MINIMIZING THE GROUND STATE ENERGY OF AN ELECTRON IN A RANDOMLY DEFORMED LATTICE

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Abstract

We provide a characterization of the spectral minimum for a random Schrödinger operator of the form $H = -\Delta + \sum_{i\in\mathbb{Z}^d} q(x-i-\omega_i)$ in $L^2(\mathbb{R}^d)$, where the single site potential q is reflection symmetric, compactly supported in the unit cube centered at 0, and the displacement parameters ω_i are restricted so that adjacent single site potentials do not overlap. In particular, we show that a minimizing configuration of the displacements is given by a periodic pattern of densest possible 2^d-clusters of single site potentials.

The main tool to prove this is a quite general phenomenon in the spectral theory of Neumann problems, which we dub "bubbles tend to the boundary." How should a given compactly supported potential be placed into a bounded domain so as to minimize or maximize the first Neumann eigenvalue of the Schrödinger operator on this domain? For square or rectangular domains and reflection symmetric potentials, we show that the first Neumann eigenvalue is minimized when the potential sits in one of the corners of the domain and is maximized when it sits in the center of the domain. With different methods we also show a corresponding result for smooth strictly convex domains.

1. Introduction and Main Results

1.1. **The Displacement Model.** The one electron model of solid state physics describes the behavior of a single electron moving under the presence of an exterior force generated by the effective potentials of a fixed configuration of nuclei in a solid. Also disregarding electron-electron interactions, this results in the one-electron Schrödinger operator

$$H = -\Delta + V$$

in $L^2(\mathbb{R}^d)$, where $-\Delta$ and V are the kinetic and potential energy of the particle, respectively.

Typically one chooses a potential V that effectively models the characteristics of a particular solid. For example, one might use a periodic potential to model a crystal or other well ordered substance. While for a material containing a sufficient number of impurities, or disorder, one might use a random potential. In this paper we consider a potential generated by identical atoms or ions located at the points $i+\omega_i$, $i\in\mathbb{Z}^d$, i.e.

$$V_\omega(x) = \sum_{i\in\mathbb{Z}^d} q(x-i-\omega_i).$$

We refer to q as the *single site potential* and consider real valued single site potentials $q\in L^\infty$ which are reflection symmetric, i.e. symmetric in each variable with the remaining variables fixed, and compactly supported in the unit cube $\Lambda_0 := (-\frac{1}{2},\frac{1}{2})^d$ of $\mathbb{R}^d$, i.e. supp $q\subset[-r,r]^d\subset$

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Λ_0, $r < 1/2$. We denote the collection of displacements by $\omega = \{\omega_i\}_{i\in\mathbb{Z}^d}$, where each $\omega_i \in [-d_{max}, d_{max}]^d$. Finally we choose $r + d_{max} = \frac{1}{2}$, which insures that adjacent single site potentials in the sum above do not overlap.

For any possible collection of displacements ω,

$$H(\omega) := -\Delta + V_\omega \tag{1}$$

with domain $H^2(\mathbb{R}^d)$, the second order Sobolev space, defines a self adjoint operator in $L^2(\mathbb{R}^d)$. We will refer to the family $H(\omega)$ as the *displacement model*. As V is uniformly bounded with respect to ω, the spectrum of $H(\omega)$, $\sigma(H(\omega))$, is uniformly bounded from below.

The question we will address is the following: How can one characterize

$$E_0 := \inf_\omega \inf \sigma(H(\omega)), \tag{2}$$

i.e. the infimum of the ground state energy of $H(\omega)$ for all possible nuclear configurations ω? In particular, is there a minimizing configuration ω^{min} such that

$$\inf \sigma(H(\omega^{min})) = E_0, \tag{3}$$

and how does it look like?

Our main result is the answer to this question:

Theorem 1.1. *A minimizing configuration ω^{min} for the ground state energy of $H(\omega)$ in the sense of* (3) *is given by*

$$\omega_i^{\min} = ((-1)^{i_1} d_{max}, \dots, (-1)^{i_d} d_{max}) \tag{4}$$

for all $i = (i_1, \dots, i_d) \in \mathbb{Z}^d$.

The energy minimizing potential $V_{\omega^{min}}$ is 2-periodic in each coordinate and given by the densest possible cluster of the nuclei in the period cell $(-\frac{1}{2}, \frac{3}{2})^d$, namely all single site potentials within the cluster move as close to the center $(\frac{1}{2}, \dots, \frac{1}{2})$ of the period cell as possible, see Figure 1. Thus, by Floquet-Bloch theory [20], E_0 is the lowest eigenvalue of $-\Delta + V_{\omega^{min}}$

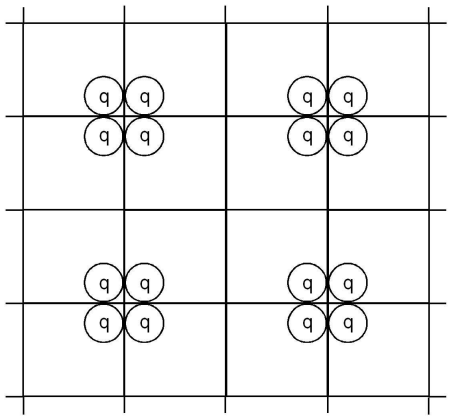

FIGURE 1. The support of $V_{\omega^{min}}$ for $d = 2$ and radially symmetric f.

restricted to $L^2((-\frac{1}{2}, \frac{3}{2})^d)$ with periodic boundary conditions. Due to the symmetry of the 2^d-cluster this is the same as the ground state energy of $-\Delta + q(x - (d_{max}, \dots, d_{max}))$ on $L^2(\Lambda_0)$ with Neumann boundary conditions. For $d = 1$ Theorem 1.1 has been conjectured and partially proven in [17].

Our interest in this result is mostly motivated by the case where the displacements ω_i, $i \in \mathbb{Z}^d$, are independent, identically distributed $\mathbb{R}^d$-valued random variables with $[-d_{max}, d_{max}]^d$ as the support of their common distribution μ. In this case we refer to $H(\omega)$ as the *random displacement model*, which is ergodic with respect to shifts in $\mathbb{Z}^d$. Thus its spectrum is almost surely deterministic, i.e. there exists $\Sigma \subset \mathbb{R}$ such that

$$\sigma(H(\omega)) = \Sigma \quad \text{for a.e. } \omega,$$

e.g. [4].

Compared to other prominent models of random Schrödinger operators, e.g. the Anderson model or Poisson model, few rigorous results are known for the random displacement model. This is mostly due to the fact that $H(\omega)$ does not depend monotonically (in form sense) on the random parameters ω_i. Even the structure of the almost sure spectrum Σ is unclear. It can be said that

$$\Sigma = \overline{\bigcup_{\omega \in C_{per}} \sigma(H(\omega))}, \tag{5}$$

where C_{per} is the set of all configurations $\omega : \mathbb{Z}^d \to \operatorname{supp} \mu$ which are periodic with respect to some sublattice of $\mathbb{Z}^d$. This follows by adapting the proof of the corresponding result for Anderson models, given e.g. in [14].

A consequence of Theorem 1.1 is

Corollary 1.2. *The infimum of the almost sure spectrum of the random displacement model is given by*

$$\inf \Sigma = E_0 = \inf \sigma(H(\omega^{min})).$$

Proof. This follows from (5) since $\omega^{min} \in C_{per}$ and, by Theorem 1.1, $\inf \sigma(H(\omega^{min})) \leq \inf \sigma(H(\omega))$ for all other $\omega \in C_{per}$. □

Note that, at least for sign-definite q, the answer to the same question for the Anderson or Poisson model is quite straightforward and found by considerations involving not much more than minimizing the potential energy: For the Anderson model, $\inf \Sigma$ is found by choosing all random couplings minimal. For the Poisson model one has $\inf \Sigma = 0$ if $q \geq 0$ and $\inf \Sigma = -\infty$ if $q \leq 0$. In fact, the latter, with few exceptions, only requires that the negative part of q doesn't vanish [1]. For the Anderson model with sign-indefinite q the description of Σ or just $\inf \Sigma$ causes difficulties similar to those for the random displacement model. Najar [18] has a result for this case in the small coupling regime, proven by perturbative arguments.

What makes our result, as well as the techniques in its proof, rather interesting is that minimizing the spectrum in the displacement model requires an understanding of the interaction between kinetic and potential energy. Physically, one can understand our result best for the case of negative potential wells q. In this case the formation of clusters of 2^d sites allows for states with low potential energy without sacrificing much kinetic energy. But we stress that Theorem 1.1 and Corollary 1.2 hold without any sign-restriction on q.

For the multi-dimensional random displacement model it is not yet known if the spectrum is localized, in the sense of being pure point, near the bottom of the spectrum. This is in contrast to the situation for Anderson and Poisson models. For the Anderson model this is a long standing result, with the hardest case of Bernoulli distributed random couplings recently settled in [2]. The new type of multi scale analysis introduced in [2] was now also used to prove the corresponding fact for the Poisson model in arbitrary dimension [9, 10]. For the one-dimensional displacement model, localization at all energies was proven in [3] and, with

different methods and under more general assumptions, in [5]. The only available result on localization for the multi-dimensional displacement model is Klopp's work [15], establishing the existence of a localized region for the semiclassical version $-h^2\Delta + V_\omega$ of (1) if h is sufficiently small.

Theorem 1.1 should serve as a first step towards understanding the spectral type of $-\Delta+V_\omega$ near $\inf\Sigma$ by identifying the periodic configuration in which $\inf\Sigma$ is attained. An important further step towards localization would be to quantify probabilistically how many other configurations have ground states close to $\inf\Sigma$, that is, to prove smallness of the integrated density of states (IDS) near $\inf\Sigma$ (or a related finite volume property). To this end it is interesting to note that for $d = 1$ the configuration given by (4) (in this case "dimerization") is only one of many minimizing periodic configurations. This will have interesting consequences for the IDS. In particular, one may not find the Lifshitz tail behavior familiar from Anderson and Poisson models and the exact asymptotics may depend strongly on the displacement distribution μ. However, we believe that, under suitable assumptions on q suggested by our proof of Theorem 1.1, in $d \geq 2$ the configuration (4) is the unique periodic minimizer. We plan to investigate this further in a separate work.

1.2. **Bubbles tend to the boundary.** Theorem 1.1 amounts to optimizing the infinitely many parameters ω_i, $i \in \mathbb{Z}^d$, with respect to minimizing the spectrum. Surprisingly, as will be shown in Section 3, its proof can be reduced to the following spectral optimization result in just one parameter.

Theorem 1.3. *Let q be as above, i.e. bounded, reflection symmetric, and supported in $[-r, r]^d$ for some $r < \frac{1}{2}$. Let $d_{max} = \frac{1}{2} - r$ and for $a \in [-d_{max}, d_{max}]^d$ let $H^N_{\Lambda_0}(a) := -\Delta + q(x - a)$ in $L^2(\Lambda_0)$ with Neumann boundary conditions on $\partial\Lambda_0$ and denote the ground state energy of $H^N_{\Lambda_0}(a)$ by $E_0(a)$. Then we have the following alternative: Either*

(i) *$E_0(a)$ is strictly maximized at $a = 0$ and strictly minimized in the 2^d corners $(\pm d_{max}, \dots, \pm d_{max})$ of $[-d_{max}, d_{max}]^d$*

or

(ii) *$E_0(a)$ is identically zero. In this case the corresponding eigenfunction is constant outside of the support of q.*

In fact, in will show that in case (i) the function $E_0(a)$ is partially strictly decreasing away from the origin, i.e. that whenever all but one of the variables $(a_1, \dots, a_d)$ are fixed, then $E(a_1, \dots, a_d)$ is strictly decreasing for the remaining variable in $[0, 1/2 - r]$ and, by symmetry, strictly increasing in $[-1/2 + r, 0]$.

A sufficient, but far from necessary condition for case (i) to hold is that q has fixed sign and does not vanish identically, as in this case $E_0(a)$ never vanishes. Case (ii) happens if the Neumann problem for $-\Delta + q$ on the support of q has lowest eigenvalue 0. Non-vanishing q with this property are easily constructed.

We find Theorem 1.3 quite interesting for its own sake, independent of its application to prove Theorem 1.1. It is a prototype of what seems to be a very general phenomenon appearing for Neumann problems on bounded domains, namely that "bubbles tend to the boundary". To this end, we have the following result for general strictly convex smooth domains and smooth potentials, proven in Section 5 with a method very different from the one we use in Section 4 to prove Theorem 1.3.

Consider an open, bounded domain $D \subset \mathbb{R}^d$ with smooth boundary. We shall assume that D is *strictly convex*. Let $q(x)$ be any bounded smooth potential whose support is a subset of D. For $a \in \mathbb{R}^d$ let $q_a(x) := q(x-a)$. In D consider the Schrödinger operator

$$H_D^N(a) = -\Delta + q_a$$

with Neumann boundary conditions on ∂D (where restriction of q_a to D is implied). We denote its ground state energy by $E_0(a)$. As shown in Lemma 2.1 of Section 2, $E_0(a)$ is continuous in a.

Denote by $G \subset \mathbb{R}^d$ the collection of vectors a such that q_a has its support also in D. Note that G is an open set.

Theorem 1.4 (Strong minimum principle for E_0). *If $E_0(a_0) = \inf_{a\in G} E_0(a)$ for some $a_0 \in G$, then $E_0(a)$ is identically zero. In this case the wave function is constant outside the support of the potential. In other words if $E_0(a)$ does not vanish identically in G, then $E_0(a_0) > \inf_{a\in G} E_0(a)$ for all $a_0 \in G$.*

The continuous function $E_0 : \overline{G} \to \mathbb{R}$ must assume its minimum. By Theorem 1.4, if $E_0(a)$ does not vanish identically, the minimum must be assumed on ∂G. In the same situation Theorem 1.3 gives the more precise result that the minimum is assumed in the corners of $\overline{G} = [-d_{max}, d_{max}]^d$.

For radially symmetric q and various types of domains D, the question of minimizing the first *Dirichlet*-eigenvalue of $-\Delta + q_a$ on D is well studied, see [12] for disks and regular polygons, or [11] for a more general class of domains which have a certain reflection property with respect to the symmetry axes of the potential.

Common to all results for Dirichlet problems is that the maximizing and minimizing positions depend on the sign of the potential. For an *obstacle* $q \geq 0$ (or "$q = \infty$", meaning a hole in the domain marked by an additional Dirichlet boundary condition) the maximizing position is in the "center" of the domain, while the first eigenvalue is minimized when the obstacle is in contact with the boundary. The reverse is true for the case of a well $q \leq 0$. As pointed out in [11], this is most easily understood, if not proven, by a perturbative argument: Consider $-\Delta + \lambda q$ on D with Dirchlet boundary condition. Its lowest eigenvalue $E_0(\lambda)$ satisfies

$$E_0'(0) = \int_D q|u_0|^2\, dx, \tag{6}$$

where u_0 is the ground state eigenfunction of the Dirichlet Laplacian. Thus $E_0(\lambda)$ changes the most (least), if q is placed where u_0 is largest (smallest), which is near the center (boundary) of D. The sign of q determines the sign of E_0' and thus reverses the role of maximizer and minimizer.

This motivation through first order perturbation theory fails for the Neumann problem. In this case (6) still applies, but the ground state of the Neumann Laplacian is constant and thus $E_0'(0)$ is independent of the placement of q. This explains why the Neumann version of the problem is more subtle than the Dirichlet problem (roughly by one order of perturbation theory). Consequently, the methods used in [12] and [11] do not extend to give similar results for the Neumann case. An exception is a remark in [12] concerning infinite spherical obstacles in spherical domains. The only other work on the Neumann case, which we found in the literature, is [16], which gives perturbative and numerical results concerning the optimal configurations of small Dirichlet holes in planar domains for maximizing the first Neumann eigenvalue.

We indeed use a second order perturbation theory formula as the starting point of the proof of Theorem 1.4, see (25) below. Our proof of Theorem 1.3 doesn't use perturbation theory, but Floquet-Bloch theory, the variational characterization of ground states, and unique continuation of harmonic functions). Still, the result may be motivated by second order perturbation theory:

In $d = 2$ (for simplicity) consider the Neumann problem $-\Delta + \lambda q$ on $L^2((-\frac{1}{2}, \frac{1}{2})^2, dxdy)$. The lowest eigenvalue $E_0(\lambda)$ satisfies the second order perturbation formula

$$E_0''(0) = -2 \sum_{k>0} \frac{(u_0, qu_k)^2}{E_k - E_0}, \tag{7}$$

where E_k and u_k are the higher eigenvalues and eigenfunctions of the Neumann-Laplacian, see Section 2.3. Considering only the leading term of (7), corresponding to $E_1 = E_2 = \pi^2$, we get

$$-\frac{4}{\pi^2} \left[\left(\int q(x,y) \sin(\pi x)\, dx\, dy \right)^2 + \left(\int q(x,y) \sin(\pi y)\, dx\, dy \right)^2 \right],$$

which is negative, independent of the sign of q. If $q = q_a$, with q_0 reflection symmetric and of fixed sign, then both integrals are zero for $a = 0$, and both integrals become maximal (in absolute value) if a is located near one of the four corners $(\pm\frac{1}{2}, \pm\frac{1}{2})$. Again, this is independent of the sign of q.

2. Preliminaries

Throughout this section $\Omega \subset \mathbb{R}^d$ will be open and bounded. The Neumann Laplacian $-\Delta_\Omega^N$ on Ω is the unique selfadjoint operator whose quadratic form is

$$\int_\Omega |\nabla f(x)|^2\, dx$$

for f in the domain $H^1(\Omega)$, the first order Sobolev space.

2.1. Continuity of Eigenvalues.

Assume that Ω satisfies the H^1-extension property, i.e. there exists a bounded operator $E : H^1(\Omega) \to H^1(\mathbb{R}^d)$ such that $(Ef)(x) = f(x)$ for all $f \in H^1(\Omega)$ and almost every $x \in \Omega$. Note that a sufficient condition for this is that Ω has Lipschitz boundary, e.g. Theorem V.4.12 of [6].

Let $q \in L^\infty(\mathbb{R}^d)$ be real-valued and define $q_a(x) = q(x - a)$ for all $a \in \mathbb{R}^d$. Let $H_\Omega^N(a) = -\Delta_\Omega^N + q_a$.

Lemma 2.1. *$H_\Omega^N(a)$ has purely discrete spectrum consisting of eigenvalues $E_0(a) \le E_1(a) \le \ldots \le E_n(a)$, counted with multiplicity, where all functions E_n are continuous in a.*

Proof. Fix $C > \|q\|_\infty$. From the extension property of Ω and boundedness of q it follows that $(-\Delta_\Omega^N + C)^{-1}$ and $(H_\Omega^N(a) + C)^{-1}$ are compact, e.g. Theorem V.4.13 of [6]. Thus $H_\Omega^N(a)$ has purely discrete spectrum $E_0(a) \le E_1(a) \le \ldots$. It remains to show that $(H_\Omega^N(a)+C)^{-1}$ is norm-continuous in a. Continuity of the eigenvalues of $(H_\Omega^N(a) + C)^{-1}$, and thus the eigenvalues of $H_\Omega^N(a)$, then follows from the min-max-characterization of eigenvalues.

Without restriction, consider continuity at $a = 0$. For any $p \in (d, \infty)$ with $p \ge 2$ one has, e.g. Theorem 4.1 of [21],

$$\begin{aligned} \|\chi_\Omega(q_a - q)(-\Delta + C)^{-1/2}\| &\le (2\pi)^{-d/p} \|\chi_\Omega(q_a - q)\|_p \|(|\cdot|^2 + C)^{-1/2}\|_p \\ &\to 0 \quad \text{as } a \to 0. \end{aligned} \tag{8}$$

As $E : H^1(\Omega) \to H^1(\mathbb{R}^d)$ is bounded, it follows that $(-\Delta + C)^{1/2} E (-\Delta_\Omega^N + C)^{-1/2}$ is bounded from $L^2(\Omega)$ to $L^2(\mathbb{R}^d)$. Combined with (8) this yields

$$\|\chi_\Omega(q_a - q)(-\Delta_\Omega^N + C)^{-1/2}\| \to 0 \quad \text{as } a \to 0. \tag{9}$$

Norm-continuity of $(H_\Omega^N(a) + C)^{-1}$ at $a = 0$ now follows from (9), boundedness of $(-\Delta_\Omega^N + C)^{1/2}(H_\Omega^N(0) + C)^{-1/2}$ and the resolvent identity

$$(H_\Omega^N(a) + C)^{-1} - (H_\Omega^N(0) + C)^{-1} = (H_\Omega^N(a) + C)^{-1}\chi_\Omega(q_a - q)(H_\Omega^N(0) + C)^{-1}.$$

□

2.2. **Positivity and non-degeneracy of the ground state.** We will frequently use that for the domains considered by us and bounded potentials q the ground state energy E_0 of $H = -\Delta_\Omega^N + q$ is non-degenerate and that the corresponding eigenfunction can be chosen strictly positive. This generally holds if, in addition to the assumptions from Section 2.1, Ω is connected. The latter guarantees that the ground state energy 0 of $-\Delta_\Omega^N$ is non-degenerate ($-\Delta_\Omega^N \varphi = 0$ implies that $\int_\Omega |\nabla\varphi|^2\, dx = 0$, i.e. $\nabla\varphi \equiv 0$ and thus φ constant by connectedness). Non-degeneracy and positivity of the ground state of H follows from the general theory of positivity preserving operators provided in Section XIII.12 and the following Appendix 1 of [20].

2.3. **Perturbation formulas.** For completeness, let us briefly recall the derivation of the eigenvalue perturbation formulas which we use in our arguments. Most significantly, this will be the first and second order perturbation formulas (31) and (25) with respect to displacements of the potential in Section 5. However, they follow in the same way as the corresponding formulas for coupling constant dependence, e.g. (7), so we will focus on the latter.

Let Ω and q satisfy the assumptions of the previous two subsections, $H(\lambda) = -\Delta_\Omega^N + \lambda q$, $E_k = E_k(\lambda)$ its eigenvalues ordered by $E_0 < E_1 \leq E_2 \leq \dots$ and $u_k = u_k(\cdot, \lambda)$ corresponding real normalized eigenfunctions. Then

$$E_0'(\lambda) = (u_0, q u_0) \tag{10}$$

and

$$E_0''(\lambda) = -2 \sum_{k>0} \frac{(u_0, q u_k)^2}{E_k - E_0}\,. \tag{11}$$

The formulas (31) and (25) below follow with the same argument, using smoothness of q and differentiating separately with respect to each component of a (the extra term $(u_0, (\Delta q_0) u_0)$ in (25) does not appear in (11) as $\partial_\lambda^2(\lambda q) = 0$).

The equation (10) is the classical Feynman-Hellmann formula, derived by using non-degeneracy of E_0 (and thus analyticity of E_0 and u_0 in λ) and the fact that $(u_0, \partial_\lambda u_0) = 0$. Differentiating (10) and using completeness of the u_k we get

$$\begin{aligned} E_0''(\lambda) &= 2(\partial_\lambda u_0, q u_0) \\ &= 2 \sum_{k>0} (q u_0, u_k)(\partial_\lambda u_0, u_k), \end{aligned} \tag{12}$$

noticing that the $k = 0$ term vanishes. Differentiating the eigenvalue equation $-\Delta u_0 + \lambda q u_0 = E_0 u_0$ yields, for every $k > 0$,

$$q u_0 = (E_0 - E_k)\partial_\lambda u_0 + (u_0, q u_0) u_0 - (-\Delta + \lambda q - E_k)\partial_\lambda u_0,$$

and thus

$$\partial_\lambda u_0 = \frac{qu_0 - (u_0, qu_0)u_0 + (-\Delta + \lambda q - E_k)\partial_\lambda u_0}{E_0 - E_k}\,. \tag{13}$$

After noting that $((-\Delta + \lambda q - E_k)\partial_\lambda u_0, u_k) = 0$, (11) follows from inserting (13) into (12).

3. Theorem 1.3 implies Theorem 1.1

Theorem 1.3 says that $\inf_a E_0(a) = E_0(a^{min})$, where a^{min} corresponds to one of the 2^d corners of the the cube $[-d_{max}, d_{max}]^d$, say $a^{min} := (d_{max}, \dots, d_{max})$. Once we know this, then the central ideas of the proof of Theorem 1.1 are (i) Neumann bracketing to go from $H(\omega)$ to operators of the type $H^N_{\Lambda_0}(a)$ and (ii) extending the ground state of the minimizer $H^N_{\Lambda_0}(a^{min})$ to $\mathbb{R}^d$ by repeated reflection.

Proof. (of Theorem 1.1) For any given configuration ω, the restriction of $H(\omega)$ to the unit cube centered at $i \in \mathbb{Z}^d$ with Neumann boundary conditions is unitarily equivalent (via translation by i) to $H^N_{\Lambda_0}(\omega_i)$, defined as in Theorem 1.3. Thus, by Neumann bracketing and Theorem 1.3,

$$\begin{aligned}
\inf \sigma(H(\omega)) &\geq \inf \sigma\left(\bigoplus_{i\in\mathbb{Z}^D} H^N_{\Lambda_0}(\omega_i)\right) \\
&\geq \inf\left\{E_0(a) :\, a \in [-d_{max}, d_{max}]^d\right\} \\
&= E_0(a^{min}).
\end{aligned}$$

This holds for arbitrary configurations ω and thus, by (2), $E_0 \geq E_0(a^{min})$.

Now consider $\omega^{min} = (\omega_i^{min})_{i\in\mathbb{Z}^d}$ as given by (4). The corresponding potential

$$V_{\omega^{min}}(x) = \sum_{i\in\mathbb{Z}^d} q(x - i - \omega_i^{min})$$

is 2-periodic in x_i for each i. By Floquet-Bloch theory [20] the bottom of the spectrum of $H(\omega^{min}) = -\Delta + V_{\omega^{min}}$ is given by the smallest eigenvalue E_0^{per} of its restriction to $\Lambda_0^2 := (-\frac{1}{2}, \frac{3}{2})^d$ with periodic boundary conditions, see Figure 2.

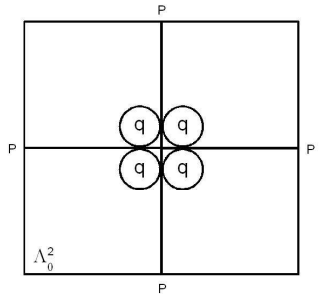

Figure 2. The period cell of $V_{\omega^{min}}$ in $d = 2$.

On Λ_0^2 the potential $V^{\omega^{min}}$ is symmetric with respect to all hyperplanes $x_i = 1/2$, $i = 1, \dots, d$. Thus E_0^{per} coincides with the smallest eigenvalue of the Neumann problem on Λ_0^2. Again by symmetry of the potential, the latter coincides with the smallest eigenvalue of the Neumann problem on Λ_0. As $\omega_0^{min} = (d_{max}, \dots, d_{max}) = a^{min}$, this eigenvalue is $E_0(a^{min})$. In summary we have shown that

$$E_0 \leq \inf \sigma(H(\omega^{min})) = E_0(a^{min}) \leq E_0.$$

Thus $E_0 = \inf \sigma(H(\omega^{min}))$, which proves Theorem 1.1. □

4. Proof of Theorem 1.3

This entire section is devoted to prove Theorem 1.3. Thus we work under the assumptions that $q \in L^\infty$ is real-valued, non-vanishing, reflection symmetric and supported in $[-r, r]^d$, $r < 1/2$.

Suppose that alternative (ii) of Theorem 1.3 is false. We will show that this implies that alternative (i) must hold.

We begin by fixing all of the components of the displacement parameter except for one, which may be chosen to be the first, and consider the lowest Neumann eigenvalue as a function only of the first coordinate, i.e. $E_0(a) := E_0(a, a_2, \dots, a_d)$. We note that $E_0(a)$ depends continuously on a (see Lemma 2.1) and that by symmetry we have

$$E_0(-a) = E_0(a).$$

For this reason we will restrict ourselves to the case $a \in [0, \frac{1}{2} - r]$ and show that

$$E_0(a_1) > E_0(a_2) \quad \text{for } 0 \le a_1 < a_2 \le 1 - r. \tag{14}$$

As the same holds for E_0 as a function of each other coordinate, we conclude from this that E_0 has a strict maximum at the origin and strict minima at the corners $(\pm d_{max}, \dots, \pm d_{max})$, i.e. we are in the situation of alternative (i).

As $(a_2, \dots, a_d)$ will be kept fixed, we will use the (slightly sloppy) abbreviation $q(x) := q(x_1, x_2 - a_2, \dots, x_d - a_d)$ for the rest of the section. For a scalar a and $e_1 = (1, 0, \dots, 0)$ we then write $q_a(x) = q(x - ae_1)$, a notation to be used also for functions other than q. By ∂_n we will denote the exterior normal derivative on the boundary of a given domain.

Lemma 4.1. *$E_0(0) > E_0(a)$ for every $a \in [0, \frac{1}{2} - r]$.*

Proof. Define the tube $L := \{x : |x_i| < \frac{1}{2}, i = 2, \dots, d\}$ and construct a periodic extension, $q_{per}(x)$, of the potential $q(x)$ on L by

$$q_{per}(x) = \sum_{i \in \mathbb{Z}} q_i(x).$$

We consider the Neumann problem on L for $-\Delta + q_{per}(x)$, see Figure 3. Let ψ denote

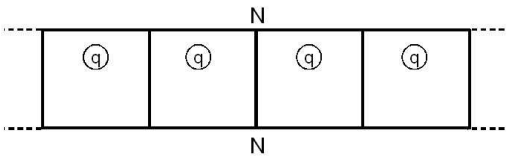

Figure 3. Periodic extension, $q_{per}(x)$, of $q(x)$

the normalized Neumann ground state of $-\Delta + q(x)$ on the unit cube Λ_0. Construct a new function Ψ on the tube L by periodically extending ψ on all of L. Symmetry of the potential implies that Ψ is a smooth solution of

$$-\Delta\Psi(x) + q_{per}(x)\psi(x) = E_0(0)\Psi(x) \tag{15}$$

on all of L. Now multiply (15) by $\Psi(x)$. Then over any unit cell C in L, periodicity of Ψ implies we may integrate by parts without creating boundary terms. In particular, this holds for the unit cell $\Lambda_a := \Lambda_0 - ae_1$, yielding

$$E_0(0) = \int_{\Lambda_a} \left(|\nabla \Psi(x)|^2 + q_{per}(x)\Psi^2(x) \right) dx. \tag{16}$$

Shifting to the right by a does not affect the result of equation (16), i.e.

$$\begin{aligned} E_0(0) &= \int_{\Lambda_0} \left(|\nabla \Psi_a(x)|^2 + q_{per}(x - ae_1)\Psi_a^2(x) \right) dx \\ &= \int_{\Lambda_0} \left(|\nabla \Psi_a(x)|^2 + q_a(x)\Psi_a^2(x) \right) dx. \end{aligned} \tag{17}$$

While $\Psi_a(x)$ does not satisfy Neumann boundary conditions on Λ_0, it is still in the form domain $H^1(\Lambda_0)$ of the Neumann operator $-\Delta + q_a(x)$ on Λ_0. Therefore, minimizing the right hand side of equation (17) over all normalized functions in $H^1(\Lambda_0)$ it is clear $E_0(0) \geq E_0(a)$.

To show that indeed $E_0(0)$ is strictly greater than $E_0(a)$ it suffices to show that, when restricted to Λ_0, Ψ_a is not equal to a multiple of the Neumann ground state eigenfunction corresponding to the potential q_a on Λ_0. Suppose, for contradiction, that Ψ_a was such a multiple. Then by construction the box $B = (-\frac{1}{2}, -\frac{1}{2} + a) \times (-\frac{1}{2}, \frac{1}{2})^{d-1}$ is disjoint from the support of the potential and Ψ_a satisfies the equation

$$-\Delta \Psi_a = E_0(0)\Psi_a \tag{18}$$

with Neumann conditions on the boundary of B. As $\Psi_a > 0$, it is the ground state of the Neumann problem on B. Thus $E_0(0) = 0$ and Ψ_a must be constant on B. This entails that Ψ_a is harmonic outside the support of the potential, and since it is constant on an open subset, by unique continuation of harmonic functions it must be constant everywhere outside the support of the potential. However this implies that alternative (ii) must hold, a contradiction. Thus $E_0(0) > E_0(a)$. □

Lemma 4.2. *For any positive integer n and $a \in (0, \frac{1}{2} - r]$, $E_0(na) > E_0((n+1)a)$ so long as $(n+1)a$ is less than or equal to $\frac{1}{2} - r$.*

Proof. To keep notations simple, we first show this for $n = 1$. Again consider the tube $L := \{x : |x_i| < \frac{1}{2}, i = 2, \ldots, d\}$. Fix a with $0 < 2a \leq \frac{1}{2} - r$ and consider a 2-periodic extension, w_{per}, of the potential

$$w(x) := q_a(x) + q_{-a+1}(x) \tag{19}$$

on L given by

$$w_{per}(x) := \sum_{i \in \mathbb{Z}} w_{2i}(x).$$

As before we consider the Neumann problem on L for $-\Delta + w_{per}(x)$, see Figure 4, and let ψ denote the Neumann ground state of $-\Delta + q_a(x)$ on the unit cube Λ_0, normalized to $\|\psi\|^2 = \frac{1}{2}$. Construct a new function Ψ on all of L by 2-periodically extending $\psi(x_1, x_2, \ldots, x_d) + \psi(-x_1 + 1, x_2, \ldots, x_d)$.

Symmetry and periodicity of the potential implies that Ψ is a smooth solution of

$$-\Delta \Psi(x) + w_{per}(x)\Psi(x) = E_0(a)\Psi(x)$$

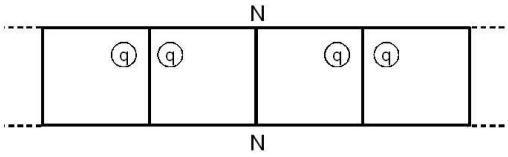

FIGURE 4. Periodic extension, $W_{per}(x)$, of $w(x) := w_a(x) + w_{-a+1}(x)$

on all of L. Now we proceed in analogy to (16) and (17), this time considering cells of length 2 instead of unit cells and again shifting by a to the right. We find

$$\begin{aligned} E_0(a) &= \int_{\{x\in L: -\frac{1}{2}-a<x_1<\frac{3}{2}-a\}} \left(|\nabla\Psi(x)|^2 + w_{per}(x)\Psi(x)^2\right) dx \\ &= \int_{\{x\in L: -\frac{1}{2}<x_1<\frac{3}{2}\}} \left(|\nabla\Psi_a(x)|^2 + (q_{2a}(x)+q_1(x))\Psi_a^2(x)\right) dx. \end{aligned} \tag{20}$$

As above we conclude that $E_0(a)$ is not smaller than the first Neumann eigenvalue $\tilde{E}$ of $-\Delta + q_{2a} + q_1$ on $\{x \in L : -\frac{1}{2} < x_1 < \frac{3}{2}\}$. A further application of the argument in the last paragraph of the proof of Lemma 4.1 shows that Ψ_a restricted to the unit 2 cell $\{x \in L : -\frac{1}{2} < x_1 < \frac{3}{2}\}$ is not a multiple of the ground state eigenfunction corresponding to $\tilde{E}$. Thus $E_0(a)$ is strictly greater than $\tilde{E}$.

Imposing an additional Neumann condition at $x_1 = \frac{1}{2}$ can not increase the lowest eigenvalue, thus

$$E_0(a) > \tilde{E} \geq \min\{E_0(2a), E_0(0)\} = E_0(2a)$$

by Lemma 4.1, which concludes the proof for $n = 1$. The crucial idea which allowed us to reduce the $n = 1$ claim to Lemma 4.1 was that the term q_{-a+1} in (19) was shifted back into the center of the cube $\{x \in L : \frac{1}{2} < x_1 < \frac{3}{2}\}$ in (20). The same mechanism can now be used to inductively prove the claim for all n. □

We can now readily complete the proof of (14): As a above was arbitrary, Lemma 4.2 implies that $E_0(a)$ is strictly decreasing on the set of all dyadic numbers in $[0, \frac{1}{2} - r]$. As this set is dense in $[0, \frac{1}{2} - r]$ and $E_0(a)$ is continuous, then $E_0(a)$ is strictly decreasing on all of $[0, \frac{1}{2} - r]$. Therefore assuming (ii) is false, (i) must be true.

5. Proof of Theorem 1.4

In Theorem 1.4 it is assumed that the domain and the potential are smooth. Thus we have by elliptic regularity that $C^\infty(\overline{D})$ is a form core for the Neumann operator $H_D^N(a) = -\Delta_D^N + q_a$. Moreover, the eigenfunctions are all in $C^\infty(\overline{D})$ and have normal derivative zero on ∂D.

We call the eigenvalues $E_k(a)$, ordered and accounting for multiplicity, and the normalized eigenfunctions $u_k(x; a)$, $k = 0, 1, \ldots$. We choose the ground state u_0 strictly positive and all other u_k real. They form an orthonormal basis in $L^2(D)$. Thus, for any function $f \in H^1(D)$ we have that

$$\sum_{k=0}^{\infty} E_k(u_k, f)^2 = \int_D \left[|\nabla f(x)|^2 + q_a(x) f(x)^2\right] dx \ , \tag{21}$$

where $(\cdot, \cdot)$ denotes the inner product on $L^2(D)$. Note that f is not in the domain of the operator, just in the form domain. See [20] and [7].

Let N denote the outward normal vector field on ∂D. It will be convenient to use that N can be extended to a smooth vector field in a neighborhood of ∂D. To see this, first work in a neighborhood of a fixed point of the surface. Without loss (i.e. up to a rigid motion) we can choose this point to be the origin and the surface to be given by

$$x_d = f(x_1, \dots, x_{d-1}) \tag{22}$$

in a vicinity of the origin, where f is smooth,

$$f(0, \dots, 0) = 0 \quad \text{and} \quad \nabla f(0, \dots, 0) = 0 \ . \tag{23}$$

Thus at a point $p = (x_1, \dots, x_{d-1}, f(x_1, \dots, x_{d-1}))$ near 0 one has

$$N(p) = \frac{(-\nabla f(x_1, \dots, x_{d-1}), 1)}{|(-\nabla f(x_1, \dots, x_{d-1}), 1)|} \ .$$

This can be extended smoothly to $x = (x_1, \dots, x_{d-1}, x_d)$ near 0 by

$$N(x) = N(x_1, \dots, x_{d-1}, f(x_1, \dots, x_{d-1})).$$

We get a global extension of N to a neighborhood of ∂D by using compactness of ∂D and a standard partition of unity argument.

In this neighborhood we define the matrix-valued smooth vector field $K = (K_{ij}) = (\partial_i N_j)$. The restriction of K to ∂D is the curvature matrix of the surface. Indeed, in the local coordinates used above, we have

$$\partial_i N_j(0) = \begin{cases} -(\partial_i \partial_j f)(0) & \text{if } 1 \le i, j \le d-1, \\ 0 & \text{if } i = d \text{ or } j = d. \end{cases}$$

We have assumed that D is strictly convex. This means that the Hessian of f is negative definite and thus at every $p \in \partial D$ the restriction of $K(p)$ to the tangent plane at p is positive definite.

The following identity for $E_0(a)$ is the main technical ingredient into our proof. Here ΔE_0 and ∇E_0 refer to the a-derivatives of E_0. Otherwise, all symbols such as ∂_i, ∇, Δ denote derivatives with respect to the spatial variable. $B(\cdot, \cdot)$ is the bilinear form

$$B(u, v) = (u, \Delta v) - (\Delta u, v).$$

Lemma 5.1 (**Second order perturbation theory**). *The ground state energy satisfies the equation*

$$\Delta E_0 - 4(u_0, \nabla u_0)\nabla E_0 = -2 \int_{\partial D} \nabla u_0 \cdot K \nabla u_0 \, dS - 2 \sum_{k \neq 0} \frac{\sum_i B(u_k, \partial_i u_0)^2}{E_k - E_0} \ . \tag{24}$$

Proof. We start with the second order perturbation theory formula

$$\Delta E_0 = (u_0, (\Delta q_a) u_0) - 2 \sum_{k \neq 0} \frac{\sum_i (u_0, (\partial_i q_a) u_k)^2}{E_k - E_0}, \tag{25}$$

see Section 2.3. Differentiating the eigenvalue equation yields

$$(\nabla q_a) u_0 = E_0 \nabla u_0 - (-\Delta + q_a) \nabla u_0$$

and therefore

$$(u_k, (\nabla q_a) u_0) = -(E_k - E_0)(u_k, \nabla u_0) + B(u_k, \nabla u_0) \ . \tag{26}$$

Hence

$$\begin{aligned}\Delta E_0 &= (u_0,(\Delta q_a)u_0) - 2\sum_{k\neq 0}\left[(E_k-E_0)(\nabla u_0,u_k)^2 - 2(\nabla u_0,u_k)\cdot B(u_k,\nabla u_0)\right]\\ &\quad - 2\sum_{k\neq 0}\frac{\sum_i B(u_k,\partial_i u_0)^2}{E_k-E_0}\end{aligned}$$

which, using (26) once more, can be rewritten as

$$\begin{aligned}\Delta E_0 &= (u_0,(\Delta q_a)u_0) + 2\sum_{k\neq 0}[B(u_k,\nabla u_0)+(u_k,(\nabla q_a)u_0)]\cdot(u_k,\nabla u_0)\\ &\quad - 2\sum_{k\neq 0}\frac{\sum_i B(u_k,\partial_i u_0)^2}{E_k-E_0}\\ &= (u_0,(\Delta q_a)u_0) + 2\sum_{k}[B(u_k,\nabla u_0)+(u_k,(\nabla q_a)u_0)]\cdot(u_k,\nabla u_0)\\ &\quad - 2[B(u_0,\nabla u_0)+(u_0,(\nabla q_a)u_0)]\cdot(u_0,\nabla u_0)\\ &\quad - 2\sum_{k\neq 0}\frac{\sum_i B(u_k,\partial_i u_0)^2}{E_k-E_0}\\ &= (u_0,(\Delta q_a)u_0) + 2(\nabla u_0,(\nabla q_a)u_0) + 2\sum_{k} B(u_k,\nabla u_0)\cdot(u_k,\nabla u_0)\\ &\quad - 2[B(u_0,\nabla u_0)+(u_0,(\nabla q_a)u_0)]\cdot(u_0,\nabla u_0)\\ &\quad - 2\sum_{k\neq 0}\frac{\sum_i B(u_k,\partial_i u_0)^2}{E_k-E_0}\ ,\end{aligned}$$

where finally the completeness relation of the u_k was used. It is clear that

$$(u_0,(\Delta q_a)u_0) + 2(\nabla u_0,(\nabla q_a)u_0) = 0$$

and using again (26) with $k=0$ we can simplify further and get

$$\begin{aligned}\Delta E_0 &= 2\sum_{k} B(u_k,\nabla u_0)\cdot(u_k,\nabla u_0) - 4(u_0,(\nabla q_a)u_0)\cdot(u_0,\nabla u_0)\\ &\quad - 2\sum_{k\neq 0}\frac{\sum_i B(u_k,\partial_i u_0)^2}{E_k-E_0}\ .\end{aligned}\tag{27}$$

Recall that $B(u,v) = (u,\Delta v) - (\Delta v,u)$ and hence

$$\sum_k B(u_k,\nabla u_0)\cdot(u_k,\nabla u_0) = \sum_k[(u_k,\Delta\nabla u_0) - (\Delta u_k,\nabla u_0)]\cdot(u_k,\nabla u_0)\ .\tag{28}$$

Since $u_0\in C^\infty(\overline{D})$ we know that the vector $\Delta\nabla u_0$ has square integrable components and hence

$$\sum_k(u_k,\Delta\nabla u_0)\cdot(u_k,\nabla u_0) = (\nabla u_0,\Delta\nabla u_0)\ .$$

The second term of (28) we write as

$$\sum_k([-\Delta+q_a]u_k,\nabla u_0)\cdot(u_k,\nabla u_0) - \sum_k(q_a u_k,\nabla u_0)\cdot(u_k,\nabla u_0)\ .$$

The second sum equals $\sum_j (\partial_j u_0, q_a \partial_j u_0)$ while the first sum is

$$\sum_j \sum_k E_k(u_k, \partial_j u_0)^2 = \sum_j \int_D [|\nabla \partial_j u_0|^2 + q_a(x)(\partial_j u_0)^2] dx$$

since $\partial_j u_0$ is in the form domain. Collecting terms we find from (28) that

$$\begin{aligned} \sum_k B(u_k, \nabla u_0) \cdot (u_k, \nabla u_0) &= \sum_j [(\partial_j u_0, \Delta \partial_j u_0) + \|\nabla \partial_j u_0\|^2] \\ &= \sum_j \int_{\partial D} (\partial_j u_0) N \cdot \nabla(\partial_j u_0)\, dS, \end{aligned} \tag{29}$$

where Green's identity was used. On an open neighborhood of ∂D we have

$$\begin{aligned} \sum_j (\partial_j u_0) N \cdot \nabla(\partial_j u_0) &= \sum_j (\partial_j u_0) \partial_j N \cdot \nabla u_0 - \sum_{j,i} (\partial_j u_0)(\partial_j N_i)(\partial_i u_0) \\ &= \nabla u_0 \cdot \nabla(N \cdot \nabla u_0) - \nabla u_0 \cdot K \nabla u_0 \ , \end{aligned} \tag{30}$$

where K is the curvature matrix defined above. Using that $N \cdot \nabla u_0 = 0$ on ∂D one has that the first term is $\nabla_t u_0 \cdot \nabla_t (N \cdot \nabla u_0)$ for points in ∂D, where ∇_t denotes the component of the gradient in the tangential directions. However, $N \cdot \nabla u_0 = 0$ and smoothness of ∂D also implies $\nabla_t (N \cdot \nabla u_0) = 0$ and thus $\nabla u_0 \cdot \nabla (N \cdot \nabla u_0) = 0$ on ∂D. Thus (29) and (30) yield

$$\sum_k B(u_k, \nabla u_0) \cdot (u_k, \nabla u_0) = -\int_{\partial D} \nabla u_0 \cdot K \nabla u_0 \, dS.$$

After substituting this and the first order perturbation formula

$$\nabla E_0 = -(u_0, (\nabla q_a) u_0) \tag{31}$$

into (27) we arrive at (24). □

Lemma 5.2. *Assume that q is a smooth potential with compact support in D. Assume that the Neumann ground state $u_0(x; a)$ for some fixed $a_0 \in G$ is constant on ∂D. Then there exists an open neighborhood of a_0 where $E_0(a_0) \geq E_0(a)$.*

Proof. By shifting coordinates we assume that $a_0 = 0$. We shall proceed by a trial function argument. Consider the problem with the shifted potential $q_a(x) := q(x - a)$. Denote by $D_a = D + a$ the shifted domain, i.e., the function $u_a(x) := u_0(x - a; 0)$ solves $-\Delta u_a + q_a u_a = E_0(0) u_a$, with a Neumann boundary condition on ∂D_a as well as being constant on ∂D_a. We shall construct a trial function ϕ in the following fashion. In the intersection of D_a with D we set $\phi = u_a$ and in $D \backslash D_a$ we set ϕ to be a constant which equals the boundary value of u_a. Note that $\phi \in H^1(D)$. By the variational principle

$$E_0(a) \leq \frac{\int_D |\nabla \phi|^2 + q_a \phi^2 dx}{\int_D \phi^2 dx} \ .$$

For $a \in G$ the right side equals

$$\frac{\int_{D \cap D_a} |\nabla u_a|^2 + q_a u_a^2 dx}{\int_D \phi^2 dx} \leq \frac{\int_{D_a} |\nabla u_a|^2 + q_a u_a^2 dx}{\int_D \phi^2 dx} = E_0(0) \frac{\int_D u_0^2 dx}{\int_D \phi^2 dx} \ . \tag{32}$$

In the case $E_0(0) = 0$, this implies $E_0(a) \leq 0$, as was to be shown.

Next we claim that for a sufficiently small

$$\frac{\int_D u_0^2 dx}{\int_D \phi^2 dx} < 1$$

if $E_0(0) > 0$ and

$$\frac{\int_D u_0^2 dx}{\int_D \phi^2 dx} > 1$$

if $E_0(0) < 0$. This yields the lemma for the remaining cases. If we denote by c the boundary value of u_0 we find that the claim follows once we show that in a vicinity of the boundary, $u_0 < c$ for $E_0(0) > 0$ and $u_0 > c$ for $E_0(0) < 0$. To see this, fix a point on the boundary, call it the origin and use the local coordinates (22) and (23) above. The normal vector at 0 is $(0, \dots, 0, 1)$ and hence the normal derivative equals $\partial_d u_0(0) = 0$. Further, since u_0 is constant on the boundary we find by differentiating $u_0(x_1, \dots, x_{d-1}, f(x_1, \dots, x_{d-1})) \equiv c$ that

$$\partial_i \partial_j u_0(0) = -\partial_d u_0(0) \partial_i \partial_j f(0) = 0$$

for $i, j = 1, \dots d-1$. Hence

$$\partial_d \partial_d u_0(0) = \Delta u_0(0) = -E_0(0) u_0(0)$$

which is negative for $E_0(0) > 0$ and positive for $E_0(0) < 0$. As this holds at all points of the boundary, we get the required property of u_0 in a vicinity of the boundary. □

We remark that in the case $E_0(a_0) \neq 0$, the above proof actually gives the strict inequality $E_0(a_0) > E_0(a)$ for a close to a_0, i.e. $E_0(a_0)$ is a strict local maximum. This is the case, for example, if q is sign-definite, and allows for a shorter argument in the following completion of the proof of Theorem 1.4.

Proof of Theorem 1.4. Assume that E_0 attains its minimum value in G say at the point a_0. This entails that $\nabla E_0(a_0) = 0$ and $\Delta E_0(a_0) \geq 0$. Using the Lemma 5.1 we find that

$$\Delta E_0(a_0) = -2 \int_{\partial D} \nabla u_0 \cdot K \nabla u_0 \, dS - 2 \sum_{k \neq 0} \frac{\sum_i B(u_k, \partial_i u_0)^2}{E_k - E_0} \ .$$

The right side is non-positive, since D is convex. It cannot be strictly negative, since that would contradict the assumption that $E_0(a)$ has a local minimum at a_0.

Thus the right side must vanish. Since D is strictly convex, the first term can vanish only if u_0 is constant on the boundary (recall that K is positive definite on the tangent space at each point of ∂D and that ∇u_0 is a tangent vector). However, Lemma 5.2 shows that $E_0(a_0) \geq E_0(a)$ in a neighborhood of a_0. Thus $E_0(a) = E_0(a_0)$ in this neighborhood. Since the set where $E_0(a_0) = E_0(a)$ is closed and open in G (the above argument applies to every a with $E_0(a_0) = E_0(a)$) the function $E_0(a)$ must be constant. Assuming now that $E_0(a)$ is constant, u_0 is constant on the boundary and moreover, there must be equality in (32). This means that

$$\int_{D_a \backslash D} |\nabla u_a|^2 dx = 0 \ .$$

Hence u_a must be constant in $D_a \backslash D$ and therefore, for small a, $0 = -\Delta u_a = E_0(a) u_a$ there. Thus, $E_0(a) \equiv 0$. Since the support of q_a is a subset of D (as $a \in G$), u_a is constant in the non-empty open set $D_a \backslash \overline{D}$, which is disjoint from the support of q_a. Since it is harmonic outside the support of q_a it must be constant there too. It follows that u_0 is constant outside the support of q. □

6. Discussion: Extensions and open problems

We conclude with some remarks about possible generalizations and open problems related to our main results.

(i) Theorem 1.3 and its proof immediately generalize to the Neumann problem on an arbitrary rectangular box $\{x : |x_i| < \ell_i, i = 1, \dots, d\}$ rather than the unit cube Λ_0, which we chose to keep notations simple. This also gives a corresponding version of Theorem 1.1, where $\mathbb{Z}^d$ is replaced by an arbitrary rectangular lattice.

(ii) In Theorems 1.1 and 1.3 we also may replace the obstacle q by an reflection symmetric hole with Dirichlet boundary conditions, often interpreted as an infinite barrier. More precisely, let $C \subset \{x : |x_i| < r, i = 1, \dots, d\}$ be closed and reflection symmetric. Let $C_a = C + a$ and $H_a^N := -\Delta$ on $\Lambda \setminus C_a$ with Neumann conditions on $\partial\Lambda$ and Dirichlet conditions on ∂C_a. Then $E_0(a)$ is minimized when the hole is in a corner of Λ_0 and $\inf \sigma(H(\omega))$ is minimized for a periodic configuration of 2^d-clusters of holes. While we expect that Theorem 1.4 also extends to this situation, at least for holes with smooth boundary, our proof does not extend directly.

(iii) Theorem 1.4 covers the situation of a radially symmetric potential (or Dirichlet hole) placed in a spherical domain, where all placements of q which touch the boundary are equivalent minimizing positions. However, in this case the methods of Lemma 5.2 may be used to also show that the maximal position occurs when the potential is centered in the domain.

To see this, suppose D is a spherical domain centered at 0 and let q be a radially symmetric potential compactly supported in D, also centered at 0. Radial symmetry of the domain and potential then imply the ground state eigenfunction, u_0, corresponding to $E_0(0)$ is radially symmetric. Thus it satisfies the conditions of Lemma 5.2. If $E_0(0) \geq 0$ one may show by reducing the problem to one dimension, or by using maximum principles, that outside the support of the potential $u_0 \leq c$, where c denotes the value of u_0 on the boundary of D. Similarly if $E_0(0) \leq 0$, $u_0 \geq c$ outside the support of the potential. One may conclude using the arguments of Lemma 5.2 that $E_0(0) \geq E_0(a)$ for every $a \in \overline{G}$. This then leads to the following alternative for the case of a spherical domain centered at 0 with radially symmetric potential: either $E_0(a) \equiv 0$, in which case the corresponding eigenfunction is constant outside the support of the potential *or* $E_0(a)$ assumes a strict maximum at $E_0(0)$ and strict minima when the support of the potential touches the boundary.

(iv) Theorems 1.3 and 1.4 are proven with very different methods and apply to mutually exclusive classes of domains (rectangular boxes vs strictly convex domains). It would be desirable to find a method of proof which covers both results, as this method would most likely also cover more general polygons and polyhedra. Particularly interesting cases would be equilateral triangles or hexagons, as they tile the plane and would lead to a corresponding extension of Theorem 1.1.

(v) One can view Theorem 1.1 as a mechanism in which the nuclei of a solid self-organize into a simple periodic pattern, given a density condition (exactly one site per cube). It would be wrong, in our opinion, to see this as a model for crystallization since the regularity of the pattern is to a large extend determined by the density condition. Real crystallization, however, cannot be explained by the interaction of one electron with nuclei alone. It is a many-body effect and the nuclear repulsion and, more importantly, the Pauli exclusion principle play a role. Further, one needs sufficiently many electrons, e.g., a half filled band. Indeed, there have been results in this direction in [13] for the Falicov-Kimball model, a variant of the Hubbard model where the nuclei are treated classically and sit on a lattice where the electrons hop. Crystallization was shown in [13] for the half filled band. In our model, without the density

condition, we expect that the nuclei would stick together. While this is an open question there is some evidence in this direction. For bosons it was shown in [13] that the nuclei indeed stick together.

It would be interesting to consider an extension of our model, a continuous analog of the Falicov-Kimball model, in which one considers a finite periodic array of cubes on a torus. Assuming the same number of spinless fermions as the number of cubes and assuming one nucleus in each cube, it is not unreasonable to expect that in an energy minimizing configuration the nuclei sit at the center of each cube. This is an interesting open question. Needless to say that the methods in this paper have no bearing on this problem. For an overview of the Falicov-Kimball model the reader may consult [8].

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