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Mathematical issues in the modeling of supersolids

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MATHEMATICAL ISSUES IN THE MODELING OF SUPERSOLIDS

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ABSTRACT. We study a model of supersolids or quantum crystals introduced in [13, 14], following recent experiments in Helium 4. This model is based on a Gross-Pitaevskii energy with a nonlocal interaction term. We give a description of the ground state in the limit of strong interaction, and relate it to a sphere packing problem. We also study the effect of rotation. In dimension one, we prove that the ground state has a periodic structure.

1. INTRODUCTION

Since the experimental achievement of Kim and Chan [15, 16, 17], who produced a solid state with superfluid properties, renewed interest for supersolidity has emerged in the physics community, both from an experimental [18, 22, 24] and theoretical point of view [13, 14, 23]. This topic is still debated in the physics community [3, 24]. The theoretical prediction of supersolidity, that is superfluid behaviour for a quantum crystal dates back to Leggett [19, 20] and Andreev Lifschitz [2]. A possible way of detecting the superfluid state can be done by rotation: the experiment by Kim and Chan [16, 17] allowed them to measure the moment of inertia of solid helium and find that it is lower than its classical value. This property is referred to as Non Classical Rotational Inertia (NCRI). This experiment has raised a lot of interest and was interpreted as a landmark of supersolidity, on the basis of papers by Leggett [19, 20]. One theoretical challenge is to estimate this NCRI.

In this paper, we consider a nonlocal Gross Pitaevskii (GP) energy which has been proposed by Josserand, Pomeau and Rica in [13, 14] to model supersolidity. Indeed, a quantum crystal can be described by a wave function and the GP energy with a nonlocal interaction potential leads to a ground state with a crystalline structure. Josserand, Pomeau and Rica derive properties under rotation, giving numerical evidence of nonclassical effects. They check that this model also provides mechanical behaviours typical of solids under small stress.

The aim of the present article is to set the GP approach of [13, 14] on a sound mathematical ground. In particular, the question of the crystalline symmetry of the ground state will be addressed. Then considerations of the effect of small rotation will be discussed. Some issues concerning the nonclassical rotational inertia fraction have been addressed in [1]. The present paper is meant to bring rigorous mathematical proofs to this supersolid framework.q

1.1. **The nonlocal Gross-Pitaevskii energy.** We will call $\mathcal{D} \subset \mathbb{R}^d$ the set occupied by the supersolid, with $d = 3$ being the most physically relevant choice. The wave function u is complex-valued, and $|u|^2$ provides the density of atoms. In [13, 14], in order to model a supersolid, the following Gross-Pitaevskii energy is introduced for u:

$$E_\varepsilon(u) = \int_{\mathcal{D}} \frac{1}{2}|\nabla u|^2 \, dx + \frac{1}{4\varepsilon^2} F(|u|^2), \tag{1.1}$$

where the function F is defined on the space of measures on $\bar{\mathcal{D}}$, by

$$F(\rho) = \int_{\bar{\mathcal{D}}} (V * \rho)(x) \; \rho(dx) \quad = \int_{\bar{\mathcal{D}}} \int_{\bar{\mathcal{D}}} V(x-y)\rho(dy) \; \rho(dx). \tag{1.2}$$

The nondimensional parameter ε accounts for the strength of the interaction and the interacting potential V is chosen to be

$$V(x) = \begin{cases} 1 & \text{if } |x| < 1 \\ 0 & \text{if not.} \end{cases} \tag{1.3}$$

This specific choice of V corresponds to putting a soft sphere interaction for each atom and provides a dispersion relation with a roton minimum [13]. It is not too realistic from an atomic point of view but as pointed out in [13], it provides a dispersion relation with a roton minimum which is a key feature. This potential allows for reasonnablle numerical simulations and provide the main behaviours of supersolids.

If instead, V is taken to be the delta function, the energy E_ε is simply the usual Gross Pitaevskii energy with an L^4 term describing interactions. This model bears an important difference with classical solids, in the sense that in classical solids, there is an integer number of atoms per unit cell, while in this quantum solid model, the average density is a free number, independent of the crystal parameters, which provides an L^2 constraint on the wave function.

We assume that $\mathcal{D}$ is a bounded, open subset of $\mathbb{R}^d$ with Lipschitz boundary. The space $H^1_0(\mathcal{D};\mathbb{C})$ is, as usual, the space of H^1 functions satisfying homogeneous Dirichlet boundary conditions. The functional is minimized in the space

$$\mathcal{A}_0(\mathcal{D}) := \left\{ u \in H^1_0(\mathcal{D};\mathbb{C}) \;:\; \fint_{\mathcal{D}} |u|^2 \, dx = 1 \right\},$$

where $\fint_{\mathcal{D}} \cdots dx$ denotes the average $\frac{1}{|\mathcal{D}|}\int_{\mathcal{D}} \cdots dx$.

Physicists have identified two regimes for the ground state: for large ε, the minimizer is constant, corresponding to a uniform density. On the other hand, for small ε, it is localized on periodic sets which are almost on a triangular lattice for large domains [13, 14], corresponding to a crystalline state. This is what we want to characterize mathematically, and this is why we also introduce periodic boundary conditions.

In the periodic setting, the domain $\mathcal{D}$ is a parallelogram, so that there exist n linearly independent vectors $v_1, \dots, v_n$ such that

$$\mathcal{D} = \left\{ \sum x_i v_i \ : \ 0 \le x_i < 1 \text{ for all } i \right\},$$

and V is understood to be the $\mathcal{D}$-periodic extension of the potential V defined in (1.3). Or equivalently, V is exactly as in (1.3), and $|x-y|$ is taken to be the distance in the periodic sense, so that

(1.4)
$$|x-y| = \inf \left\{ \left| x - y + \sum n_i v_i \right| \ : \ n_i \in \mathbb{Z} \text{ for all } i \ \right\} \qquad \text{in the periodic setting.}$$

The space $H^1_{per}(\mathcal{D};\mathbb{C})$ denotes $\mathcal{D}$-periodic functions in $H^1_{loc}(\mathbb{R}^d;\mathbb{C})$ and the energy is then minimized in

$$\mathcal{A}_{per}(\mathcal{D}) := \left\{ u \in H^1_{per}(\mathcal{D};\mathbb{C}) \ : \ \fint_{\mathcal{D}} |u|^2 \, dx = 1 \right\}.$$

Under rotation along the vertical axis, the energy in the rotating frame becomes

$$E_{\varepsilon,\Omega}(u) = E_\varepsilon(u) - \Omega \int_{\mathcal{D}} A \cdot \mathrm{Im}(\bar{u} \nabla u) \, dx, \tag{1.5}$$

where Ω is the rotational velocity, and $A(x,y) = (-y,x)$ when $d=2$ and $A(x,y,z) = (-y,x,0)$ when $d=3$.

When Ω is small, $\inf E_{\varepsilon,\Omega}$ can be expanded as $\inf E_\varepsilon - (1/2) I \Omega^2$, where I is the effective moment of inertia of the solid. Leggett [19] suggested as a criterion for supersolidity the existence of a nonclassical rotational inertia fraction defined as $(I_0 - I)/I_0$, where I_0 is the classical moment of inertia of the crystal phase. Thus, we need to understand and estimate the ground state for $\Omega = 0$ and for small Ω.

Our aim is to characterize the minimizers of $E_{\varepsilon,\Omega}$. When ε is small, minimizers of $E_{\varepsilon,\Omega}$ are expected to be almost minimizers of

$$G_\Omega(u) = \int_{\mathcal{D}} \frac{1}{2} |\nabla u|^2 dx - \ \Omega \int_{\mathcal{D}} A \cdot \mathrm{Im}(\bar{u} \nabla u) \, dx$$

in the set of minimizers of F since the energy (1.5) reads

$$E_{\varepsilon,\Omega}(u) = G_\Omega(u) + \frac{1}{4\varepsilon^2} F\left(|u|^2\right)$$

and thus the two terms are of different order.

1.2. **Ground state of F and sphere packing problem.** If S is any measurable subset of any Euclidean space, we will use the notation

$$\begin{aligned}\mathcal{M}(S) &:= \{\text{nonnegative measures } \rho \text{ on } S : \rho(S) = |S|\},\\ \mathcal{M}_{ac}(S) &:= \{\rho \in \mathcal{M}(S) \ : \ \rho \ll \mathcal{L}^d\},\end{aligned}$$

where $\mathcal{L}^d$ is the Lebesgue measure of $\mathbb{R}^d$ and $|S| := \mathcal{L}^d(S)$.

Our first result is a complete description of the minimizers of F in $\mathcal{M}_{ac}$, which is related to a sphere packing problem:

Theorem 1.1. *Suppose that $\mathcal{D}$ is a bounded, open subset of $\mathbb{R}^d$ with Lipschitz boundary, and that* diam $\mathcal{D} > 1$. *Define*

$$n(\mathcal{D}) := \max\{k : \exists x_1, \dots, x_k \in \mathcal{D} \text{ such that } |x_i - x_j| > 1 \ \ \forall i \neq j\}. \tag{1.6}$$

Then

$$\min_{\mathcal{M}_{ac}(\mathcal{D})} F = |\mathcal{D}|^2/n(\mathcal{D}),$$

and a measure ρ in $\mathcal{M}_{ac}(\mathcal{D})$ minimizes F if and only if there exist $n(\mathcal{D})$ pairwise disjoint closed sets $A_1, \dots, A_{n(\mathcal{D})} \subset \bar{\mathcal{D}}$, such that

$$\operatorname{dist}(A_i, A_j) \geq 1 \text{ if } i \neq j, \tag{1.7}$$

and

$$\int_{A_i} \rho \, dx \ = \ \frac{|\mathcal{D}|}{n(\mathcal{D})} \tag{1.8}$$

for all i.

An important point due to the choice of the interaction potential is that the self interaction of an A_i is a constant on each set, which eventually gets added to the energy.

When the number $n(\mathcal{D})$ is large, the optimal location of the points x_i in (1.6) is proved [7] to be close to a hexagonal lattice in 2D. In 3D, 2 configurations are optimal: hexagonal close packing and face centered cubic close packing.

Remark 1. A description of minimizers of F in $\mathcal{M}$, rather than $\mathcal{M}_{ac}$ is somewhat easier and will be obtained as a byproduct of the proof.

Remark 2. In fact the boundary of $\mathcal{D}$ can be quite irregular. The proof we give works as long as $\mathcal{L}^d(\partial\mathcal{D}) = 0$.

We will denote by $\mathcal{M}^*_{ac}(\mathcal{D})$ the set of minimizers of F in $\mathcal{M}_{ac}$:

$$\mathcal{M}^*_{ac}(\mathcal{D}) := \{\rho \in \mathcal{M}_{ac}(\mathcal{D}) \ : \exists A_1, \dots, A_n \subset \mathcal{D} \text{ satisfying } (1.7), (1.8)\}\,. \tag{1.9}$$

It is clear that $\mathcal{M}^*_{ac}(\mathcal{D})$ is nonempty.

1.3. **Ground state with rotation.** We will prove that the ground states of $E_{\varepsilon,\Omega}$ are almost given by the minimizers of G_Ω restricted to the space of minimizers of F. For that purpose, we define

$$E_{0,\Omega}(u) := \begin{cases} G_\Omega(u) & \text{if } |u|^2 \in \mathcal{M}^*_{ac}(\mathcal{D}), \\ +\infty & \text{if not.} \end{cases} \tag{1.10}$$

This functional arises as a sort of $\varepsilon \to 0$ limit of $E_{\varepsilon,\Omega}$. The next result makes this limit precise. We define

$$\mathcal{A}^*_0(\mathcal{D}) := \left\{ u \in H^1_0(\mathcal{D};\mathbb{C}) \ : |u|^2 \in \mathcal{M}^*_{ac} \right\},$$
$$\mathcal{A}^*_{per}(\mathcal{D}) := \left\{ u \in H^1_{per}(\mathcal{D};\mathbb{C}) \ : \ |u|^2 \in \mathcal{M}^*_{ac} \right\}.$$

Theorem 1.2. *If u_ε minimizes $E_{\varepsilon,\Omega}(\cdot) = G_\Omega(\cdot) + \frac{1}{4\varepsilon^2}F(|\cdot|^2)$ in $\mathcal{A}_0(\mathcal{D})$, then $\{u_\varepsilon\}_{\varepsilon\in(0,1]}$ is strongly precompact in $H^1(\mathcal{D})$, and the limit of any convergent subsequence minimizes G_Ω in $\mathcal{A}^*_0(\mathcal{D})$. Similarly, if u_ε minimizes $E_{\varepsilon,\Omega}$ in $\mathcal{A}_{per}(\mathcal{D})$, then $\{u_\varepsilon\}_{\varepsilon\in(0,1]}$ is strongly precompact in $H^1(\mathcal{D})$, and the limit of any convergent subsequence minimizes G_Ω in $\mathcal{A}^*_{per}(\mathcal{D})$.*

In particular Theorem 1.2 implies that the problem

$$\text{find } u_0 \in \mathcal{A}^*_0(\mathcal{D}) \text{ such that } G_\Omega(u_0) = \min_{\mathcal{A}^*_0(\mathcal{D})} G_\Omega \tag{1.11}$$

has a solution. This is actually the first step of the proof of Theorem 1.2. The rest of the proof is based on energy estimates, which imply that minimizers of $E_{\varepsilon,\Omega}$ are bounded in H^1, hence converge weakly in H^1. This allows to pass to the limit in the energy and the constraint. Since the convergence of the energy implies that $\int |\nabla u_\varepsilon|^2$ converges, we have strong convergence in H^1.

1.4. **The one-dimensional case.** In the special case of dimension one, it is possible to compute explicitly the minimizers of F and the limit points of minimizers of E_ε. Note that in such a case no angular momentum terms are present, so we will consider the functional

$$E_\varepsilon(u) = \int_{\mathcal{D}} \frac{1}{2}|u'|^2 + \frac{1}{4\varepsilon^2}(V * |u|^2)|u|^2 \, dx. \tag{1.12}$$

and its $\varepsilon \to 0$ limit

$$E_0(u) := \begin{cases} \int_{\mathcal{D}} \frac{1}{2}|u'|^2 & \text{if } |u|^2 \in \mathcal{M}^*_{ac}(\mathcal{D}), \\ +\infty & \text{if not.} \end{cases} \tag{1.13}$$

in the spaces $\mathcal{A}_{per}(\mathcal{D})$ and $\mathcal{A}_0(\mathcal{D})$, where $\mathcal{D} \subset \mathbb{R}$ is an open interval. We will write $G_0(u)$ for the Dirichlet energy $\int \frac{1}{2}|u'|^2 \, dx$.

We assume that $\mathcal{D} = (0, L)$ for some $L > 0$, and consider the problem

$$\text{find } u_0 \in \mathcal{A}^*_0(\mathcal{D}) \text{ such that } E_0(u_0) = \min_{\mathcal{A}^*_0(\mathcal{D})} E_0, \tag{1.14}$$

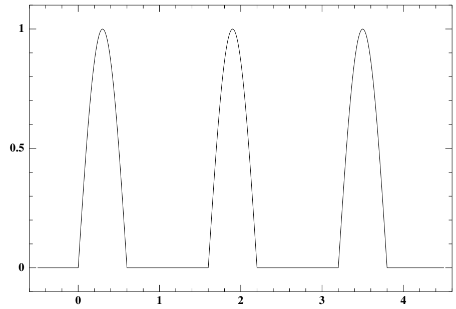

FIGURE 1. The minimizer u_p introduced in Proposition 1.1 The bumps are of size h_p and separated by a distance 1.

together with the corresponding periodic problem. We write $\lceil L \rceil$ to denote the smallest integer that is greater than or equal to L.

Proposition 1.1. *There is a unique nonnegative minimizer for problem* (1.14) *with Dirichlet boundary conditions, and it is given explicitly by*

$$u_0(x) = \begin{cases} \sqrt{\frac{2L}{h_0 \bar{n}_0}} \sin(\frac{\pi}{h_0}(x - x_i)) & \text{if } x \in (x_i, x_i + h_0) \\ & \quad \text{for some } i \in \{0, \dots \bar{n}_0 - 1\} \\ 0 & \text{if not} \end{cases}$$

where $\bar{n}_0, h_0$ and x_i are defined by

$$\bar{n}_0 = \lceil L \rceil, \qquad h_0 = (L - (\bar{n}_0 - 1))/\bar{n}_0, \qquad x_i = i(1 + h_0).$$

Moreover, $E_0(u_0) = \pi^2 L / 2h_0^2$.

Similarly, if we consider periodic boundary conditions, then there is a positive minimizer that is unique modulo translations, and is given by

$$u_p(x) = \begin{cases} \sqrt{\frac{2L}{h_p \bar{n}_p}} \sin(\frac{\pi}{h_p}(x - x_i)) & \text{if } x \in (x_i, x_i + h_p) \\ & \quad \text{for some } i \in \{0, \dots \bar{n}_p - 1\} \\ 0 & \text{if not} \end{cases}$$

where $\bar{n}_p, h_p$ and x_i are defined by

$$\bar{n}_p = \lceil L \rceil - 1, \qquad h_p = (L - \bar{n}_p)/\bar{n}_p, \qquad x_i = i(1 + h_p).$$

And $E_0(u_0) = \pi^2 L / 2h_p^2$.

Note that for both the Dirichlet and the periodic problem, h_0, h_p are bounded by C/L, so that the support of a minimizer is sharply concentrated for L large. Note also that h_0, h_p tend to zero as L approaches an integer from above.

Dimension one also allows for explicit computations of the next order in the asymptotic expansion of E_ε. Indeed, we have the following

Theorem 1.3. *Assume that $L > 2$, and let $\mathcal{D} = [0, L] \subset \mathbb{R}$ with periodic boundary conditions. Suppose that u_ε minimizes $E_\varepsilon(\cdot)$ in $H^1_{per}(\mathcal{D})$. Then there exist $C > c > 0$ such that*

$$E_\varepsilon(u_p) - C\varepsilon^{2/5} \leq E_\varepsilon(u_\varepsilon) \leq E_\varepsilon(u_p) - c\varepsilon^{2/5}.$$

The result in Theorem 1.3 is stated only in terms of energy, giving the next order expansion in powers of ε. However, the proof indicates that the support of the minimizer u_ε is concentrated at distance of order $\varepsilon^{2/5}$ from the support of its limit u_p, up to an error of size $\exp(-C/\varepsilon)$. We consider only the periodic case for simplicity, but similar results hold for the Dirichlet data.

Although we do not have results in dimension $d \geq 2$, we believe that a similar expansion for the energy and boundary layer should be true. However, this would require a better understanding of the minimizers of F (that is $\mathcal{M}^*_{ac}(\mathcal{D})$).

1.5. **Large ε.** Finally, we prove that in the case of weak interaction, that is, when $\varepsilon \to \infty$ (and $\Omega = 0$), the minimizer is homogeneous (that is, $|u| = 1$). Note that this result holds only for the periodic boundary conditions, but is valid in any dimension:

Proposition 1.2. *Let $\mathcal{D} = [-L/2, L/2]^d$ with periodic boundary conditions. If*

$$\varepsilon > \sqrt{\omega_d}, \tag{1.15}$$

where ω_d is the volume of the unit ball of $\mathbb{R}^d$, then

$$E_{\varepsilon,0}(1) \leq E_{\varepsilon,0}(u)$$

for all $u \in H^1_{per}(\mathcal{D})$ such that $\int |u|^2 = |\mathcal{D}|$. (Here 1 denotes the constant function.) Moreover, if equality holds then $u = 1$.

The proof of this result is based on the decomposition of u in Fourier series, and on estimates of the energy in this basis.

1.6. **Open problems.** The main difficulties, due to the nonlocal term in the equation, are the uniqueness and periodicity of minimizers.

In the one-dimensional setting, we have an explicit expression of the limit of u_ε as $\varepsilon \to 0$, and it is periodic, even with Dirichlet boundary conditions. We also expect that, for any ε (or at least for ε small enough), the minimizer of E_ε with periodic boundary conditions is periodic. The difficulty one faces in proving such a result is to have a uniqueness result for a nonlocal equation: indeed, the Euler-Lagrange equation reads

$$-u'' + \frac{1}{\varepsilon^2}\left(V * u^2\right) u = \lambda_\varepsilon u$$

and we are not able to prove any kind of uniqueness or maximum principle. This is also open in dimension 2 and 3. In the two-dimensional setting, it is already a very difficult issue, related to the sphere packing problem [7, 10, 11] and optimal partition and eigenvalue problems [5, 6, 12], to prove the uniqueness (modulo symmetries) or periodicity of minimizers of the $\varepsilon = 0$ problem (1.11), even when $\Omega = 0$. Apart from this problem, minimizing G_Ω among all minimizers of F should give information on the connected components A_i. For instance, their boundary is probably Lipschitz, and any boundary point of A_i should be at distance 1 from another A_j. An interesting point of view in proving this would be to consider the boundary of each A_j as a free boundary, and derive an Euler-Lagrange equation satisfied by ∂A_j.

Another question in the one-dimensional setting is to study the limit $L \to \infty$. This limit is justified by the fact that physically, the interaction length, which is set to 1 here, is much smaller than the size of the sample. Thus, it would be interesting to study the corresponding asymptotics. This is implicitly what is done in [14]. As pointed out above, in this limit, the minimizers of F become sums of Dirac masses, and the above results do not apply to this case. The corresponding proofs would require a more detailed study of the asymptotic expansion of the energy and of the boundary layer near each peak of the density.

In the two-dimensional case, a difficult issue is the presence of vortices. According to numerics [14], it seems that there are no visible vortices. However, the density is exponentially small between the A_j. We give the proof of this fact in dimension 1 (see Lemma 4.1 below), but it may be adapted to dimension 2. Hence, investigating the presence of vortices in this region will probably be very difficult, since one can add or remove a vortex with a change in the energy of order $e^{-C/\varepsilon}$. However, proving that there is no vortex in each A_j is probably more tractable, and would use estimates on ground states of Schrödinger operators with magnetic potential, in the spirit of [8, 9] for instance.

1.7. **Back to nonclassical rotational effects.** We fix $\varepsilon > 0$, $d = 2$, and study the limit $\Omega \to 0$. The nonclassical rotational inertia fraction (NCRIF) is defined by

$$NCRIF = \frac{I_0 - I}{I_0},$$

where I is the moment of inertia of the system, that is the second derivative of the energy with respect to Ω, and I_0 is the classical moment of inertia, that is, $I_0 = \int_{\mathcal{D}} |x|^2|u_0|^2$, where u_0 is the minimizer of $E_{\varepsilon,0}$. This minimizer satisfies an elliptic equation, which allows to apply the Harnack inequality: u_0 is positive in $\mathcal{D}$. A perturbation argument then allows to prove that for Ω small enough, the same property holds for $u_{\varepsilon,\Omega}$, the minimizer of $E_{\varepsilon,\Omega}$, hence one can write

$$u_{\varepsilon,\Omega} = \rho_{\varepsilon,\Omega} e^{i\Omega S_{\varepsilon,\Omega}}.$$

If we assume uniqueness of the minimizer of $E_{\varepsilon,0}$, which is likely to be a difficult issue, as we have mentionned above, then we can derive an explicit expression for $NCRIF$, since we can expand $\rho_{\varepsilon,\Omega}$ and $S_{\varepsilon,\Omega}$ in powers of Ω^2, justify the expansion and find

$$NCRIF = \frac{\int_{\mathcal{D}} u_0^2|\nabla S_0 - x^\perp|^2}{\int_{\mathcal{D}} |x|^2 u_0^2} = \frac{\inf_{S\in H^1(\mathcal{D})} \int_{\mathcal{D}} u_0^2|\nabla S - x^\perp|^2}{\int_{\mathcal{D}} |x|^2 u_0^2}.$$

In [1], we have derived the lower bound

$$NCRIF \geq \frac{1}{\varepsilon^2}\frac{\pi^2}{16} e^{-2\sqrt{2}T/\varepsilon}.$$

This relies on the extra strong assumption that u_0 is periodic with a periodic cell of diameter T, in order to apply the Harnack inequality and get

$$\inf u_0 \geq \frac{1}{\varepsilon^2}\frac{\pi}{4} e^{-\sqrt{2}T/\varepsilon} \sup u_0.$$

The issues of the uniqueness and periodicity are, to our opinion, a key point in this analysis.

We give in Section 2 the proof of Theorem 1.1, together with a generalization to other interaction potentials. In Section 3, we prove the convergence of minimizers in the limit $\varepsilon \to 0$ (Theorem 1.2). The one-dimensional case is studied in details in Section 4, with the proof of Proposition 1.1 and Theorem 1.3. Finally, Section 5 is devoted to the proof of Proposition 1.2.

2. Minimizers of the interaction

We give in this section the proof of Theorem 1.1. It covers both the periodic case and the non-periodic case. The proofs are identical in the two cases, the only difference being that in the periodic case, $|x - y|$ is understood as in (1.4)

2.1. **Preliminaries.** In this subsection and part of the next, it is convenient to work on a closed set; this is used in the proof of Lemma 2.2 below. We will write such a set as $\bar{\mathcal{D}}$, although in fact our arguments are valid for rather general closed sets, not only for those that arise as the closure of open sets $\mathcal{D}$ as in the statement of Theorem 1.1.

First we prove

Lemma 2.1. *The functional F as defined in* (1.2), (1.3) *is lower semicontinuous with respect to weak convergence of measures in $\mathcal{M}(\bar{\mathcal{D}})$, i.e.*

$$\text{if } \rho_k \in \mathcal{M}(\mathcal{D}), \rho_k \rightharpoonup \rho, \text{ then } F(\rho) \le \liminf_k F(\rho_k)$$

Proof. The point is that

$$F(\rho) = (\rho \times \rho)(\{(x,y) : |x-y| < 1\})$$

where $\rho \times \rho$ denotes the product measure on $\bar{\mathcal{D}} \times \bar{\mathcal{D}}$. It is well-known (see [4] Chapter 1, for example) that $\rho_k \rightharpoonup \rho$ if and only if $\rho_k \times \rho_k \rightharpoonup \rho \times \rho$, and also that if $\rho_k \times \rho_k \rightharpoonup \rho \times \rho$ then $\rho \times \rho(O) \le \liminf_k \rho_k \times \rho_k(O)$ for every O that is relatively open in $\bar{\mathcal{D}} \times \bar{\mathcal{D}}$. Since $\{(x,y) : |x-y| < 1\}$ is open, the lemma follows. □

Lemma 2.2. *F has a minimizer in $\mathcal{M}(\bar{\mathcal{D}})$.*

Proof. Let $\{\rho_k\} \subset \mathcal{M}(\bar{\mathcal{D}})$ be a minimizing sequence such that $F(\rho_k) \to \inf_{\mathcal{M}(\bar{\mathcal{D}})} F(\cdot)$. Standard facts about weak convergence of measures imply that there exists a subsequence (still denoted by ρ_k) and a measure $\rho \in \mathcal{M}(\bar{\mathcal{D}})$ such that $\rho_k \rightharpoonup \rho$. Then the previous lemma implies that $F(\rho) \le \inf_{\mathcal{M}} F(\cdot)$. □

Note that the above standard argument does not yield the existence of minimizers in $\mathcal{M}_{ac}(\mathcal{D})$, since this space is not closed with respect to weak convergence of measures.

Next we find optimality conditions:

Lemma 2.3. *If ρ minimizes F in $\mathcal{M}(\bar{\mathcal{D}})$, then*

$$|\mathcal{D}|^{-1} F(\rho) = \min_{x \in \bar{\mathcal{D}}} \; V * \rho(x) \tag{2.1}$$

and

$$V * \rho = |\mathcal{D}|^{-1} F(\rho) \qquad \rho - a. \ e. \tag{2.2}$$

(ie, the set $S := \{x \in \bar{\mathcal{D}} \ : \ F * \rho(x) > |\mathcal{D}|^{-1} F(\rho)\}$ satisfies $\rho(S) = 0$).

The same optimality conditions (2.1), (2.2) *are satisfied by a measure ρ that minimizes F in $\mathcal{M}_{ac}(\mathcal{D})$.*

Proof. Let ρ_0 minimize F in $\mathcal{M}(\bar{\mathcal{D}})$. Note that $\mathcal{M}(\bar{\mathcal{D}})$ is a convex set, so that if $\rho_1 \in \mathcal{M}(\bar{\mathcal{D}})$, then $\rho_\alpha = \alpha\rho_1 + (1-\alpha)\rho_0 \in \mathcal{M}(\bar{\mathcal{D}})$ for every $\alpha \in [0,1]$. Thus

$$0 \le \lim_{\alpha\to 0} \frac{1}{\alpha}(F(\rho_\alpha) - F(\rho_0)) = \int_{\bar{\mathcal{D}}} V * \rho_0(\rho_1 - \rho_0),$$

In other words,

$$\int_{\bar{\mathcal{D}}} \left(V * \rho_0 - \frac{F(\rho_0)}{|\mathcal{D}|} \right) \rho_1 \ge 0 \tag{2.3}$$

for every $\rho_1 \in \mathcal{M}(\bar{\mathcal{D}})$. In particular, taking $\rho_1 = |\mathcal{D}|\delta_x$ for arbitrary $x \in \mathcal{D}$, we deduce that $V*\rho_0(x) \ge |\mathcal{D}|^{-1}F(\rho_0)$, and therefore that $\inf V*\rho_0 \ge |\mathcal{D}|^{-1}F(\rho_0)$.

Also, note that

$$\int_{\bar{\mathcal{D}}} \left(V * \rho_0 - \frac{F(\rho_0)}{|\mathcal{D}|} \right) \rho_0 = F(\rho_0) - \frac{F(\rho_0)}{|\mathcal{D}|} \int_{\bar{\mathcal{D}}} \rho_0 = F(\rho_0) - F(\rho_0) = 0.$$

However, we have shown above that $V * \rho_0 - |\mathcal{D}|^{-1}F(\rho_0) \ge 0$, so we deduce that $V * \rho_0(x) - |\mathcal{D}|^{-1}F(\rho_0) = 0$ at ρ_0 -a.e. $x \in \mathcal{D}$.

Finally, if ρ_0 minimizes F in $\mathcal{M}_{ac}$, then since $\mathcal{M}_{ac}$ is convex, we find as before that ρ_0 satisfies (2.3) for every $\rho_1 \in \mathcal{M}_{ac}$. It is clear that $V * \rho_0$ is continuous, so it follows that $V * \rho_0 \ge \frac{F(\rho_0)}{|\mathcal{D}|}$ everywhere. Then the remainder of the proof is exactly as in the previous case. $\square$

2.2. **Characterization of minimizers.** In this section we present the proof of Theorem 1.1. We first provide a simpler proof with some (not so) restrictive hypothesis in Section 2.2.1, then a full proof in Section 2.2.2

A trivial but useful fact is that

$$\int_{\bar{\mathcal{D}}} V * \rho(x)\, dx = \int_{\bar{\mathcal{D}}} V(x-y)\, dx\, \rho(dy) = \left(\int_{\bar{\mathcal{D}}} V\ dx \right) \int_{\bar{\mathcal{D}}} \rho(dy) = |\mathcal{D}| \int_{\bar{\mathcal{D}}} V\, dx. \tag{2.4}$$

Let us recall that $n(\mathcal{D})$ is defined by (1.6). We also define

$$\bar{n}(\bar{\mathcal{D}}) = \max\{k : \exists x_1, \dots, x_k \in \bar{\mathcal{D}} \text{ such that } |x_i - x_j| \ge 1 \ \ \forall i \ne j\}. \tag{2.5}$$

>From these definitions, it is clear that $n(\mathcal{D}) \le \bar{n}(\bar{\mathcal{D}})$. In many cases, we have in fact equality: for example, in dimension one, $\mathcal{D} = (0, L)$, and equality holds iff L is *not* an integer. In such a case, $n(\mathcal{D}) = \bar{n}(\bar{\mathcal{D}}) = [L]+1$, where $[L]$ is the integer part of L. On the contrary, if n is an integer, then $n(\mathcal{D}) = L$ and $\bar{n}(\bar{\mathcal{D}}) = L + 1$.

2.2.1. *The case $n = \bar{n}$.*

Proof of Theorem 1.1. This proof is valid only in the case $n(\mathcal{D}) = \bar{n}(\bar{\mathcal{D}})$. Throughout the proof we will write $B(x)$ to denote the open ball $B(x, 1)$ of radius 1 centered at x.

Given a measure $\rho \in \mathcal{M}_{ac}(\mathcal{D})$, we will extend it to a measure on $\bar{\mathcal{D}}$, still denoted by ρ, by specifying that $\rho(A) = \rho(A \cap \mathcal{D})$ for $A \subset \bar{\mathcal{D}}$. Thus we can identify $\mathcal{M}_{ac}(\mathcal{D})$ with a subset of $\mathcal{M}(\bar{\mathcal{D}})$.

Step 1: upper bound. Let $\rho \in \mathcal{M}^*_{ac}(\mathcal{D})$ be defined in (1.9), so that we can associate to ρ a family of sets $A_1, \ldots, A_n$ satisfying (1.7) and (1.8). Then (1.7) immediately implies that

$$\forall x \in A_i, \qquad B(x) \cap \left(\cup_{j=1}^n A_j\right) \subset A_i. \tag{2.6}$$

Next, note that (1.7), (1.8) imply that $\rho(\mathcal{D} \setminus \cup A_j) = 0$. According to (2.6), we infer that for any $x \in A_i$,

$$V * \rho(x) = \rho(B(x)) \le \rho(A_i) = \frac{|\mathcal{D}|}{n}.$$

Computing the energy, we thus find that $F(\rho) \le |\mathcal{D}|^2/n$, hence

$$\inf_{\mathcal{M}_{ac}(\mathcal{D})} F \le \sup_{\mathcal{M}^*_{ac}(\mathcal{D})} F \le \frac{|\mathcal{D}|^2}{n}. \tag{2.7}$$

We point out for future reference that the verification of (2.7) did not use the assumption $n = \bar{n}$.

Step 2: lower bound. Let ρ be a minimizer of F in $\mathcal{M}(\bar{\mathcal{D}})$, which exists due to Lemma 2.2. Then, it satisfies the Euler-Lagrange equations (2.1) and (2.2). We claim that there exist n points $x_1, \ldots, x_n \in \bar{\mathcal{D}}$ such that

$$|x_i - x_j| \ge 1 \text{ whenever } i \ne j, \text{ and } V * \rho(x_i) = \frac{\min_{\mathcal{M}} F(\bar{\mathcal{D}})}{|\mathcal{D}|} \ \forall i. \tag{2.8}$$

In order to prove it, we define

$$T := \{x \in \bar{\mathcal{D}} \ : \ V * \rho(x) = \inf_x V * \rho = |\mathcal{D}|^{-1} \inf_{\mathcal{M}(\bar{\mathcal{D}})} F\}.$$

According to (2.1), T has a non-empty intersection with any set J such that $\rho(J) > 0$. In particular, T is not empty, and we can find $x_1 \in T$. We then argue by induction: suppose that we have found $x_1, \ldots, x_{j-1}$ satisfying (2.8), and assume that $j \le n$. Since $V * \rho(x_i) \le \min_{\mathcal{M}} F(\bar{\mathcal{D}}) \le \inf_{\mathcal{M}_{ac}(\mathcal{D})} F$, we infer from Step 1 that

$$\begin{aligned}
\rho(\bar{\mathcal{D}}) = |\mathcal{D}| > |\mathcal{D}| \frac{j-1}{n} &\ge \sum_{i=1}^{j-1} V * \rho(x_i) \\
&= \sum_{i=1}^{j-1} \rho(B(x_i)) \ge \rho\left(\cup_{i=1}^{j-1} B(x_i)\right).
\end{aligned}$$

Thus $\rho(\bar{\mathcal{D}} \setminus (\cup_{i=1}^{j-1} B(x_i)) > 0$, so we can find $x_j \in T \setminus (\cup_{i=1}^{j-1} B(x_i))$. Together with the induction hypothesis, this implies that $\{x_1, \ldots, x_j\}$ satisfy (2.8). This completes the induction proof and hence establishes the claim (2.8).

Next, the definition of $\bar{n}$ and the fact that $n = \bar{n}$ implies that if $x_1, \ldots, x_n$ are any points such that $|x_i - x_j| \geq 1$ for all $i \neq j$, then $\cup B(x_j) \supset \bar{\mathcal{D}}$. So for the points $x_1, \ldots, x_n$ satisfying (2.8), we find that

$$|\mathcal{D}| = \rho(\bar{\mathcal{D}}) = \rho(\cup_{i=1}^{\bar{n}} B(x_i)) \leq \sum_{i=1}^{\bar{n}} \rho(B(x_i)) = \sum_{i=1}^{\bar{n}} V * \rho(x_i) = \frac{\bar{n}}{|\mathcal{D}|} \inf_{\mathcal{M}(\bar{\mathcal{D}})} F.$$

Since $\mathcal{M}_{ac}(\mathcal{D}) \subset \mathcal{M}(\bar{\mathcal{D}})$, it follows from this and Step 1 that that

$$\frac{|\mathcal{D}|^2}{\bar{n}} \leq \inf_{\mathcal{M}(\bar{\mathcal{D}})} F \leq \inf_{\mathcal{M}_{ac}(\mathcal{D})} F \leq \frac{|\mathcal{D}|^2}{n}$$

and thus that equality holds throughout when $n = \bar{n}$. It also follows that F attains its infimum in $\mathcal{M}_{ac}$, and that every measure in $\mathcal{M}_{ac}^*$ is a minimizer.

Step 3: any absolutely continuous minimizer belongs to $\mathcal{M}_{ac}^*(\bar{\mathcal{D}})$. We now assume that $\rho \in \mathcal{M}_{ac}$ is a minimizer, and denote by $x_1, \ldots, x_n$ the points constructed in step 2. We then have $\rho(B(x_i)) = |\mathcal{D}|/n$. We thus define

$$A_j = B(x_j) \cap \operatorname{supp} \rho, \qquad j = 1, \ldots, n.$$

Then, according to (2.1) and (2.2), $V * \rho = |\mathcal{D}|/n$ in A_j. Hence, $\rho(A_j) = |\mathcal{D}|/n$: (1.8) is satisfied. We next prove that (1.7) holds. In order to do so, first note that

$$\forall i \neq j, \quad \rho(B(x_i) \cap B(x_j)) = 0. \tag{2.9}$$

Indeed, as remarked above, $\mathcal{D} \subset \cup B(x_i)$, so $\rho(\mathcal{D}) \leq \sum \rho(B(x_i)) = \sum \rho(A_i) = |\mathcal{D}| = \rho(\mathcal{D})$, hence $\rho\left(\cup B(x_i)\right) = \sum \rho(B(x_i))$, which implies (2.9). Since $B(x_i) \cap B(x_j)$ is open and $\operatorname{supp} \rho$ is closed, we deduce from (2.9) that $\operatorname{supp} \rho \cap B(x_i) \cap B(x_j) = \emptyset$ whenever $i \neq j$, hence

$$\forall i \neq j, \quad A_i \cap B(x_j) = \emptyset. \tag{2.10}$$

If $y_i \in A_i$, then $V * \rho(y_i) = \rho(B(y_i)) = |\mathcal{D}|/n$, according to the definition of A_i. Hence, by (2.10), the points $(\{x_1, \ldots, x_n\} \cup \{y_i\}) \setminus \{x_i\}$ again satisfy (2.8), where we know that $\inf F = |\mathcal{D}|^2/n$. Thus, repeating the reasoning that led to (2.10), we find that $A_j \cap B(y_i) = \emptyset$ for all $j \neq i$, ie $|y_i - y_j| \geq 1$ for any $y_j \in A_j, j \neq i$. Since y_i was an arbitrary point in A_i, this proves (1.7). □

2.2.2. *The case* $n \neq \bar{n}$. We write $B(a, x)$ to denote the *open* ball of radius a about the point x, with respect to the relevant distance (Euclidean or periodic) so that $B(a, x) := \{y \in \mathcal{D} : |x - y| < a\}$, with $|x - y|$ understood in the suitable way.

It is convenient to define, for $a > 0$,

$$F_a(\rho) := \int_{\bar{\mathcal{D}}} V_a * \rho \, d\rho \qquad \text{where } \; V_a(x) := \begin{cases} 1 & \text{if } |x| < a \\ 0 & \text{if not.} \end{cases}$$

We first note that the result of the last subsection (ie, Theorem 1.1 in the case $n = \bar{n}$) remains valid if F is replaced by F_a.

Lemma 2.4. *Define*

$$n(\mathcal{D}, a) := \max\{k : \exists x_1, \dots, x_k \in \mathcal{D} \text{ such that } |x_i - x_j| > a \quad \forall i \neq j\}$$

and assume that $a > 0$ satisfies

$$n(\mathcal{D}, a) = \max\{k : \exists x_1, \dots, x_k \in \bar{\mathcal{D}} \text{ such that } |x_i - x_j| \geq a \quad \forall i \neq j\}. \tag{2.11}$$

Then

$$\min_{\mathcal{M}_{ac}(\mathcal{D})} F_a = |\mathcal{D}|^2 / n(\mathcal{D}; a)$$

and the minimum is attained. In fact, a measure ρ in $\mathcal{M}_{ac}(\mathcal{D})$ minimizes F_a if and only if there exist $n(\mathcal{D}; a)$ pairwise disjoint closed sets $A_1, \dots, A_{n(\mathcal{D};a)} \subset \mathcal{D}$, such that

$$\operatorname{dist}(A_i, A_j) \geq a \text{ if } i \neq j, \tag{2.12}$$

and

$$\rho(A_i) = \frac{|\mathcal{D}|}{n(\mathcal{D}; a)} \tag{2.13}$$

for all i.

We will use the notation

$$\mathcal{M}^*_{ac}(\mathcal{D}; a) := \{\rho \in \mathcal{M}_{ac}(\mathcal{D}) \ : \exists A_1, \dots, A_n \subset \mathcal{D} \text{ satisfying } (2.12), (2.13)\}. \tag{2.14}$$

Note that if $\rho \in \mathcal{M}^*_{ac}(\mathcal{D}; a)$ for some $a > 0$, the definitions easily yield

$$\rho(\mathcal{D} \setminus \cup A_j) = 0. \tag{2.15}$$

When $a = 1$, this lemma is exactly the result proved in the last subsection, and in particular assumption (2.11) is exactly the condition $n = \bar{n}$. It is easy to see that this assumption holds for all but countable many a.

Proof. This follows from the result of the previous subsection by a simple rescaling. $\square$

We now use the above lemma to deduce the *proof of Theorem 1.1.* Throughout the proof we will write n and $n(a)$ instead of $n(\mathcal{D})$ (as defined in the statement of the theorem) and $n(\mathcal{D};a)$ (as defined in Lemma 2.4) respectively. Note that $n = n(a)$ for $a = 1$. We will also write $\bar{n}(a)$ to denote the right-hand side of (2.11). It is clear that $n(a) \le \bar{n}(a)$ for all a, and also that $n, \bar{n}$ are nonincreasing functions of a.

We first remark that there exists $\delta > 0$ such that

$$n = n(a) = \bar{n}(a) \quad \text{for all } a \in (1, 1+\delta). \tag{2.16}$$

To see this, note that by the definition of n, there exist points $x_1, \ldots, x_n \in \mathcal{D}$ such that $|x_i - x_j| > 1$ whenever $i \ne j$, and so it is clear that $n \le n(a)$ whenever $a < \min\{|x_i - x_j| : i \ne j\} =: 1 + \delta$. Then properties of a noted above imply that $n(a) \le \bar{n}(a) \le \bar{n}(1)$ for $a \in (1, 1+\delta)$, proving (2.16).

Note that $V_a \to V$ almost everywhere as $a \searrow 1$. For any $\rho \in \mathcal{M}_{ac}$, it therefore follows from the dominated convergence theorem, Lemma 2.4, and (2.16) that

$$F(\rho) = \lim_{a \searrow 1} F_a(\rho) \ge \liminf_{a \searrow 1} \frac{|\mathcal{D}|^2}{n(a)} = \frac{|\mathcal{D}|^2}{n}.$$

On the other hand, when considering the case $n = \bar{n}$, we proved that $F(\rho) \le \frac{|\mathcal{D}|^2}{n}$ for all $\rho \in \mathcal{M}^*_{ac}(\mathcal{D})$. (This proof did not use the assumption $n = \bar{n}$; see (2.7)). We deduce that $\min_{\mathcal{M}_{ac}(\mathcal{D})} F = \frac{|\mathcal{D}|^2}{n}$, and this minimum is attained by measures in $\mathcal{M}^*_{ac}(\mathcal{D})$.

Finally, suppose that ρ is a minimizer of F in $\mathcal{M}_{ac}$, so that $F(\rho) = \frac{|\mathcal{D}|^2}{n}$. Since the derivation of the optimality conditions (2.1), (2.2) in Lemma 2.3 holds for minimizers in $\mathcal{M}_{ac}$, we can repeat arguments from Step 2 of the proof of Theorem 1.1 in the case $n = \bar{n}$ to find points $x_1, \ldots, x_n \in \mathcal{D}$ such that $V * \rho(x_i) = F(\rho)$ and $|x_i - x_j| \ge 1$ for $i \ne j$. We then define $A_j = B(x_j) \cap \operatorname{supp} \rho$ for $j = 1, \ldots, n$, and by repeating the arguments from Step 3 of the $n = \bar{n}$ proof, we verify that these sets satisfy (1.7), (1.8), which shows that $\rho \in \mathcal{M}^*_{ac}(\mathcal{D})$. □

2.3. **A generalization.**

The above results extend to the functional

$$F_E(\rho) = \int_{\mathcal{D}} V_E * \rho \, d\rho, \qquad \text{where } V_E(x) = \begin{cases} 1 & \text{if } x \in E \\ 0 & \text{if not} \end{cases} \tag{2.17}$$

for suitable sets E.

Theorem 2.1. *Suppose that E is a bounded, open subset of $\mathbb{R}^d$ with $0 \in E$, and that E is even in the sense that $x \in E \iff -x \in E$.*

Given a set $S \subset \mathbb{R}^d$, define $n(\mathcal{D}, S)$ by

$$n(\mathcal{D}, S) := \sup\{k : \exists x_1, \ldots, x_k \in \bar{\mathcal{D}} \text{ such that } x_i - x_j \notin S \ \ \forall i \ne j\}.$$

Then $\min_{\mathcal{M}} F_E = |\bar{\mathcal{D}}|^2/n(\mathcal{D}, E)$ *and the minimum is attained. Moreover, a measure* ρ *in* $\mathcal{M}$ *minimizes* F_E *if and only if there exist* $n(\mathcal{D}, E)$ *pairwise disjoint closed sets* $A_1, \ldots, A_{n(\mathcal{D},E)} \subset \bar{\mathcal{D}}$*, such that if* $x_i \in A_i, x_j \in A_j$*, and* $i \neq j$*, then* $x_i - x_j \notin E$*; and in addition* $\rho(A_i) = \frac{|\bar{\mathcal{D}}|}{n(\mathcal{D},E)}$ *for all* i*.*

If E *also satisfies the condition* $\mathcal{L}^d(\partial E) = 0$*, then* $\min_{\mathcal{M}_{ac}} F_E = |\bar{\mathcal{D}}|^2/n(\mathcal{D}, \bar{E})$*. In this case a measure* ρ *minimizes* F_E *in* $\mathcal{M}_{ac}$ *if and only if there exist* $n(\mathcal{D}, \bar{E})$ *pairwise disjoint closed sets* $A_1, \ldots, A_n \subset \bar{\mathcal{D}}$*, such that if* $x_i \in A_i, x_j \in A_j$*, and* $i \neq j$*, then* $x_i - x_j \notin \bar{E}$*; and in addition* $\rho(A_i) = |\bar{\mathcal{D}}|/n(\bar{E})$ *for all* i*.*

It is natural to assume that E is open, since then F_E is lower semicontinuous on the space of nonnegative measures, exactly as the proof of Lemma 2.1. (The same argument shows that if E is closed, then F_E is upper semicontinuous.)

We omit the proof of Theorem 2.1, apart from the following remarks: The part of the proof that deals with minimizers in $\mathcal{M}$ is a straightforward adaptation of the proof of Lemma 2.4; it is just necessary to replace $B(a, x)$ by $x + E$ throughout. The part of the proof concerning minimizers in $\mathcal{M}_{ac}$ is likewise an adaptation of the proof of Theorem 1.1; the point is that if ρ is absolutely continuous and $\mathcal{L}^d(\partial E) = 0$, then $F_E(\rho) = F_{\bar{E}}(\rho) = \lim_{r\searrow 0} F_{E_r}(\rho)$ where $E_r := \{x \in \mathbb{R}^d \ : \ \mathrm{dist}(x, E) < r\}$.

We do not know what are the most general hypotheses on a set E for a result of the above sort to hold, and have only written the hypotheses that allow the earlier proof to go through more or less without change.

3. Asymptotic $\varepsilon \to 0$: derivation of $E_{0,\Omega}$

In other sections of this paper, A denotes the infinitesimal generator of rotation about the z-axis. In this section we allow somewhat more general vector fields A, since it makes absolutely no difference to the proof. Thus, throughout this section,

$$G_\Omega(u) := \int_{\mathcal{D}} \frac{1}{2}|\nabla u|^2 - \Omega A \cdot \mathrm{Im}(\bar{u}\nabla u)\ dx$$

and $A \in L^\infty(\mathcal{D}; \mathbb{R}^d)$ is a fixed vector field. In fact it will be apparent from our proof that the result holds for a much larger class of functionals G.

Proof of Theorem 1.2. For concreteness we consider the Dirichlet problem; the proofs for the periodic problem are almost exactly the same. Throughout the proof we will write for example $\mathcal{A}_0, \mathcal{M}$, and so on instead of $\mathcal{A}_0(\mathcal{D}), \mathcal{M}(\mathcal{D})$ when there is no possibility of confusion.

We will repeatedly use the fact that

$$G_\Omega(u) \geq \frac{1}{4}\|\nabla u\|^2_{L^2} - \Omega^2|\mathcal{D}|\|A\|^2_{L^\infty(\mathcal{D})}, \qquad \text{for } u \in \mathcal{A}_0. \tag{3.1}$$

1. We first show that G_Ω attains its minimum in $\mathcal{A}_0^*$. Let $\{u_k\} \subset \mathcal{A}_0^*$ be a sequence such that $G_\Omega(u_k) \to \inf_{\mathcal{A}_0^*} G_\Omega$.

In view of (3.1), we can extract a subsequence (still labelled u_k) and a function $u_0 \in H_0^1$ such that such that $u_k \to u_0$ strongly in L^2 and $\nabla u_k \to \nabla u_0$ weakly in L^2. In particular, it follows that $|u_k|^2 \to |u_0|^2$ in L^1, and hence $|u_0|^2 \in \mathcal{M}_{ac}$. Also, standard lowersemicontinuity results (see also Step 4 below) imply that $G_\Omega(u_0) \le \inf_{\mathcal{A}_0^*} G_\Omega$. So we only need to show that u_0 belongs to $\mathcal{A}_0^*$. This however is easy, since the lowersemicontinuity of F implies that

$$F(|u_0|^2) \le \liminf_{k\to\infty} F(|u_k|^2) = \min_{\mathcal{M}_{ac}} F,$$

since every $|u_k|^2$ is a minimizer for F in $\mathcal{M}_{ac}$. Since $|u_0|^2 \in \mathcal{M}_{ac}$, it follows that it minimizes F in $\mathcal{M}_{ac}$. Hence we conclude from Theorem 1.1 that $|u_0|^2 \in \mathcal{M}_{ac}^*$, or equivalently that $u_0 \in \mathcal{A}_0^*$.

2. Now let u_ε minimize $E_{\varepsilon,\Omega}$ in $\mathcal{A}_0$, and let u_0 minimize G_Ω in $\mathcal{A}_0^*$. Then $|u_0|^2$ minimizes F, by Theorem 1.1, so that

$$\begin{aligned} G_\Omega(u_\varepsilon) &= E_{\varepsilon,\Omega}(u_\varepsilon) - \frac{1}{4\varepsilon^2} F(|u_\varepsilon|^2) \\ &\le E_{\varepsilon,\Omega}(u_0) - \frac{1}{4\varepsilon^2} F(|u_0|^2) \\ &= G_\Omega(u_0). \end{aligned} \tag{3.2}$$

Thus we deduce from (3.1) that $\{u_\varepsilon\}_{\varepsilon\in(0,1]}$ is uniformly bounded in H^1. Similarly

$$\begin{aligned} F(|u_\varepsilon|^2) = {} & 4\varepsilon^2 \left[E_{\varepsilon,\Omega}(u_\varepsilon) - G_\Omega(u_\varepsilon)\right] \\ \le {} & 4\varepsilon^2 \left[E_{\varepsilon,\Omega}(u_0) - G_\Omega(u_\varepsilon)\right] \\ = {} & 4\varepsilon^2 \left[G_\Omega(u_0) + \frac{1}{4\varepsilon^2} F(|u_0|^2) - G_\Omega(u_\varepsilon)\right] \\ \le {} & \min_{\mathcal{M}_{ac}} F + C\varepsilon^2. \end{aligned} \tag{3.3}$$

3. In view of (3.2), (3.1), and Rellich's compactness theorem, we may extract a subsequence (still labelled u_ε) and a function $u_* \in H_0^1$ such that $u_\varepsilon \to u_*$ strongly in L^2 and $\nabla u_\varepsilon \rightharpoonup \nabla u_*$ weakly in L^2. In particular, it follows $|u_\varepsilon|^2 \to |u_*|^2$ in L^1, and also that $|u_*|^2 \in L^1 \subset \mathcal{M}_{ac}$. Since F is continuous with respect to the L^1 norm, this convergence and (3.3) imply

$$F(|u_*|^2) = \lim F(|u_\varepsilon|^2) = \min_{\mathcal{M}_{ac}} F.$$

It then follows from the characterization of minimizers of F in Theorem 1.1 that $u_* \in \mathcal{A}_0^*$. Moreover, it follows from (3.2) and the lower semicontinuity of

G_Ω that

$$\min_{\mathcal{A}_0^*} G_\Omega \leq G_\Omega(u_*) \leq \liminf_{\varepsilon\to 0} G_\Omega(u_\varepsilon) \leq \limsup_{\varepsilon\to 0} G_\Omega(u_\varepsilon) \leq G_\Omega(u_0) = \min_{\mathcal{A}_0^*} G_\Omega.$$

Therefore u_* minimizes G_Ω in $\mathcal{A}_0^*$, and

$$\lim_{\varepsilon\to 0} G_\Omega(u_\varepsilon) = G_\Omega(u_*). \tag{3.4}$$

4. It only remains to prove that $u_\varepsilon \to u_*$ strongly in H^1. This is easy, however, because the weak H^1 convergence $u_\varepsilon \rightharpoonup u_*$ implies that

$$\int_{\mathcal{D}} A\cdot \mathrm{Im}(\bar u_\varepsilon \nabla u_\varepsilon)\ dx \quad \to \quad \int_{\mathcal{D}} A\cdot \mathrm{Im}(\bar u_* \nabla u_*)\ dx,$$

so we deduce from (3.4) that $\|\nabla u_\varepsilon\|_{L^2} \to \|\nabla u_*\|_{L^2}$, and this together with weak convergence implies that $\nabla u_\varepsilon \to \nabla u_*$ strongly in L^2. □

4. One dimensional case

In this section we consider one-dimensional problems. It is easy to check that $E_\varepsilon(|u|) \leq E_\varepsilon(u)$, and similarly E_0. Since we are interested in minimizers, we will therefore often implicitly restrict our attention to nonnegative functions.

The analysis here is *much* simpler than in higher dimensions, but the results we establish here presumably give at least some indication of what to expect when $n \geq 2$.

4.1. Minimizers of the $\varepsilon = 0$ problem.

In this subsection we consider the problem (1.14), which we recall here:

$$\text{find } u_0 \in \mathcal{A}_0^*(\mathcal{D}) \text{ such that } E_0(u_0) = \min_{\mathcal{A}_0^*(\mathcal{D})} E_{0,\Omega}.$$

Recall that $\lceil L\rceil$ to denote the smallest integer that is greater than or equal to L. We now give the

Proof of Proposition 1.1. In the Dirichlet case, Theorem 1.1 implies that $\mathcal{A}_0$ consists of functions supported in $n(\mathcal{D})$ sets $A_1, \ldots A_{n(\mathcal{D})}$, each one separated from all others by distance at least 1. Hence there are numbers $a_k < b_k$, $k = 1, \ldots, n(\mathcal{D})$ such that (after relabelling the A_i if necessary) $A_i \subset [a_i, b_i]$ for all i, and $b_i + 1 \leq a_{i+1}$ for $i = 1, \ldots, n(\mathcal{D}) - 1$. Moreover, the choice of $n(\mathcal{D})$ makes it impossible for some A_j to have nonempty intersection with the convex hull of some other A_i.

Then, since (1.8) implies that $\int_{a_i}^{b_i} |u|^2 = \frac{L}{n(\mathcal{D})}$ for every i,

$$\int_{\mathcal{D}} |u'|^2 = \sum_{i=1}^{n(\mathcal{D})} \int_{a_i}^{b_i} |u'|^2 \geq \sum_{i=1}^{n(\mathcal{D})} \frac{\pi^2}{(b_i-a_i)^2} \int_{a_i}^{b_i} |u|^2 = \frac{L}{n(\mathcal{D})} \sum_{i=1}^{n(\mathcal{D})} \frac{\pi^2}{(b_i-a_i)^2},$$

with equality if and only if the restriction of u to each interval (a_i, b_i) is a scaled and normalized sine function multiplied by a constant of modulus 1. Moreover, Jensen's inequality implies that

$$\sum \frac{1}{(b_i - a_i)^2} \geq \frac{n(\mathcal{D})}{(n(\mathcal{D})^{-1} \sum (b_i - a_i))^2} \geq n(\mathcal{D})/h_0^2,$$

with equality if and only if $b_i - a_i = h_0$ for every i. This implies that, if we assume that $u_0 \geq 0$, it is the function defined in the statement of the theorem. The proof of the periodic case is essentially the same. □

4.2. **Minimizers of E_ε for $0 < \varepsilon \ll 1$.** This section is devoted to the proof of Theorem 1.3. We first prove three technical lemmas, then give the proof of the theorem. We use the notation of Proposition 1.1, namely

$$\bar{n}_p = \lceil L \rceil - 1, \qquad h_p = (L - \bar{n}_p))/\bar{n}_p. \tag{4.1}$$

Recall also the notation $\tau_y u(x) := u(x - y)$.

The starting point of the proof of the theorem is the fact that a minimizer u_ε of E_ε is close (after a suitable translation) to the minimizer u_p of the $\varepsilon = 0$ problem. The first lemma records a quantitative consequence of this fact. Thus u_ε has n "bumps" separated by regions in which it is exponentially small. In the proof of the theorem, we extract $3n$ parameters, related to a local mass, kinetic energy, and a length-scale associated with each of these bumps. The second lemma is used, in the proof of the theorem, to bound E_ε below by a function depending only on these parameters, and the third lemma gives a lower bound for this function of $3n$ variables.

Lemma 4.1. *Given $\delta > 0$, there exists $\varepsilon_0 > 0$ such that for $0 < \varepsilon < \varepsilon_0$, if u_ε is a nonnegative minimizer in $\mathcal{H}^1_{per}(\mathcal{D})$ of E_ε and*

$$y \mapsto \|u_p - \tau_y u_\varepsilon\|_{H^1} \text{ is minimized for } y = 0 \tag{4.2}$$

then there exists a constant $C > 0$ depending only on L such that

$$u_\varepsilon(x) \leq 2\left(1 + \frac{\pi L}{h_p}\right) e^{-C\frac{\delta^{5/2}}{\varepsilon}} \quad \text{for all } x \text{ such that } dist(x, supp\, u_p) > \delta. \tag{4.3}$$

Remark 3. Note that because $\mathcal{D} = (0, L]$ with periodic boundary conditions is compact, the function $y \in \mathcal{D} \mapsto \|u_p - \tau_y u_\varepsilon\|_{H^1}$ attains its minimum, and we can arrange by a suitable translation that this minimum is attained at $y = 0$.

Remark 4. Tracking the dependence of the constants in the proof of Lemma 4.1, it is possible to give an explicit expression for the constant C: $C = L/(2\sqrt{6} h_p \bar{n}_p)$.

Proof. Let u_ε be a sequence satisfying the assumptions of the theorem. We first point out that

$$\begin{aligned} \frac{1}{2}\int_0^L (u_\varepsilon')^2 &= E_\varepsilon(u_\varepsilon) - \frac{1}{4\varepsilon^2}F(u_\varepsilon) \leq E_\varepsilon(u_p) - \frac{1}{4\varepsilon^2}F(u_p) = \frac{1}{2}\int_0^L (u_p')^2 \\ &= \frac{\pi^2 L}{2h_p^2}. \end{aligned} \tag{4.4}$$

Moreover, since $\fint u_\varepsilon^2 = 1$, one can find $x \in \mathcal{D}$ such that $u_\varepsilon(x) \leq 1$. Hence,

$$\|u\|_{L^\infty(\mathcal{D})} \leq 1 + \sqrt{L}\left(\int_0^L (u_\varepsilon')^2\right)^{1/2} \leq 1 + \frac{\pi L}{h_p}. \tag{4.5}$$

Next, we claim that $u_\varepsilon \to u_p$ in H^1. Indeed, it follows from Theorem 1.2 (and also from inequality (4.4)) that $\{u_\varepsilon\}$ is precompact in H^1, and that every limit of a convergent subsequence is a minimizer for the limiting problem. However, every such minimizer is a translate of u_p, and since $\|\tau_{-y}u_p - u_\varepsilon\|_{H^1} = \|u_p - \tau_y u_\varepsilon\|_{H^1}$ it follows from (4.2) that the only possible limit of a convergent subsequence is u_p.

Moreover, the convergence of u_ε in H^1 implies that

$$V * u_\varepsilon^2 \longrightarrow V * u_p^2 \quad \text{in } H^1.$$

It is easy to check that

$$\forall x \in \mathcal{D}, \quad \left(V * u_p^2\right)(x) \geq \frac{L}{\bar{n}_p} + c\left[\text{dist}\left(x, \text{supp}(u_p)\right)\right]^3,$$

where c is a constant independent of ε. Hence, if $\text{dist}(x, \text{supp } u_p) \geq \delta/2$, we can find $\varepsilon_0 > 0$ such that, for any $0 < \varepsilon < \varepsilon_0$,

$$\left(V * u_\varepsilon^2\right)(x) \geq \frac{L}{\bar{n}_p} + \frac{c}{2}\left[\text{dist}\left(x, \text{supp}(u_p)\right)\right]^3 \tag{4.6}$$

Next we record the Euler-Lagrange equation for u_ε, which is

$$u_\varepsilon'' = \frac{1}{\varepsilon^2}(V * u_\varepsilon^2)u_\varepsilon - \lambda_\varepsilon u_\varepsilon, \qquad \lambda_\varepsilon = \fint_{\mathcal{D}} (u_\varepsilon')^2 + \frac{1}{\varepsilon^2} V * u_\varepsilon^2 \cdot u_\varepsilon^2 \, dx. \tag{4.7}$$

Note that

$$E_\varepsilon(u_\varepsilon) \leq E_\varepsilon(u_p) = \frac{1}{4\varepsilon^2}\frac{L^2}{\bar{n}_p} + \frac{\pi^2}{2h_p^2}L.$$

Clearly $\lambda_\varepsilon < \frac{4}{L}E_\varepsilon(u_\varepsilon)$, so $\lambda_\varepsilon < \frac{L}{\varepsilon^2 \bar{n}_p} + \frac{2\pi^2}{h_p^2}$. So it follows from (4.6), (4.7) that

$$-\varepsilon^2 u_\varepsilon'' + \left(\frac{c}{2}\,\text{dist}(x, \text{supp}(u_p))^3 - \frac{2\pi^2}{h_p^2}\varepsilon^2\right) u_\varepsilon \leq 0, \tag{4.8}$$

whenever dist $(x, \text{supp } u_p) \geq \delta/2$. Taking ε_0 smaller if necessary, we may assume that $\varepsilon^2 < (h_p^2\delta^3)/(64\pi^2)$, so that (4.8) becomes

$$-u_\varepsilon'' + \frac{c}{4\varepsilon^2}\operatorname{dist}(x, \operatorname{supp}(u_p))^3 u_\varepsilon \leq 0, \tag{4.9}$$

whenever dist $(x, \text{supp } u_p) \geq \delta/2$. Without loss of generality, we may assume that a connected component of $\{x,\ \operatorname{dist}(x, \operatorname{supp}(u_p)) \geq \delta/2\}$ is an open interval (a, b). On this connected component, we use the function

$$U(x) = \|u_p\|_{L^\infty}\left(e^{-\frac{\sqrt{c}\delta^{3/2}}{4\varepsilon\sqrt{2}}(x-a)} + e^{\frac{\sqrt{c}\delta^{3/2}}{4\varepsilon\sqrt{2}}(b-x)}\right)$$

as a supersolution. Hence, on (a, b),

$$u_\varepsilon(x) \leq U(x) \leq 2\|u_p\|_{L^\infty} e^{-\frac{\sqrt{c}\delta^{3/2}}{4\varepsilon\sqrt{2}}\left(\operatorname{dist}(x,\operatorname{supp}(u_p)) - \frac{\delta}{2}\right)}.$$

If $\operatorname{dist}(x, \operatorname{supp} u_p) > \delta$, we infer (4.3), with $C = \sqrt{c}/8\sqrt{2}$. □

The next lemma quantifies the fact that one cannot confine the entire mass of a one-dimensional wave function in a small interval, if the kinetic energy is bounded. As remarked earlier, it will be used to bound E_ε below by a function of finitely many variables.

Lemma 4.2. *Given an interval $J = (a, b) \subset \mathbb{R}$, let*

$$p(m, k, J) := \sup\left\{\int_J u^2\, dx \ :\ \int_{\mathbb{R}} u^2\, dx = m,\ \int_{\mathbb{R}} u'^2\, dx = k\right\}$$

Then there exists a function $f : [0, \infty) \to [0, \infty)$ such that

$$p(m, k, J) = mf\left(|J|\sqrt{\frac{k}{m}}\right), \tag{4.10}$$

and in addition f satisfies

$$f(s) \leq 1 \quad \text{for all } s, \text{ and } f(s) = 1 \text{ if } s \geq \pi, \tag{4.11}$$

$$f(s) = 1 - \frac{1}{2\pi}(\pi - s)^3 + O\left((\pi - s)^4\right) \qquad \text{for } s \leq \pi. \tag{4.12}$$

As a result, there exists a constant $c > 0$ such that $f(s) \leq 1 - c(\pi - s)^{+\,3}$ for every $s \geq 0$.

Proof. **1**. We will eventually prove the lemma when $J = (-\frac{1}{2}, \frac{1}{2})$. We first show that the general case follows by a change of variables. Indeed, suppose $J = (a, b)$, and for m, k given, consider any $u \in H^1(\mathbb{R})$ such that $\|u\|_{L^2}^2 = m, \|u'\|_{L^2}^2 = k$. Let $x_0 = \frac{1}{2}(a + b)$ and $L = b - a$, and define a new variable

$y = \frac{x-x_0}{L}$. Next define $U(y) = u(x)$, and let $m' = \|U\|_{L^2}^2 = m/L$, $k' := \|U'\|_{L^2}^2 = Lk$ and $J' = (-\frac{1}{2}, \frac{1}{2})$. Note that

$$\int_J u^2\,dx = L\int_{J'} U^2\,dy$$

Hence if the conclusion holds for $J' = (-\frac{1}{2}, \frac{1}{2})$, then

$$p(m,k,J) = Lp(m',k',J') = Lm' f(|J'|\sqrt{\frac{k'}{m'}}) = mf(|J|\sqrt{\frac{k}{m}}).$$

2. We henceforth fix $J = (-\frac{1}{2}, \frac{1}{2})$. By a scaling argument similar to that given above, we can also assume that $m = 1$, so that in fact

$$f(s) = \sup\left\{\int_J u^2\ dx\ :\ \|u\|_{L^2} = 1, \|u'\|_{L^2} = s\right\}. \tag{4.13}$$

It is clear that $f(s) \le 1$ for all s. For $s \ge \pi$, define

$$u(x) = \begin{cases} \sqrt{\frac{2s}{\pi}}\cos(sx) & \text{if } |x|\ \le\ \pi/2s \\ 0 & \text{if not,} \end{cases}$$

and note that $\|u\|_{L^2} = 1$, $\|u'\|_{L^2} = s$, and $\int_J u^2 = 1$. Hence $f(s) = 1$ for $s \ge \pi$.

3. It remains to prove (4.12), which is the real content of the lemma. To do this, fix $s < \pi$. We first claim that the supremum in (4.13) is attained. To see this, let u_k be a sequence such that $\|u_k\|_{L^2} = 1$ and $\|u_k'\|_{L^2} = s$, and such that $\int_J u_k^2 \nearrow f(s)$. Let $u \in H^1(\mathbb{R})$ be a function such that $u_k \to u$ locally in L^2, and $u_k' \rightharpoonup u$ weakly in L^2. Then

$$\int_J u^2\,dx = f(s), \qquad \|u\|_{L^2} \le 1, \quad \|u'\|_{L^2} \le s.$$

Let us write $a = \|u\|_{L^2}$ and $b = \frac{1}{s}\|u'\|_{L^2}$, so that $0 < a, b \le 1$. We consider two cases:

case 1: suppose $b \le a \le 1$. Then define $U(x) = (ab)^{-1/2}u(ax/b)$. Then one can check that $\|U\|_{L^2} = 1$, $\|U'\|_{L^2} = s$, and

$$\int_J U^2\ dx = \frac{1}{a}\int_{-\frac{a}{2b}}^{\frac{a}{2b}} u^2\ dx \ge \int_J u^2 dx = f(s).$$

Then U satisfies the constraints and attains the supremum on the right-hand side of (4.13). Note also that we get strict inequality, and hence a contradiction, if $a < 1$.

case 2: suppose $a < b \le 1$. First, define U_0 to be the symmetric rearrangement of u (see [21] for example), so that U_0 is even and nonincreasing in $(0,\infty)$. Then

$$\int_J U_0^2\,dx \ge \int_J u^2\,dx = f(s), \quad \|U_0\|_{L^2} = a, \quad \|U_0'\|_{L^2} = b's \le bs = \|u'\|_{L^2}.$$

If $b' \le a$ then we are back to case 1, and this leads to a contradiction since $a < 1$. If not, we define $U_1(x)$ by

$$U_1(x) := \begin{cases} U_0(0) & \text{if } |x| \le \delta \\ U_0(|x|-\delta) & \text{if } |x| \ge \delta, \end{cases}$$

where δ is chosen so that $\|U_1\|_{L^2} = b'$. Note also that $\|U_1'\|_{L^2} = \|U_0'\|_{L^2} = b'$, regardless of the choice of δ. Also, since U_0 attains its maximum at $x = 0$, $\int_J U_1^2 \ge \int_J U_0^2 \ge f(s)$. Finally, let $U_2 = \frac{1}{b'}U_1$. Then U_2 satisfies the constraints $\|U_2\|_{L^2} = 1$, $\|U_2'\|_{L^2} = s$, and $\int_J U_2^2 \ge f(s)$, so the supremum on the right-hand side of (4.13) is attained.

4. Now let u_s denote a function such that

$$\int_J u_s^2\,dx = f(s), \qquad \|u_s\|_{L^2} = 1, \quad \|u_s'\|_{L^2} = s.$$

Standard arguments show that $u_s > 0$ everywhere. The Euler-Lagrange equation satisfied by u_s is

$$\chi_J u_s = \lambda u_s + \mu u_s''$$

where λ, μ are Lagrange multipliers. Here $\chi_J(x) = 1$ if $x \in J$ and 0 otherwise. This equation cannot be satisfied if $\mu = 0$, so it can be rewritten

$$-u_s'' = (\nu\chi_J + \eta\chi_{J^c})u_s \tag{4.14}$$

for certain constants ν, η, where J^c denotes the complement of J. Note that this is essentially the equation for a one-dimensional quantum particle in a square well, so that if we like, we can find a complete description of solutions by consulting basic quantum mechanics textbooks. From this, or by solving directly, we find that (4.14) has square-integrable solutions only if $\nu > 0$ and $\eta < 0$, so we can rewrite the equation as

$$-u_s'' = (\alpha^2\chi_J - \beta^2\chi_{J^c})u_s. \tag{4.15}$$

We further see that L^2 solutions exist only if $\beta = \alpha\tan(\alpha/2)$, and when this holds, all square-integrable solutions are multiples of

$$\psi_\alpha(x) := \begin{cases} \cos\alpha x & \text{if } |x| \le \frac{1}{2} \\ \cos(\alpha/2)\exp\left[\beta\left(\frac{1}{2} - |x|\right)\right] & \text{if } |x| \ge \frac{1}{2}. \end{cases}$$

It follows from this that for $s < \pi$, $u_s = \psi_\alpha/\|\psi_\alpha\|_{L^2}$ for some $\alpha = \alpha(s)$ such that $\psi_\alpha > 0$ and $\|\psi_\alpha'\|_{L^2}/\|\psi_\alpha\|_{L^2} = s$. Note that $\psi_\alpha > 0$ iff $\alpha < \pi$. We now define

$$g(\alpha) := \|\psi'_\alpha\|_{L^2}/\|\psi_\alpha\|_{L^2}, \quad h(\alpha) = \|\psi_\alpha\|_{L^2}^{-2}\int_J \psi_\alpha^2\,dx.$$

It follows from what we have said that $f(s) = h(\alpha)$ for some $\alpha \in (0,\pi)$ such that $g(\alpha) = s$. We will show that in fact g is one-to-one in $(0,\pi]$, so that $f(s) = h(g^{-1}(s))$, where g^{-1} denotes the inverse of the restriction of g to $(0,\pi]$.

5. We next explicitly compute $g(\alpha)$ and $h(\alpha)$. We integrate to find that

$$\|\psi_\alpha\|_{L^2}^2 = \frac{1}{2}\left(1 + \frac{1}{\alpha}\sin\alpha\right) + \frac{1}{\beta}\cos^2\frac{\alpha}{2}$$

We substitute $\beta = \alpha\tan\frac{\alpha}{2}$ and write $\frac{1}{2}\sin\alpha = \sin\frac{\alpha}{2}\cos\frac{\alpha}{2}$, then simplify to find

$$\|\psi_\alpha\|_{L^2}^2 = \frac{1}{2} + \frac{1}{\alpha}\cot\frac{\alpha}{2}.$$

Similarly, noting that $\psi_\alpha'^2 = \alpha^2\psi_\alpha^2$ in J and $\psi_\alpha'^2 = \beta^2\psi_\alpha^2$ elsewhere, and rewriting as above, we see that

$$\|\psi'_\alpha\|_{L^2}^2 = \frac{\alpha^2}{2}(1 + \frac{1}{\alpha}\sin\alpha) + \beta\cos^2\frac{\alpha}{2} = \frac{\alpha^2}{2} + \alpha\sin\alpha.$$

Thus

$$g(\alpha) = \alpha\left[\frac{\alpha + 2\sin\alpha}{\alpha + 2\cot\frac{\alpha}{2}}\right]^{1/2}$$

Similarly,

$$h(\alpha) = \frac{\alpha + \sin\alpha}{\alpha + 2\cot\frac{\alpha}{2}}.$$

It is easy to check that g^2, and hence g, is an increasing function on $(0,\pi)$, as is h for that matter. Thus $f(s) = h(g^{-1}(s))$. Now (4.12) follows by calculus. Indeed, we compute that $g(\pi) = \pi$, $\quad g'(\pi) = \frac{1}{2}$ which implies that $g^{-1}(s) = \pi + 2(s-\pi) + O((s-\pi)^2)$ near $s = \pi$. We also check that $h(\pi) = 1$, $h'(\pi) = h''(\pi) = 0$ and $h'''(\pi) = \frac{3}{2\pi}$. Substituting the expansion for $g^{-1}(s) - \pi$ into the Taylor series for h at $\alpha = \pi$ yields (4.12). $\square$

The last technical lemma is

Lemma 4.3. *Let $L > 2$ be as in Theorem 1.3, let $c > 0$ be given, and define $\bar{n}_p, h_p$ by* (4.1)*. Then, for any positive numbers $(m_i)_{1\le i\le \bar{n}_p}, (\alpha_i)_{1\le i\le \bar{n}_p}, (\ell_i)_{1\le i\le \bar{n}_p}$ such that*

$$\sum_{i=1}^{\bar{n}_p} m_i = L, \quad \sum_{i=1}^{\bar{n}_p} \ell_i = \bar{n}_p h_p,$$

we have

$$\sum_{j=1}^{\bar{n}_p} m_j^2 + c(\pi - \ell_j\alpha_j)^{+\ 6} + 2\varepsilon^2 m_j\alpha_j^2 \ \geq\ \frac{L^2}{\bar{n}_p} + 2\varepsilon^2\frac{\pi^2}{h_p^2}L - C\varepsilon^{2/5}. \tag{4.16}$$

Proof. Let us write $q_0((m_j),(\alpha_j),(\ell_j))$ to denote the left-hand side of (4.16). Fix $(m_j),(\alpha_j),(\ell_j)$ that minimize $q_0(\cdot,\cdot,\cdot)$ subject to the constraints on $\sum m_i$ and $\sum \ell_i$. If we let $\tilde{m}_j = L/\bar{n}_p, \tilde{\ell}_j = h_p, \tilde{\alpha}_j = \pi/h_p$ for all j, then

$$q_0((m_j),(\alpha_j),(\ell_j)) \leq q_0((\tilde{m}_j),(\tilde{\alpha}_j),(\tilde{\ell}_j)) = \frac{L^2}{\bar{n}_p} + 2\varepsilon^2\frac{\pi^2}{h_p^2}L. \tag{4.17}$$

The constraint $\sum m_i = L$ implies that

$$\sum_{i=1}^{\bar{n}_p} m_i^2 \ = \ \frac{L^2}{\bar{n}_p} + \sum_{i=1}^{\bar{n}_p}(m_i - \frac{L}{\bar{n}_p})^2.$$

Thus

$$\sup_j (m_j - \frac{L}{\bar{n}_p})^2 \ \leq\ \sum_{i=1}^{\bar{n}_p}(m_j - \frac{L}{\bar{n}_p})^2 \ \leq\ 2\varepsilon^2\frac{\pi^2}{h_p^2}L.$$

>From (4.17) we also see that

$$\sup_j m_j\alpha_j^2 \ \leq\ \sum_{j=1}^{\bar{n}_p} m_j\alpha_j^2 \ \leq\ \frac{\pi^2}{h_p^2}L.$$

Combining these, we deduce that $m_j\alpha_j^2 \geq \frac{L}{\bar{n}_p}\alpha_j^2 - O(\varepsilon)$ for every j. Hence

$$q_0((m_j),(\alpha_j),(\ell_j)) \geq \frac{L^2}{\bar{n}_p} + \sum_{j=1}^{\bar{n}_p} c(\pi - \ell_j\alpha_j)^{+\ 6} + 2\varepsilon^2\frac{L}{\bar{n}_p}\alpha_j^2 - C\varepsilon^3.$$

It now suffices to show

$$q_1((\alpha_j),(\ell_j)) := \sum_{j=1}^{\bar{n}_p} c(\pi - \ell_j\alpha_j)^{+\ 6} + 2\varepsilon^2\frac{L}{\bar{n}_p}\alpha_j^2 \ \geq\ 2\varepsilon^2\frac{\pi^2}{h_p^2}L - C\varepsilon^{2/5}. \tag{4.18}$$

To do this, let $(\alpha_j^*),(\ell_j^*)$ minimize q_1 subject to the constraint $\sum \ell_j^* = \bar{n}_p h_p$. Clearly $q_1((\alpha_j^*),(\ell_j^*)) \leq 2\varepsilon^2\frac{\pi^2}{h_p^2}L$, which implies that $\pi - \ell_j\alpha_j \leq C\varepsilon^{1/3}$. Since $\ell_j \leq \sum \ell_j = C$, it follows that $\alpha_j \geq C > 0$ for all j.

The first-order optimality conditions for $(\alpha_j^*),(\ell_j^*)$ are

$$6c\left(\pi - \ell_j^*\alpha_j^*\right)^{+\,5}\ell_j = 4\varepsilon^2\frac{L}{\bar{n}_p}\alpha_j^* \qquad 6c\left(\pi - \ell_j^*\alpha_j^*\right)^{+\,5}\alpha_j^* = \lambda$$

for all j, where λ is a Lagrange multiplier. These imply that $4\varepsilon^2\frac{L}{\bar n_p}\alpha_j^{*\ 2} = \lambda\ell_j^*$, and hence that

$$6c\left(\pi - \frac{4\varepsilon^2}{\lambda}\frac{L}{\bar n_p}\left(\alpha_j^*\right)^3\right)^{+5}\alpha_j^* = \lambda. \tag{4.19}$$

We also deduce that

$$\lambda\bar n_p h_p = \sum_j \lambda\ell_j^* = 4\varepsilon^2\frac{L}{\bar n_p}\sum_j a_j^{*\,2} = O(\varepsilon^2).$$

which implies that $\lambda = O(\varepsilon^2)$. For $\lambda > 0$, the equation $6c(\pi - \frac{4\varepsilon^2}{\lambda}\frac{L}{\bar n_p}x)^{+5}x = \lambda$ has at most two roots, say $x_- < x_+$. Since $\lambda = O(\varepsilon^2)$, one of these roots must $x_- = O(\varepsilon^2)$. However, we have already shown that $\alpha_j \geq C$ for all j, and so it follows that $\alpha_j^* = x_+$ for every j. In particular, all α_j^* are equal, which implies that all λ_j^* are equal. Thus $\lambda_j^* = h_p$ for all j. It follows that

$$q_1((\alpha_j),(\ell_j)) \geq \bar n_p \inf_\alpha\left[c(\pi - h_p\alpha)^{+6} + 2\varepsilon^2\frac{L}{\bar n_p}\alpha^2\right]$$

Now it is easy to deduce (4.18). □

Proof of Theorem 1.3. **1. upper bound**: We define a one-parameter family of test functions v_h, and we then optimize over h. Let

$$v_h(x) = \begin{cases} \sqrt{\frac{2L}{h\bar n_p}}\sin(\frac{\pi}{h}(x - x_i)) & \text{if } x \in (x_i, x_i + h) \\ & \quad\text{for some } i \in \{0,\dots\bar n_p - 1\} \\ 0 & \text{if not}\end{cases}$$

where $\bar n_p$ and x_i are defined by

$$\bar n_p = \lceil L\rceil - 1, \qquad x_i = i(1 + h_p), \qquad h_p = \frac{1}{\bar n_p}(L - \bar n_p).$$

The assumption that $L > 2$ implies that $\frac12 < \frac{L}{\bar n_p} \leq 1$. We have normalized v_h so that $⨍_{\mathcal D} v_h^2\,dx = 1$. We easily see that

$$\|v_h'\|_{L^2}^2 = \left(\frac{\pi}{h}\right)^2\|v_h\|_{L^2}^2 = \left(\frac{\pi}{h}\right)^2 L. \tag{4.20}$$

Let $h_p = \frac{1}{\bar n_p}(L - \bar n_p)$. If $h \leq h_p$ then components of the support of v_h are separated by distance at least 1, and so

$$F(|v_h|^2) = \min_{\mathcal M_{ac}} F = F(u_p) = L^2/\bar n_p \tag{4.21}$$

On the other hand, if $h > h_p$, then for $x \in (0,h)$,

$$V * v_h^2(x) = \int_0^h v_h^2 dx = L/\bar n_p \quad \text{ if } h_p - h \leq x < h_p,$$

since then $\{y \in \operatorname{supp} u : x-1 < y < x+1\} = (0,h)$. If $h_p < x < h$ say, then $x+1 \le 1+h$, so

$$V * v_h^2(x) \le \int_0^h v_h^2 dx + \int_{1+h_p}^{1+h} v_h^2 dx \le \frac{L}{\bar{n}_p} + C\frac{(h-h_p)^3}{h^3}.$$

The same bound holds for $0 < x < h - h_p$. On these intervals, v_h^2 is bounded by $C(h-h_p)^2/h^3$, so

$$\begin{aligned}\int_0^h V * v_h^2 \cdot v_h^2 dx &\le \frac{L}{\bar{n}_p}\int_0^h v_h^2 + C\frac{(h-h_p)^3}{h^3}\int_{(0,h-h_p)\cup(h,h_p)} v_h^2\, dx \\ &\le \left(\frac{L}{\bar{n}_p}\right)^2 + C\frac{(h-h_p)^6}{h^6}.\end{aligned}$$

Summing the contributions from different components of the support of v_h, we find that

$$E_\varepsilon(v_h) \le \frac{1}{4\varepsilon^2}\left[\frac{L^2}{\bar{n}_p} + Cn_p\frac{[(h-h_p)^+]^6}{h^6}\right] + \frac{\pi^2}{2h^2}L. \tag{4.22}$$

where $(h-h_p)^+ = \max\{0, h-h_p\}$. Let h_ε minimize the right-hand side of (4.22). One can then check by calculus that $h_\varepsilon - h_p \approx \varepsilon^{2/5}$ and that $E_\varepsilon(v_{h_\varepsilon}) \le E_\varepsilon(u_p) - c\varepsilon^{2/5}$, proving the upper bound.

2. lower bound. Let u_ε denote a minimizer of E_ε in $H^1_{per}(\mathcal{D})$ which satisfies the hypotheses of Lemma 4.1. For $i = 1,\ldots,\bar{n}_p$, let $I_j = (y_j, y_{j+1})$, where $y_j = \frac{1}{2}(x_j + x_{j+1}) + h/2$. Thus each y_i is the midpoint between two adjacent maxima of u_p, and each I_i is centered at a max of u_p. We will use the notation

$$m_j = \int_{I_j} u_\varepsilon^2\, dx, \qquad F_{ij} := \iint_{I_i\times I_j} V(x-y)u_\varepsilon^2(x)u_\varepsilon^2(y)\, dx\, dy$$

so that $\int_{\mathcal{D}} V * u^2 \cdot u^2 dx = \sum_{i,j} F_{ij}$. Note that for every j,

$$F_{jj} = m_j^2 - \iint_{\{x,y\in I_j\times I_j\ :\ |x-y|\ge 1\}} u_\varepsilon^2(x)u_\varepsilon^2(y)\, dx\, dy \ge m_j^2 - Ce^{-C/\varepsilon}$$

by Lemma 4.1. Also, clearly $F_{ij} = 0$ if $|i-j| \ge 2$. For each j, we define an interval $K_j \subset I_j \cup I_{j+1}$ such that $|K_j| = 1$ and

$$\int_{K_j^-} u_\varepsilon^2\, dx \;=\; \int_{K_j^+} u_\varepsilon^2\, dx \;=\; \frac{1}{2}\int_{K_j} u_\varepsilon^2\, dx =: \frac{1}{2}\kappa_j,$$

where $K_j^- := K_j \cap I_j$ and $K_j^+ := K_j \cap I_{j+1}$. Since $V(x-y) = 1$ if $x \in K_j^- \subset I_j$ and $y \in K_j^+ \subset I_{j+1}$, we see that

$$F_{j+1,j} = F_{j,j+1} \geq \left(\int_{K_j^-} u_\varepsilon^2(x)dx \right) \left(\int_{K_j^+} u_\varepsilon^2(y)dy \right) = \frac{1}{4}\kappa_j^2.$$

Thus

$$\begin{aligned} \int_{\mathcal{D}} V * u_\varepsilon^2 \cdot u_\varepsilon^2 dx \ &\geq \ \sum_j (m_j^2 + \frac{1}{2}\kappa_j^2) - Ce^{-C/\varepsilon} \\ &\geq \ \sum_j [m_j^2 + \frac{1}{2}(\frac{\kappa_{j-1}+\kappa_j}{2})^2] - Ce^{-C/\varepsilon}. \end{aligned} \tag{4.23}$$

Note also that

$$\frac{1}{2}(\kappa_{j-1} + \kappa_j) = \int_{K_{j-1}^+} u_\varepsilon^2\, dx + \int_{K_j^-} u_\varepsilon^2\, dx = m_j - \int_{J_j} u_\varepsilon^2\, dx. \tag{4.24}$$

for $J_j := I_j \setminus (K_{j-1}^+ \cup K_j^-)$. We now change a little bit the function u_ε in order to have $u_\varepsilon \in H_0^1(I_j)$, so that, extending it by 0 outside I_j, we may apply Lemma 4.2. Indeed, recall that, according to Lemma 4.1, $u_\varepsilon(y_j) \leq Ce^{-C/\varepsilon}$. Hence, one can find an affine function v such that

$$\|v\|_{W^{1,\infty}(I_j)} \leq Ce^{-\frac{C}{\varepsilon}}, \quad u_\varepsilon + v \in H_0^1(I_j).$$

Hence, denoting by w_ε the function equal to $u_\varepsilon + v$ in I_j and 0 elsewhere, we apply Lemma 4.2 to w_ε, finding that

$$\int_{J_j} w_\varepsilon^2 \leq m \left[1 - c\left(\pi - |J_j|\sqrt{\frac{k}{m}} \right)^{+\ 3} \right],$$

where

$$k = \int_{\mathbb{R}} (w_\varepsilon')^2, \quad m = \int_{\mathbb{R}} w_\varepsilon^2.$$

Hence, using the fact that $\|w_\varepsilon - u_\varepsilon\|_{W^{1,\infty}(I_j)} \leq Ce^{-C/\varepsilon}$ and that the function $s \mapsto (\pi - s)^{+\ 3}$ is uniformly continuous on $\mathbb{R}^+$, we have

$$\int_{J_j} u_\varepsilon^2\, dx \leq m_j \left[1 - c(\pi - |J_j|\alpha_j)^{+3}\right] + Ce^{-\frac{C}{\varepsilon}} \quad \text{for } \alpha_j = \left(\frac{1}{m_j} \int_{I_j} (u_\varepsilon')^2\, dx \right)^{1/2}. \tag{4.25}$$

We combine (4.24) and (4.25) and substitute into (4.23) to obtain

$$\int_{\mathcal{D}} V * u_\varepsilon^2 \cdot u_\varepsilon^2 dx \ \geq \ \sum_j \left[m_j^2 + c(\pi - |J_j|\alpha_j)^{+6} \right] - Ce^{-C/\varepsilon}.$$

Since $\int_{\mathcal{D}}(u_\varepsilon')^2\,dx = \sum_j m_j\alpha_j^2$, we finally conclude that

$$E_\varepsilon(u_\varepsilon) \geq \sum_j \left[\frac{1}{4\varepsilon^2}\left(m_j^2 + c(\pi - |J_j|\alpha_j)^{+6}\right) + \frac{1}{2}m_j\alpha_j^2\right] - Ce^{-C/\varepsilon}. \tag{4.26}$$

Note that $\sum m_j = |\mathcal{D}| = L$, and $\sum |J_j| = L - \bar{n}_p = \bar{n}_p h_p$. This last fact follows from the fact that $\mathcal{D} = \cup_{j=1}^{\bar{n}_p}(J_j \cup K_j)$, since $|K_j| = 1$ for every j and the union is disjoint. Thus the lower bound follows from Lemma 4.3. □

5. Minimizers of E_ε for large ε

We give in this section the

Proof of Proposition 1.2. Let us first point out that

$$\omega_d = \|V\|_{L^1} = (V * 1)(x), \quad \forall x \in \mathcal{D}.$$

This will be useful in the sequel.

Fix $u \in H^1_{per}(\mathcal{D})$ such that $\int |u|^2 = |\mathcal{D}|$, and write $u = 1 + h$. We may assume that $u \geq 0$, since $E_\varepsilon(|u|) \leq E_\varepsilon(u)$. Hence, $h \geq -1$ and

$$\int_{\mathcal{D}}(2h + h^2)\,dx = \int_{\mathcal{D}}(1+h)^2\,dx \; - \; \int_{\mathcal{D}} 1\,dx \; = \; 0.$$

Using this fact, one easily checks that

$$\begin{aligned} E_\varepsilon(u) - E_\varepsilon(1) &= \int_{\mathcal{D}} \frac{1}{2}|\nabla h|^2 dx \; + \frac{1}{4\varepsilon^2}\left[V * (1+h)^2 \cdot (1+h)^2 - V * 1 \cdot 1\right] dx \\ &= \int_{\mathcal{D}} \frac{1}{2}|\nabla h|^2 dx \; + \frac{1}{4\varepsilon^2}\int_{\mathcal{D}} V * (2h + h^2)\cdot(2h+h^2)\; dx. \end{aligned}$$

Note also that

$$\begin{aligned} &\frac{1}{4}\int_{\mathcal{D}} V * (2h+h^2)\cdot(2h+h^2)\; dx \\ &\qquad = \int_{\mathcal{D}} V * h \cdot h + V * h \cdot h^2 + \frac{1}{4}V * h^2 \cdot h^2\,dx \\ &\qquad = \int_{\mathcal{D}} V * h \cdot h \; + \; V * (1 + h/2)^2 \cdot h^2 - V * 1 \cdot h^2\,dx \\ &\qquad \geq \int_{\mathcal{D}} V * h \cdot h\,dx \; - \; \omega_d \|h\|^2_{L^2}, \end{aligned}$$

hence

$$E_\varepsilon(u) - E_\varepsilon(1) \geq \int_{\mathcal{D}} \frac{1}{2}|\nabla h|^2 dx \; + \frac{1}{\varepsilon^2}\int_{\mathcal{D}} V * h \cdot h\,dx \; - \; \frac{1}{\varepsilon^2}\omega_d\|h\|^2_{L^2}. \tag{5.1}$$

We are now going to prove that if (1.15) holds, then the right-hand side of (5.1) is non-negative, and vanishes only when $h \equiv 0$. We will do this using Fourier series, and we first fix notation: for $f \in L^2(\mathcal{D})$ we write

$$\widehat{f}(n) := \frac{1}{L^d}\int_{\mathcal{D}} f(x) e^{-i\pi n\cdot x/L}\, dx$$

so that

$$f(x) = \sum_{\mathbb{Z}^d} \widehat{f}(n) e^{i\pi n\cdot x/L}.$$

We have the usual identities, which scale in L as follows:

$$\int_{\mathcal{D}} f(x)\overline{g(x)}\, dx \; = L^d \sum_{\mathbb{Z}^d} \widehat{f}(n)\overline{\widehat{g}(n)},$$

$$\widehat{(f*g)}\ (n) = L^d \widehat{f}(n)\ \widehat{g}(n),$$

Using these we check that

$$\text{(5.2)}\quad \frac{1}{2}\int_{\mathcal{D}} |\nabla h|^2\, dx + \frac{1}{\varepsilon^2}\int_{\mathcal{D}} V*h\cdot h\, dx \; = \; L^d \sum_{\mathbb{Z}^d}\left(\frac{\pi^2}{2}\frac{|n|^2}{L^2} + \frac{L^d}{\varepsilon^2}\widehat{V}(n)\right)|\widehat{h}(n)|^2.$$

Next, we write $\mathcal{F}V(\xi) = \int_{\mathbb{R}^d} V(x)e^{-ix\cdot\xi}\, dx$ for the Fourier transform on $\mathbb{R}^d$, so that $\mathcal{F}V(n\pi/L) \; = \; L^d\widehat{V}(n)$. Since V is even and nonnegative,

$$\begin{aligned}\mathcal{F}V(\xi) &= \int_{\mathbb{R}^d}\frac{1}{2}(V(x)+V(-x))e^{-ix\cdot\xi}\, dx = \int_{\mathbb{R}^d} V(x)\frac{1}{2}\left[e^{-ix\cdot\xi}+e^{ix\cdot\xi}\right]\, dx \\ &= \int_{\mathbb{R}^d} V(x)\ \cos(x\cdot\xi)\, dx = \int_{\{|x|<1\}} \cos(x\cdot\xi)\, dx.\end{aligned}$$

In particular,

$$L^d\widehat{V}(n) \geq \omega_d \inf_{|s|\leq |n|\pi/L} \cos s \geq \omega_d\left(1 - \frac{\pi^2}{2}\frac{|n|^2}{L^2}\right).$$

It follows from this, (5.2) and (5.1) that

$$\begin{aligned} E_\varepsilon(u) - E_\varepsilon(1) \;&\geq\; L^d \sum_{\mathbb{Z}^d}\left[\frac{\pi^2|n|^2}{2L^2} + \frac{\omega_d}{\varepsilon^2}\left(1-\frac{\pi^2|n|^2}{2L^2}\right) - \frac{\omega_d}{\varepsilon^2}\right]|\widehat{h}(n)|^2 \\ &=\; L^d \sum_{\mathbb{Z}^d}\left[\frac{\pi^2|n|^2}{2L^2}\left(1-\frac{\omega_d}{\varepsilon^2}\right)\right]|\widehat{h}(n)|^2 \\ &\geq\; 0,\end{aligned}$$

with equality iff $h \equiv 0$. This completes the proof of the proposition. □

Remark 5. In the preceding proof, we have used an exact decomposition of the energy of $1+h$. However, the crucial point is that $u \equiv 1$ is a critical point of E_ε under the constraint $\int u^2 = |\mathcal{D}|$, and that the second derivative of E_ε is positive definite for ε sufficiently large. Under this condition, using the fact that the minimizer of u_ε converges to 1 as ε tends to infinity, it is possible to argue by contradiction and prove that there exists $\varepsilon_1 > 0$ such that for any $\varepsilon > \varepsilon_1$, the unique minimizer is $u \equiv 1$. However, this kind of proof does not give any information on ε_1. In particular, ε_1 may depend on L.

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