For (a),  $0 < M \le Z$ , the (relative) compactness of all minimizing sequences for  $e_{\varepsilon}^{Z}(M)$  was proved by Lions [37, Corollary II.2.]. Let  $u_{\varepsilon} \in \mathcal{H}^{M}$  with  $\mathcal{E}_{\varepsilon}^{Z}(u_{\varepsilon}) = e_{\varepsilon}^{Z}(M)$ . By Lemma 17, there exists a generalized minimizer of  $e_{0}^{Z}(M)$ ,  $\{u^{i}\}_{i=0}^{N}$ , such that (1.19) and (1.20) hold for  $i = 0, \ldots, N$ , and

$$\mathscr{F}_0^Z(\{u^i\}_{i=0}^N) = e_0^Z(M) = \lim_{n \to \infty} e_{\varepsilon_n}^Z(M).$$

By Remark 10, N=0 and  $u_{\varepsilon} \xrightarrow[\varepsilon \to 0^+]{} u^0$  in  $\mathscr{L}^2(\mathbb{R}^3)$ , which attains the minimum in  $e_0^Z(M)$ .

For (b), first note that if there is a sequence  $\varepsilon_n \xrightarrow[n \to \infty]{} 0^+$  for which  $e^Z_{\varepsilon_n}(M)$  attains its minimum at  $u_n \in \mathscr{H}^M$ , then by the same argument as for (a) we obtain the conclusion of the Theorem with  $M_{\varepsilon_n} = M$ . It therefore suffices to consider sequences  $\varepsilon_n \xrightarrow[n \to \infty]{} 0^+$  for which the minimum in  $e^Z_{\varepsilon_n}(M)$  is not attained. By part (ii) of Lemma 16, for each n there exist s  $m_n^0 \in (0,M)$  such that

$$e_{\varepsilon_n}^Z(M) = e_{\varepsilon_n}^Z(m_n^0) + e_{\varepsilon_n}^0(M - m_n^0),$$

and there exists  $u_n \in \mathscr{H}^1(\mathbb{R}^3)$  with  $\|u_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = m_n^0$  and  $\mathscr{E}_{\varepsilon_n}^Z(u_n) = e_{\varepsilon_n}^Z(m_n^0)$ . For each n, we may choose functions  $v_n \in \mathscr{H}^1(\mathbb{R}^3)$  with compact support and  $\|v_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = M - m_n^0$  and for which

$$\mathscr{E}_{\varepsilon_n}^0(v_n) < e_{\varepsilon_n}^0(M - m_n^0) + \varepsilon_n.$$

Next, choose radii  $\rho_n$  in the smooth cut-off  $\omega_{\rho_n}$  defined in (4.3), such that  $\tilde{u}_n = u_n \omega_{\rho_n}$  satisfies both

$$\|\tilde{u}_n - u_n\|_{\mathcal{L}^2(\mathbb{R}^3)}^2 \xrightarrow[n \to \infty]{} 0 \text{ and } |\mathcal{E}_{\varepsilon_n}^Z(\tilde{u}_n) - \mathcal{E}_{\varepsilon_n}^Z(u_n)| \xrightarrow[n \to \infty]{} 0.$$

We also choose vectors  $\overrightarrow{\xi}_n \in \mathbb{R}^3$  such that  $\widetilde{u}_n$  and  $v_n(\cdot + \overrightarrow{\xi}_n)$  have disjoint supports for each n, and  $|\overrightarrow{\xi}_n| \xrightarrow[n \to \infty]{} \infty$ . Set

$$U_n(\overrightarrow{x}) := \widetilde{u}_n(\overrightarrow{x}) + v_n(\cdot + \overrightarrow{\xi}_n),$$

so that

$$\|U_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 = \|\tilde{u}_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 + \|v_n\|_{\mathscr{L}^2(\mathbb{R}^3)}^2 \xrightarrow[n \to \infty]{} M, \quad \text{and} \quad |\mathscr{E}_{\varepsilon_n}^Z(U_n) - e_{\varepsilon_n}^Z(M)| \xrightarrow[n \to \infty]{} 0.$$

By Lemma 15,  $\mathscr{E}^Z_{\varepsilon_n}(U_n) \xrightarrow[n \to \infty]{} e^Z_0(M)$ , so applying (i) of Theorem 7 there exists  $\{u^i\}_{i=0}^{\infty} \in \mathscr{H}^M_0$  for which (1.19) and (1.20) hold, and

$$\mathscr{F}_0^Z(\{u^i\}_{i=0}^{\infty}) = e_0^Z(M).$$

By Remark 10,  $u^i \equiv 0$  for all  $i \geq 1$  and  $u^0 = \mathbb{1}_{\mathbb{B}_M}$  minimizes  $e_0^V(M)$ . From (1.19) we conclude that

$$U_n = \tilde{u}_n + v_n(\cdot + \overrightarrow{\xi}_n) \xrightarrow[n \to \infty]{} u^0 \text{ in } \mathscr{L}^2(\mathbb{R}^3).$$

Since for every fixed compact set  $K \subset \mathbb{R}^3$  we have  $U_n = u_n$  pointwise almost everywhere in K and for all sufficiently large n, it follows that  $u_n \xrightarrow[n \to \infty]{} u^0$  in  $\mathcal{L}^2_{loc}(\mathbb{R}^3)$  and pointwise almost everywhere up to a subsequence. Consequently, we have  $v_n \xrightarrow[n \to \infty]{} 0$  and  $u_n \xrightarrow[n \to \infty]{} u^0$  globally in  $\mathcal{L}^2(\mathbb{R}^3)$ . In conclusion, taking

$$M_{\varepsilon_n} := m_n^0,$$

$$e^Z_{\varepsilon_n}(M_{\varepsilon_n}=m_n^0)$$
 is attained at  $u_{\varepsilon_n}=u_n, M_{\varepsilon_n} \xrightarrow[n \to \infty]{} M$ , and  $u_n \xrightarrow[n \to \infty]{} u^0=\mathbb{1}_{\mathbb{B}_M}$  in  $\mathscr{L}^2(\mathbb{R}^3)$ .

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