The spectral minimum for random displacement models

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Abstract

Consider a one-dimensional Schrödinger operator with potential V given as follows: Fix a *single site potential* f which is supported in an interval of length less than 1. Construct V by placing a translate of f into each unit interval $[n, n+1]$ for integer n, where otherwise the positions of each translate are arbitrary. Which configuration of single sites minimizes the spectral minimum of the Schrödinger operator with potential V? This question is equivalent to finding the spectral minimum of the random displacement model. We conjecture that the minimum is realized through *pair formation* of the single sites. We provide a partial proof of this conjecture and additional numerical evidence for its correctness.

Keywords: Random Schrödinger Operator, Spectral Theory

1 Introduction

The study of Schrödinger operators with random potentials has not only revealed the need for probabilistic tools in spectral theoretic investigations but also provided motivation for exploring numerous questions in the "classical" spectral theory of Schrödinger operators. The goal of this note is to discuss one such question that remains unsolved, even for the simplest case of one-dimensional Schrödinger operators. We formulate a conjecture on the solution of this problem and prove a partial result toward its verification. In addition, we present the results of numerical calculations, providing additional evidence for the correctness of our conjecture (the public domain software package SLEIGN2 by P. Bailey, N. Everitt and T. Zettl, available at math.niu.edu/ zettl/SL2/, was used for these calculations). We hope completion of the rigorous proof of our conjecture will be an interesting challenge for further research in this area.

1.1 The Model

Our basic object of study is the so-called *random displacement model*, a random Schrödinger operator of the form

$$H_\omega^D = -\frac{d^2}{dx^2} + \sum_{n\in\mathbb{Z}} f(x-n-d_n(\omega)) \tag{1}$$

in $L^2(\mathbb{R})$. We assume that the *single site potential* $f \neq 0$ is real-valued, compactly supported and locally integrable. Starting from the periodic potential $\sum_n f(x-n)$, the n-th potential site is displaced by $d_n(\omega)$, which are chosen to be independent and identically distributed (i.i.d.) random variables, each of them with distribution supported in the interval $[-d_{max}, d_{max}]$. The simplest way to realize this is to choose $d_n(\omega)$ as the n-th component ω_n of the random sequence $\omega = (\omega_n) \in [-d_{max}, d_{max}]^{\mathbb{Z}} =: \Omega$. Ω becomes a probability space with the infinite product measure $\mathbf{P} = \bigotimes_{n\in\mathbb{Z}} \mu^D$, where the Borel probability measure μ^D on $[-d_{max}, d_{max}]$ is the common distribution of the ω_n, i.e. $\mathbf{P}(\omega_n \in B) = \mu^D(B)$ for all Borel sets $B \subset [-d_{max}, d_{max}]$.

For simplicity we also assume that $\operatorname{supp} f \subset [-s, s]$, where $s + d_{max} \leq 1/2$. This means that the supports of adjacent terms in $\sum_n f(x-n-d_n(\omega))$ do not overlap. This also guarantees that the differential expressions on the r.h.s. of (1) are in limit point case at $\pm\infty$ for all ω. Thus they define unique self-adjoint operators in $L^2(\mathbb{R})$ in the sense of Sturm-Liouville theory (or through form methods), denoted by H_ω^D.

In fact, we are not dealing with a single Schrödinger operator, but with the rather large family of operators H_ω^D, indexed by the random parameter $\omega \in \Omega$. Nevertheless, it is known that the spectrum of H_ω^D is *almost surely deterministic*, i.e. there exists a set $\Sigma^D \subset \mathbb{R}$ such that

$$\sigma(H_\omega^D) = \Sigma^D \quad \text{for } \mathbf{P}\text{-almost every } \omega \in \Omega. \tag{2}$$

This follows from the general theory of ergodic operators, which applies to H_ω^D, e.g. [2].

1.2 Questions and known results

The two main spectral theoretic questions for H_ω^D are now: (1) What is the structure of the almost sure spectrum Σ^D? (2) What is the spectral type of H_ω^D, i.e. does its spectrum consist of eigenvalues, singular continuous spectrum or absolutely continuous spectrum?

One might expect that the first question is more elementary than the second question, and therefore that they should be answered in the given order. It is quite surprising that the opposite is true for the random displacement model. The second question has recently been answered in [1] (see also a remark in [6] on a proof under the most general assumptions): If the random variables are non-trivial, i.e. the support of μ contains at least two points, then almost surely the spectrum of H_ω^D is the closure of its eigenvalues and contains no continuous spectrum. On the other hand, not much is known about the structure of Σ^D.

To understand the reasons for this paradoxical situation better, let us compare the displacement model with the Anderson model, where more complete answers are known. The Anderson model (in its continuum form) is the random operator

$$H_\omega^A = -\frac{d^2}{dx^2} + \sum_{n\in\mathbb{Z}} q_n(\omega) f(x-n). \tag{3}$$

Randomness enters here through the random coupling constants $q_n(\omega)$, which are i.i.d. and whose support μ^A is supposed to be contained in a finite interval: $\operatorname{supp}\mu^A \subset [q_{min}, q_{max}]$. The single site potential f is as above with $\operatorname{supp} f \subset [-1/2, 1/2]$. It is again known that almost surely $\sigma(H_\omega^A) = \Sigma^A$, $\sigma(H_\omega^A)$ is the closure of its eigenvalues and no continuous spectrum exists (e.g. [2, 3]).

To study the structure of Σ^A and Σ^D we have the following basic result which covers both models (where $\overline{M}$ denotes the closure of a set M):

Theorem 1 *(a)*

$$\Sigma^A = \overline{\bigcup_{\{q_n\}\in S^A} \sigma\left(-\frac{d^2}{dx^2} + \sum_{n\in\mathbb{Z}} q_n f(x-n)\right)}, \tag{4}$$

where S^A is the set of all periodic sequences $\{q_n\}$ (with arbitrary period) such that $q_n \in$ supp μ^A for all n.

(b)

$$\Sigma^D = \overline{\bigcup_{\{d_n\}\in S^D} \sigma\left(-\frac{d^2}{dx^2} + \sum_{n\in\mathbb{Z}} f(x-n-d_n)\right)}, \tag{5}$$

where S^D is the set of all periodic sequences $\{d_n\}$ (with arbitrary period) such that $d_n \in$ supp μ^D for all n.

A proof of this result (based on Weyl sequences and elementary probabilistic arguments) for the case of the Anderson model can be found in [5]. The same methods can be used for the displacement model. Theorem 1 reduces the determination of the spectra of random Schrödinger operators to the case of periodic Schrödinger operators, but of course a rather large number of them, indexed by S^A and S^D, respectively. It shows that Σ^A and Σ^P have *band structure*, since this is known for periodic potentials. Of course, most gaps may be closed due to the large union which is to be taken.

For the Anderson model more can be said under additional assumptions:

Theorem 2 *If f has fixed sign, i.e. $f \geq 0$ or $f \leq 0$, and if supp $\mu^A = [q_{min}, q_{max}]$, then*

$$\Sigma^A = \bigcup_{q\in[q_{min},q_{max}]} \sigma\left(-\frac{d^2}{dx^2} + q\sum_{n\in\mathbb{Z}} f(x-n)\right). \tag{6}$$

In particular,

$$\inf \Sigma^A = \begin{cases} \inf\sigma\left(-d^2/dx^2 + q_{min}\sum_n f(x-n)\right) & \text{if } f \geq 0, \\ \inf\sigma\left(-d^2/dx^2 + q_{max}\sum_n f(x-n)\right) & \text{if } g \leq 0. \end{cases} \tag{7}$$

A particularly simple special case is given by $f = \chi_{[-1/2,1/2]}$, where $\Sigma^A = [q_{min}, \infty)$.

Theorem 2 is found in [5] and follows quite easily from Theorem 1(a). Let us sketch the argument: First, the constant sequences $\{q_n \equiv q \in \operatorname{supp} \mu^A\}$ are contained in S^A, and thus the r.h.s. of (6) is contained in Σ^A by (4). For the other inclusion, we may focus on the case $f \geq 0$ ($f \leq 0$ is easily reduced to this case). Let $\{q_n\} \in S^A$ be L-periodic and $[a, b]$ the k-th stability interval of the L-periodic operator $-d^2/dx^2 + \sum_n q_n f(x-n)$. Also let $[a_1, b_1]$ and $[a_2, b_2]$ be the k-th stability intervals of $-d^2/dx^2 + q_{min} \sum_n f(x-n)$ and $-d^2/dx^2 + q_{max} \sum_n f(x-n)$, both understood as L-periodic operators. By the variational principle we have $a_1 \leq a \leq a_2$ and $b_1 \leq b \leq b_2$. Since the stability intervals of $-d^2/dx^2 + q \sum_n f(x-n)$ depend continuously on q, it follows that $\sigma(-d^2/dx^2 + \sum_n q_n f(x-n))$ is contained in the r.h.s. of (6). Since the latter is closed, this completes the proof of (6). (7) follows immediately.

The above proof depends on a *monotonicity* property of the Anderson model: If, say, $f \geq 0$ and $q_n^{(1)} \geq q_n^{(2)}$ for all n, then $-d^2/dx^2 + \sum q_n^{(1)} f(x-n) \geq -d^2/dx^2 + \sum q_n^{(2)} f(x-n)$ in form sense. For this reason Theorem 2 does not extend to the random displacement models, since H_ω^D depends *non-monotonically* on the random variables d_n, even if f is assumed to be sign-definite. Particularly striking is the fact that $\inf \Sigma^A$ is quite easily characterized by (7), while it is far from clear how to characterize $\inf \Sigma^D$. It is the goal of the rest of this paper to study this problem, both theoretically and numerically.

1.3 Conjectures and a new result

Based on (5) it is natural to ask if there is a minimizer $\{d_n\} \in S^D$, i.e. a periodic sequence $\{d_n\}$ such that

$$\inf \Sigma^D = \inf \sigma \left(-\frac{d^2}{dx^2} + \sum_n f(x-n-d_n) \right). \tag{8}$$

The existence of a minimizer is not obvious, but would correspond to the Anderson model with sign-definite f, where the constant sequences $\{q_n = q_{min}\}$ and $\{q_n = q_{max}\}$, respectively, are minimizers. The answer to this question should to some extend depend on properties of f and $\operatorname{supp} \mu^D$. Under natural additional assumptions we state

Conjecture 1 *In addition to the previous assumptions let $f(x) \leq 0$ and $f(x) = f(-x)$ for all x and $\operatorname{supp} \mu^D = [-d_{max}, d_{max}]$. Then (8) is satisfied for the sequence $(d_n^{pair}) = (\dots, d_{max}, -d_{max}, d_{max}, -d_{max}, \dots)$.*

In other words: The energy in the random displacement model is minimized by *pair formation* of the single site potentials, meaning that adjacent displacements take values d_{max} and $-d_{max}$. Note that there are actually two sequences of the type (d_n^{pair}), depending on whether $d_0 = d_{max}$ or $d_0 = -d_{max}$).

If the conjecture is correct, then (d_n^{pair}) would minimize the spectrum of $-d^2/dx^2 + \sum_n f(x-n-d_n)$ not only within periodic sequences, but within all sequences (d_n) with $d_n \in [-d_{max}, d_{max}]$, $n \in \mathbb{Z}$. This can easily be seen by an argument using periodic approximations and strong resolvent convergence.

Unfortunately, we have only partial rigorous results towards the proof of Conjecture 1. To state them, define for $k \in \mathbb{N}$

$$\Sigma_k := \bigcup_{\{d_n\} \in S_k^D} \sigma\left(-\frac{d^2}{dx^2} + \sum_n f(x-n-d_n)\right), \tag{9}$$

where S_k^D are the k-periodic sequences within S^D. Thus we have $\Sigma^D = \overline{\bigcup_k \Sigma_k}$. We can prove that $\{d_n^{pair}\}$ is the unique minimizer within all 2-periodic sequences:

Theorem 3 *If $\{d_n\} \in S_2^D$ and $\{d_n\} \neq \{d_n^{pair}\}$, then*

$$\inf \sigma\left(-\frac{d^2}{dx^2} + \sum_n f(x-n-d_n)\right) > \inf \sigma\left(-\frac{d^2}{dx^2} + \sum_n f(x-n-d_n^{pair})\right). \tag{10}$$

In particular,

$$\inf \Sigma_2 = \inf \sigma\left(-\frac{d^2}{dx^2} + \sum_n f(x-n-d_n^{pair})\right). \tag{11}$$

The proof of Theorem 3 is presented in Section 2.

We believe that

$$\inf \Sigma_k \geq \inf \Sigma_2 \tag{12}$$

for all $k \geq 3$. Together with Theorem 1 this would imply Conjecture 1. Section 3 contains a discussion of numerical evidence for (12). In particular, we will provide evidence for

Conjecture 2 *If k is odd, then*

$$\inf \Sigma_k > \inf \Sigma_2. \tag{13}$$

Intuitively this can be explained by the idea that pair formation should be energetically optimal: An attempt of forming pairs out of an odd number of sites leaves one site "stranded".

It is obvious that for even $k = 2n$ one has $\inf \Sigma_{2n} \leq \inf \Sigma_2$, since a 2-periodic potential is also $2n$-periodic. Therefore Conjecture 1 means that $\inf \Sigma_{2n} = \inf \Sigma_2$. One may ask if a chain of n pairs is the unique minimizer of Σ_{2n} or if other configurations may give the same spectral minimum. The latter is the case. Already for $k = 4$ it turns out that a "pair-antipair-configuration" gives the same minimum, which is due to symmetries of the corresponding eigenfunctions. This is also discussed in Section 3.

While much of our interest in Conjecture 1 is based on mathematical and aesthetic reasons, we point out that its verification can also be seen as a first step toward physically motivated applications. One of them would be the study of so-called *Lifshitz tails of the density of states* near the bottom of the spectrum in the random displacement model. This phenomenon is well studied for the Anderson model (see e.g. [2, Section VI.2] for a recent review). The above mentioned differences between the Anderson and displacement models suggest that the latter might exhibit a weaker form of Lifshitz tails. In addition to characterizing the minimizing configurations for which $\inf \Sigma^D$ is obtained, this would also require to estimate the probability that restrictions of H_ω^D to finite intervals have eigenvalues below $\inf \Sigma^D + \varepsilon$, i.e. not only minimizing configurations, but also close-to-minimizing configurations need to be considered.

We finally mention that we have not looked at the multidimensional version of our problem, not even numerically. In dimension $d \geq 2$, H_ω^D is defined similarly as in (1), the displacements d_n are now vector-valued random variables. One may expect that pair formation should be replaced by *$2d$-cluster formation* as the energetically optimal configuration, but this will be even harder to prove than Conjecture 1.

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2 Pair formation for configurations of period 2

Let f satisfy all assumptions made in Theorem 3, i.e. $f \not\equiv 0$, $f \leq 0$, integrable, symmetric to the origin, and supported in $[-s, s]$ for some s with $s + d_{max} \leq 1/2$. If $\{d_n\} \in [-d_{max}, d_{max}]^{\mathbb{Z}}$ is 2-periodic, then the bottom of the spectrum of $H = -d^2/dx^2 + \sum_n f(x - n - d_n)$ is given by the smallest eigenvalue of the restriction of H to any interval of length 2 with periodic boundary conditions, see e.g. [4]. We see that our problem is reduced to minimizing $\inf \sigma(H_{b_1,b_2})$ over $(b_1, b_2) \in [1/2 - d_{max}, 1/2 + d_{max}]^2$, where

$$H_{b_1,b_2} = -\frac{d^2}{dx^2} + f(x - b_1) + f(x - 1 - b_2) \tag{14}$$

in $L^2(0, 2)$ with periodic boundary conditions. The use of periodic boundary conditions implies that $\inf \sigma(H_{b_1,b_2})$ only depends on the distance of the centers b_1 and $1 + b_2$. We may thus choose $b_1 = 1/2 + d$, $b_2 = 1/2 - d$ with a single parameter $d \in [-d_{max}, d_{max}]$, resulting in a potential which is symmetric to 1. Due to symmetry of the potential the ground state φ of the problem with periodic boundary conditions coincides with the ground state of the Neumann problem. Since also $\varphi'(1) = 0$ we see that $\inf \sigma(H_{1/2+d,1/2-d}) = \inf \sigma(H^N_{1/2+d})$, where

$$H_b^N = -\frac{d^2}{dx^2} + f(x - b) \tag{15}$$

on $L^2(0,1)$ with Neumann boundary conditions at 0 and 1. The ground state energy $\lambda_0(b)$ of H_b^N is symmetric with respect to $b = 1/2$. Since $1/2 + d_{max} \leq 1 - s$, Theorem 3 is a consequence of

Theorem 4 *The ground state energy $\lambda_0(b)$ of H_b^N is strictly decreasing for $b \in [1/2, 1-s]$.*

We will prove Theorem 4 through several Lemmas.

Lemma 1 *Let $1/2 < b \leq 1 - s$ be fixed, $E = \lambda_0(b)$ the smallest eigenvalue of H_b^N and u the corresponding eigenfunction normalized such that $u(0) = 1$. Then $u(1) > 1$.*

Proof: Since $E < 0$ there is $\alpha < 0$ such that $E = -\alpha^2$. Since u is the ground state we have $u(x) > 0$ for all $x \in [0,1]$ and (by a Sturm comparison argument) $u(x)^2 - u'(x)^2/\alpha^2 > 0$ for all $x \in [0,1]$. Thus we can introduce hyperbolic coordinates for $(u(x), u'(x))$, i.e. there are unique $a(x) \in (0, \infty)$ and $t(x) \in (-\infty, \infty)$ such that

$$u(x) = a(x) \cosh t(x), \quad u'(x)/\alpha = a(x) \sinh t(x). \tag{16}$$

Differentiating $a^2 = u^2 - (u'/\alpha)^2$ and $u'/u = \alpha \tanh t$ and using $u'' = (f_b(x) + \alpha^2)u$ (where $f_b(x) := f(x-b)$), we get first order differential equations for t and a:

$$\begin{aligned} t' &= \frac{f_b}{\alpha} \cosh^2 t + \alpha, & (17) \\ (\ln a)' &= -\frac{f_b}{2\alpha} \sinh(2t). & (18) \end{aligned}$$

Due to the Neumann boundary conditions we have $t(0) = t(1) = 0$. f_b vanishes on $[0, b-s]$ and $[b+s, 1]$. Thus we get from (17) that $t(b-s) = \alpha \cdot (b-s)$ and $t(b+s) = -\alpha \cdot (1-b-s)$, and, in particular,

$$t(b-s) + t(b+s) = \alpha \cdot (2b-1) > 0. \tag{19}$$

We will now show that

$$t(b-r) > -t(b+r) \quad \text{for all } r \in [0, s]. \tag{20}$$

Suppose on the contrary that $t(b-r_0) = -t(b+r_0)$ for some $r_0 \in [0, s]$. We get from (17) that

$$\begin{aligned} \frac{d}{dr} t(b-r) &= -\frac{f_b(b-r)}{\alpha} \cosh^2 t(b-r) - \alpha \\ &= -\frac{f(r)}{\alpha} \cosh^2 t(b-r) - \alpha & (21) \end{aligned}$$

and

$$\frac{d}{dr}(-t(b+r)) = -\frac{f(r)}{\alpha}\cosh^2(-t(b+r)) - \alpha. \tag{22}$$

Uniqueness of solutions of the corresponding initial value problem at $r = r_0$ implies $t(b-r) = -t(b+r)$ for all r, which for $r = s$ contradicts (19). Thus (20) is proven.

Integrating (17) we get

$$\begin{aligned}
\ln a(b+s) - \ln a(b-s) &= -\frac{1}{2\alpha}\int_{b-s}^{b+s} f_b(x)\sinh(2t(x))\,dx \\
&= \frac{1}{2\alpha}\int_0^s |f(r)|\left[\sinh(2t(b-r)) + \sinh(2t(b+r))\right]\,dr \\
&> 0.
\end{aligned} \tag{23}$$

Here we have used that by (20) $\sinh(2t(b-r)) + \sinh(2t(b+r)) > 0$ for all $r \in [0, s]$ and that $f \neq 0$. This implies the Lemma since $u(1) = a(1) = a(b+s)$ and $u(0) = a(0) = a(b-s)$. $\square$

The following lemma is of general nature. Denote by $t_y(x, \tau, q)$ and $a_y(x, \tau, q)$ the solutions of

$$t'(x) = \frac{q(x)}{\alpha}\cosh^2 t(x) + \alpha, \tag{24}$$

$$(\ln a(x))' = -\frac{q(x)}{2\alpha}\sinh(2t(x)), \tag{25}$$

with initial values at y given by $t_y(y, \tau, q) = \tau$ and $a_y(y, \tau, q) = 1$. Here q is a real-valued integrable function.

Lemma 2 *For fixed x such that (24) has a solution on $[y, x]$, one has*

$$\partial_\tau t_y(x, \tau, q) = \frac{1}{a_y(x, \tau, q)^2} \quad \textit{for a.e. } \tau. \tag{26}$$

Proof: By exchanging ∂_x and ∂_τ and using (24) we calculate

$$\begin{aligned}
\partial_x \partial_\tau t_y(x, \tau, q) &= \partial_\tau\left[\frac{q(x)}{\alpha}\cosh^2 t_y(x, \tau, q) + \alpha\right] \\
&= \frac{q(x)}{\alpha}\sinh(2t_y(x, \tau, q))\partial_\tau t_y(x, \tau, q) \\
&= -2(\ln a_y(x, \tau, q))'\partial_\tau t_y(x, \tau, q).
\end{aligned} \tag{27}$$

Since $a_y(y,\tau,q) = 1$ this implies $\ln \partial_\tau t_y(x,\tau,q) = -2\ln a_y(x,\tau,q)$, and therefore (26). In fact, under our assumptions ∂_x and ∂_τ only commute for almost every pair (x,τ). Thus, after x-integration of (27), one gets (26) for almost every τ. $\square$

For the next lemma we return to the specific situation of Theorem 4 and Lemma 1.

Lemma 3 *For almost every $b \in [1/2, 1-s]$ we have*

$$\frac{d}{db} t_0(1,0,f_b) = \alpha(a_0(1,0,f_b)^{-2} - 1) < 0. \tag{28}$$

Proof: Solving (17) successively from 0 to $b-s$, $b-s$ to $b+s$, and $b+s$ to 1, we get

$$\begin{aligned} t_0(1,0,f_b) &= t_{b+s}(1, t_{b-s}(b+s, t_0(b-s,0,0), f_b), 0) \\ &= t_{b+s}(1, t_{b-s}(b+s, \alpha(b-s), f_b), 0) \\ &= t_{b+s}(1, t_{-s}(s, \alpha(b-s), f_b), 0) \\ &= t_{-s}(s, \alpha(b-s), f) + \alpha(1-b-s). \end{aligned}$$

Also, by linearity of (18) and the fact that $a_0(x,0,f_b)$ stays constant on $[0,b-s]$ and $[b+s,1]$, we have

$$a_0(1,0,f_b) = a_{b-s}(b+s, \alpha(b-s), f_b) = a_{-s}(s, \alpha(b-s), f).$$

Thus by Lemma 2

$$\begin{aligned} \frac{d}{db} t_0(1,0,f_b) &= \alpha(a_{-s}(s,\alpha(b-s),f)^{-2} - 1) \\ &= \alpha(a_0(1,0,f_b)^{-2} - 1) \quad \text{for a.e. } b. \end{aligned}$$

The latter is negative since $a_0(1,0,f_b) = u(1)$, where u is as in Lemma 1, i.e. $u(1) > 1$. $\square$

We need a final lemma to study the α-dependence of the solutions (17) and (18), for which we write $t(x,b,\alpha)$ and $a(x,b,\alpha)$.

Lemma 4 *For every $\alpha > 0$ one has*

$$\begin{aligned} \partial_\alpha t(x,b,\alpha) &= a(x,b,\alpha)^{-2} \int_0^x \left(1 - \frac{f_b(y)}{\alpha} \cosh^2 t(y,b,\alpha)\right) a(y,b,\alpha)^2 \, dy \\ &> 0. \end{aligned} \tag{29}$$

Proof: We calculate

$$\begin{aligned}\partial_x\partial_\alpha t = \partial_\alpha\partial_x t &= 1 - \frac{f_b}{\alpha^2}\cosh^2 t + \frac{f_b}{\alpha}\sinh(2t)\cdot\partial_\alpha t \\ &= 1 - \frac{f_b}{\alpha^2}\cosh^2 t + (\ln a^{-2})'\partial_\alpha t.\end{aligned}$$

Since $\partial_\alpha t(0, b, \alpha) = 0$, (29) follows by variation of the constant. Similar to the proof of Lemma 2 we first conclude this for almost every α. But (29) extends to hold for all α since both sides are continuous in α (by analytic dependence of solutions on α). Positivity now follows from $f_b \leq 0$. □

We can now complete the **proof of Theorem 4:** Let $\alpha(b) := \sqrt{-\lambda_0(b)}$. That $\lambda_0(b)$ is the ground state of a Neumann problem for every b means that $t(1, b, \alpha(b)) = 0$ for all $b \in [1/2, 1-s]$. Differentiation gives

$$0 = (\partial_b t)(1, b, \alpha(b)) + (\partial_\alpha t)(1, b, \alpha(b)) \cdot \alpha'(b).$$

We have $(\partial_b t)(1, b, \alpha(b)) < 0$ for almost every b by Lemma 3 and $(\partial_\alpha t)(1, b, \alpha(b)) > 0$ for all b by Lemma 4. We conclude that $\alpha'(b) > 0$ for almost every b. This yields

$$\lambda_0(b_2) - \lambda_0(b_1) = -2\int_{b_1}^{b_2} \alpha'(b)\alpha(b)\, db < 0$$

for arbitrary $1/2 \leq b_1 < b_2 \leq 1 - s$, which concludes the proof. □

3 Numerical results

3.1 Eigenvalues and eigenfunctions for period 2

Here we present some numerical results which illustrate Theorem 3, and shed some additional light on the fact that pair formation should be energetically optimal.

We choose as the single site potential

$$f(x) = \min(0, 16x^2 - 1), \tag{30}$$

i.e. a parabolic well of depth 1 and supported in $[-1/4, 1/4]$. As discussed in Section 2, to find $\inf \Sigma_2$ for this case we need to minimize the ground state energy $\lambda_0(a)$ of the operator $H^{(a)} = -d^2/dx^2 + V^{(a)}(x)$ on $L^2(0, 2)$ with periodic boundary conditions, where (with $f_c(x) = f(x - c)$)

$$V^{(a)}(x) = \sum_{k\in\mathbb{Z}}(f_{2k+a}(x) + f_{2(k+1)-a}(x)). \tag{31}$$

The non-overlapping case treated in Section 2 corresponds to $a \in [1/4, 3/4]$. Figure 1 shows $\lambda_0(a)$ as a function of $a \in [0, 1]$, thereby allowing overlap of adjacent single site potentials up to the extreme case where two copies of f have the same center, resulting in a single well of depth 2. Figure 1 confirms Theorem 3 by showing that $\lambda_0(a)$ is strictly increasing in $[0.25, 0.5]$ and strictly decreasing in $[0.5, 0.75]$. The value of $\lambda_0(a)$ gets even smaller when the sites start to overlap and reaches its absolute minimum when two sites sit on top of each other, a result which we haven't checked theoretically. This can be understood physically since the lowest possible ground state energy should be found for a well of maximal depth. If overlap is not allowed, then pair formation ($a = 1/4$ or $a = 3/4$) comes closest to the case where two sites form a single deep well.

Figures 2 to 7 further illustrate this fact by showing the corresponding eigenfunctions. Here we consider a slightly different model by using the single site potential

$$\tilde{f}(x) = \min(0, x^2 - 1) \tag{32}$$

and constructing periodic potentials with periods being multiples of 4 by placing one translate of $\tilde{f}$ in each interval of length 4. Figures 2 to 7 show the potential and ground state eigenfunction of Schrödinger operators on $L^2(0, 8)$ with periodic boundary conditions for three different cases.

The potential in Figure 2 is $\tilde{f}(x-2) + \tilde{f}(x-6)$, corresponding to maximally separated wells for the 8-periodic problem. Its ground state (Figure 3) has two separated maxima, reflecting the fact that a quantum mechanical particle is equally likely to be found in either one of the two wells.

Figures 4 and 5 show the potential $\tilde{f}(x-3) + \tilde{f}(x-5)$ and ground state for the case of pair formation. The ground state still has two separate maxima, but essentially has a plateau in the region of the double well.

Finally, Figure 6 shows the potential $2\tilde{f}(x-4)$, i.e. the case of maximal overlap of two sites. The single deep will in the potential yields a single well defined peak in the eigenfunction (Figure 7).

3.2 Evidence for Conjectures 1 and 2

We continue to work with the single site potential $\tilde{f}$ given by (32) and displacement models whose periods are a multiple of 4. For $k \in \mathbb{N}$ and $1 \le d_\ell \le 3$, $\ell = 1, \cdots, k$, define

$$V(x; d_1, \ldots, d_k) = \sum_{\ell=1}^{k} \tilde{f}(x - 4(\ell - 1) - d_\ell)$$

and let $H(d_1, \ldots, d_k)$ be the self-adjoint realization of $-d^2/dx^2 + V(x; d_1, \ldots, d_k)$ in $L^2(0, 4k)$ with periodic boundary conditions. Conjectures 1 and 2 now correspond to the claim that

$$\inf \sigma(H(d_1, \ldots, d_k)) \begin{cases} \ge & \inf \sigma(H(3,1)) \quad \text{if } k \text{ is even,} \\ > & \inf \sigma(H(3,1)) \quad \text{if } k \text{ is odd.} \end{cases} \tag{33}$$

We have numerically checked this for k up to 8 and configurations $(d_1, \ldots, d_k)$ where all d_ℓ take values 1, 2 or 3, corresponding to a position at the left, center or right of the ℓ-th interval of length 4. We used single precision calculations in SLEIGN2, where $k = 8$ was the largest number of sites accurately calculable within this precision.

For an odd number $k = 2n+1$ of sites, the energy seems to be minimized for the configuration

$$(3, \underbrace{1, \ldots, 1}_{n \text{ times}}, \underbrace{3, \ldots, 3}_{n \text{ times}}), \tag{34}$$

and equivalent configurations found by rotation and reflection. We have confirmed this for $n = 1, 2$ and 3. It means that two sites form a pair and all others move as close to the pair as possible, where $[0, 4k]$ is thought of as a circle. The corresponding energies converge to the energy for pair formation quite rapidly:

$$\begin{aligned}
\inf \sigma(H(3,1,3)) &= -0.47346 \\
\inf \sigma(H(3,1,1,3,3)) &= -0.47642 \\
\inf \sigma(H(3,1,1,1,3,3,3)) &= -0.47666 \\
\inf \sigma(H(3,1)) &= -0.47668
\end{aligned}$$

For $k = 2n$ even with $n \geq 2$ it is not true that pair formation $(3, 1, \ldots, 3, 1)$ or $(1, 3, \ldots, 1, 3)$ are the only minimizing configurations. This can be understood by considering the ground state eigenfunction φ of $H(3,1)$ on $L^2(0,8)$. Due to the symmetries of the potential, φ' vanishes at 0, 4 and 8. This allows to construct an eigenfunction ψ of $H(d_1, \ldots, d_k)$ on $L^2(0, 4k)$ by continuously joining rescaled copies of $\varphi|_{[0,4]}$ and $\varphi|_{[4,8]}$ as long as all d_ℓ are 1 or 3 and we make sure that $\psi(4k) = \psi(0)$. As seen in Section 2, φ is symmetric to $x = 4$, strictly increasing in $[0, 4]$ and strictly decreasing in $[4, 8]$. We conclude that one gets $\psi(4k) = \psi(0)$ if and only if k is even and exactly half of the d_ℓ's are 1, the others 3. This yields $\binom{k}{k/2}$ configurations which all minimize $\inf \sigma(H(d_1, \ldots, d_k))$.

For example, for $k = 4$ one gets the pair-antipair-configuration $(3, 1, 1, 3)$, and for general $k = 2n$ a minimizer of the form

$$(3, \underbrace{1, \ldots, 1}_{n-1 \text{ times}}, \underbrace{3, \ldots, 3}_{n-1 \text{ times}}, 1).$$

This explains why the ground state energies of the odd number configurations (34) converge rapidly to $\inf \sigma(H(3,1))$, even if they contain only one pair and thus look locally very different from a chain of pairs.

Our numerical calculations for $k = 4, 6$ and 8 confirm that there should be no minimizing configurations other than the $\binom{k}{k/2}$ just described. Thus pair formation would be the unique minimizer up to degeneration due to symmetry.

A final observation, which might be worth noticing, concerns the configurations with the *largest* possible ground state energy. Theorem 3 shows that for $k = 2$ this happens for the configuration $(2, 2)$ (or equivalent), i.e. for maximal distance of the two sites. One might guess that the maximizing configuration is $(2, \ldots, 2)$ (or equivalent) for all k, i.e. a simple periodic chain of k sites. It came as a surprise to us that this was confirmed numerically for $k = 3, 4$ an 5, but not for $k \geq 6$. For example, we found that $(1, 2, 1, 2, 3, 2)$ is a maximizer for $k = 6$. We prefer to think of this as a numerical error since we have no other explanation.

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Figure 1: The ground state energy of $H^{(a)}$

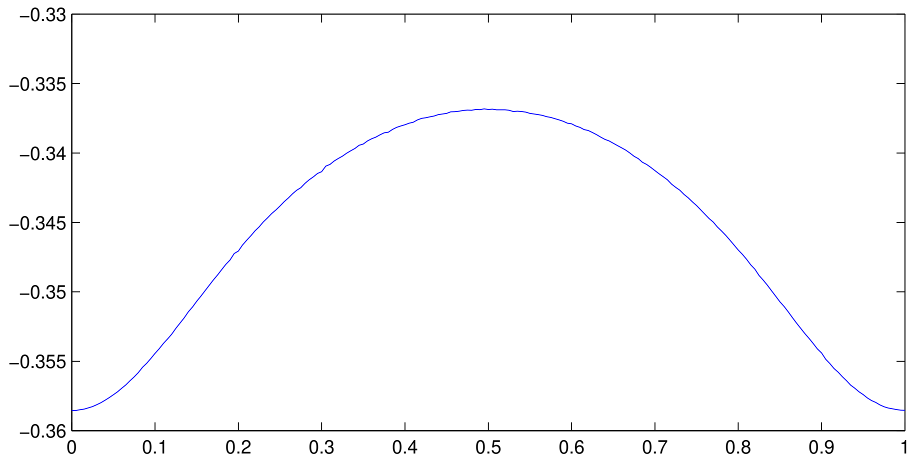

Figure 2: Distant wells

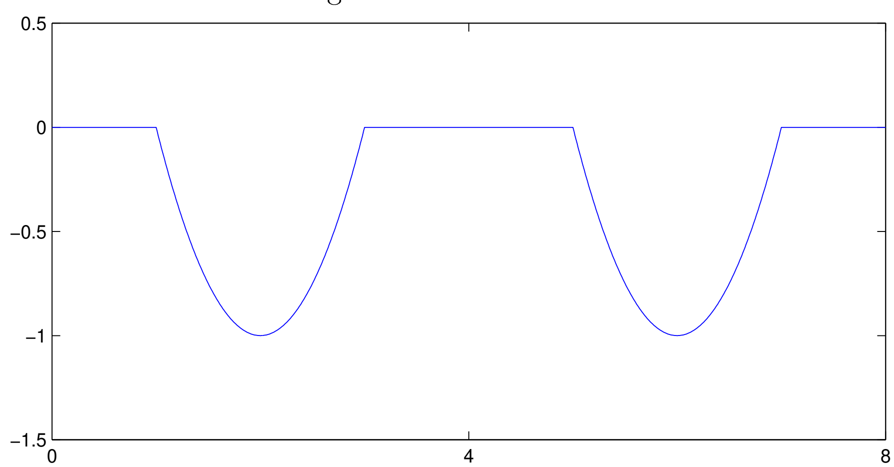

Figure 3: Eigenfunction for distant wells

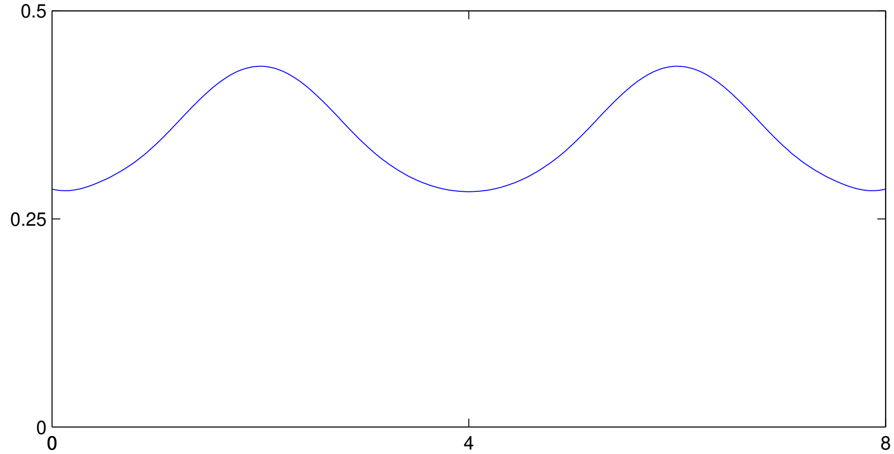

Figure 4: Pair formation

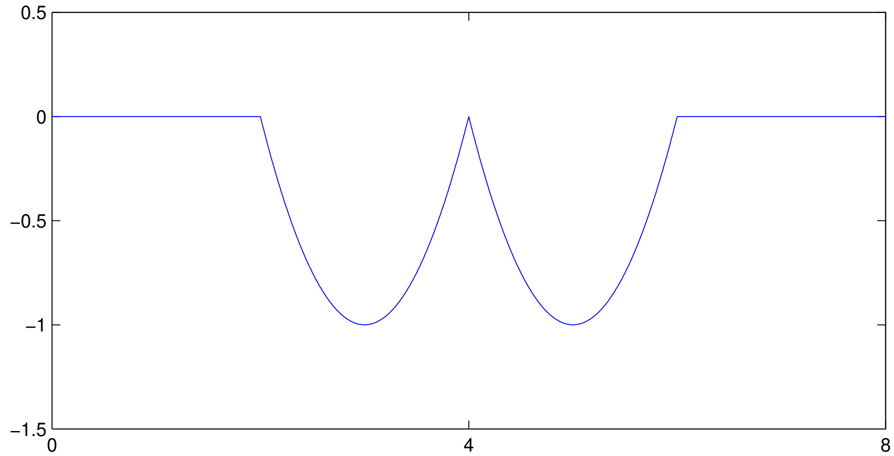

Figure 5: Eigenfunction for pair formation

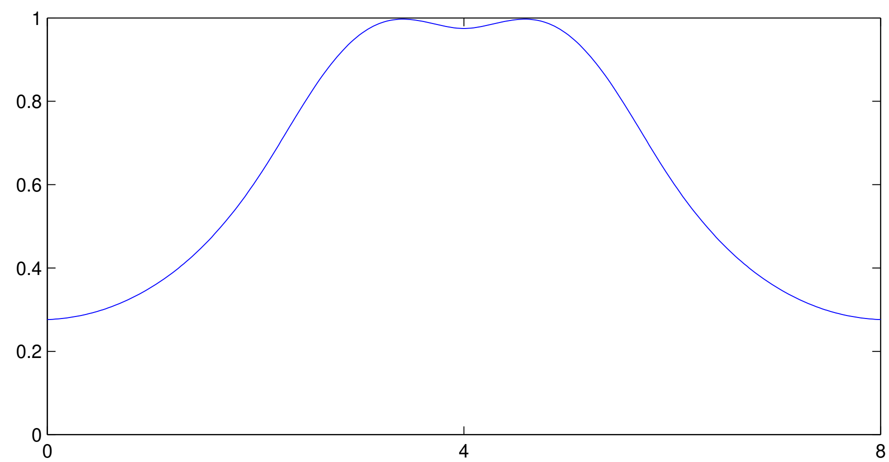

Figure 6: Maximal overlap

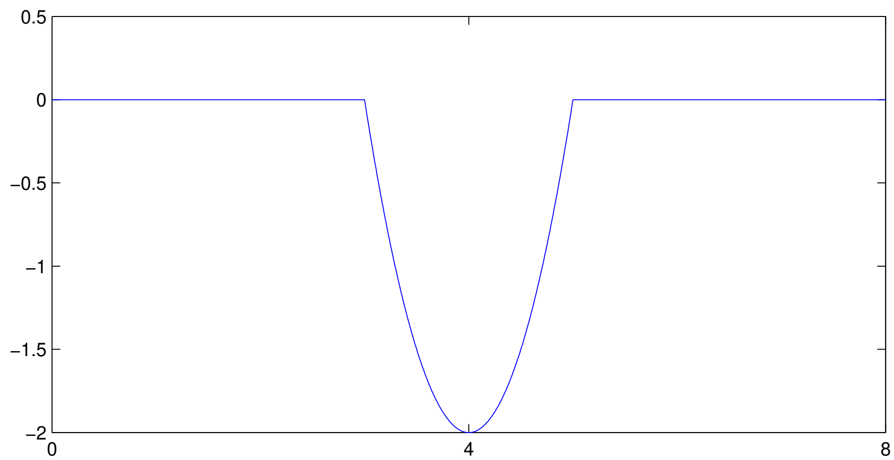

Figure 7: Eigenfunction for maximal overlap