DISCRETE VS. CONTINUOUS IN THE SEMICLASSICAL LIMIT

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Abstract. We compare the bottom of the spectrum of discrete and continuous Schrödinger operators with periodic potentials with barriers at the boundaries of their fundamental domains (see Figure 3). Our results show that these energy levels coincide in the semiclassical limit and we provide an explicit rate of convergence. We demonstrate the optimality of our results by using Bohr-Sommerfeld quantization conditions for potentials exhibiting non-degenerate wells, and by numerical experiments for more general potentials. We also investigate the dependence of the spectrum of the discrete semiclassical Schrödinger operator on the semiclassical parameter h and show that it can be discontinuous.

1. Introduction and statement of results

Suppose that $V \in C^\infty(\mathbb{R}^n;\mathbb{R})$ is periodic with respect to $\mathbb{Z}^n$: $V(x+\gamma) = V(x)$, $\gamma \in \mathbb{Z}^n$. We make the following general assumptions on V (see Figure 3):

$$\exists \text{ a fundamental domain of } \mathbb{Z}^n,\ F, \text{ such that } V|_{\partial F} > \min V. \tag{1.1}$$

To V we associate discrete and continuous Schrödinger operators,

$$(P_{\rm d}(h)v)(\gamma) := \sum_{j=1}^{n} (2v(\gamma) - v(\gamma+e_j) - v(\gamma-e_j)) + V(h\gamma)v(\gamma), \quad \gamma \in \mathbb{Z}^n, \tag{1.2}$$

and

$$P_{\rm c}(h)u(x) := -\Delta u(x) + V(hx)u(x), \quad x \in \mathbb{R}^n, \tag{1.3}$$

which are selfadjoint on $\ell^2(\mathbb{Z}^n)$ and $L^2(\mathbb{R}^n)$ (with domain $H^2(\mathbb{R}^n)$), respectively.

Motivated by questions considered by Detherage–Stier–Srivastava [DSS24] (we refer to that paper for background and pointers to related work) we provide the following general result:

Theorem. *Suppose that V satisfies (1.1) and $P_\bullet$ are defined in (1.2) and (1.3). Then*

$$d(h) := \frac{\min \operatorname{Spec}(P_{\rm d}(h))}{\min \operatorname{Spec}(P_{\rm c}(h))} = 1 + \mathcal{O}(h). \tag{1.4}$$

As a consequence, the bottom of the spectrum of the discrete operator $P_{\rm d}(h)$ can be determined by studying the (often more tractable) continuous Schrödinger operator

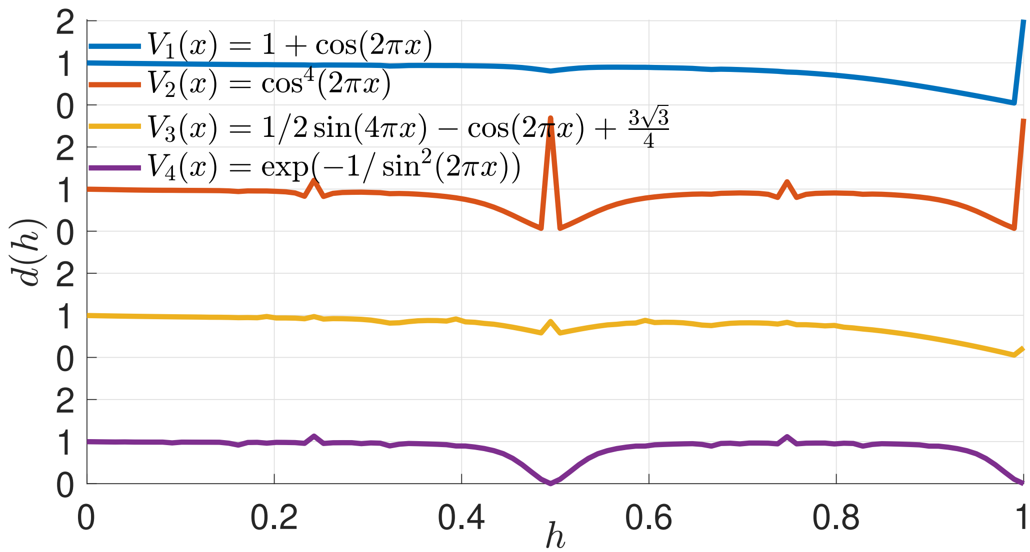

FIGURE 1. Plots of $d(h)$ in (1.4) sampled at rational values, $h \in \mathbb{Q}$ for four different potentials. The results of [DSS24] show that $d(h) \leq 1$ for $h \notin \mathbb{Q}$. The spikes indicate dramatic discontinuities of the spectrum of $P_{\rm d}(h)$ at rational points – see §4.2 – where $d(h) > 1$.

$P_{\rm c}(h)$, and vice versa. The proof of the theorem follows standard semiclassical arguments, similar to, though much simpler than, those in Helffer–Sjöstrand [HelSj89b] and Becker–Zworski [BeZw19, §5].

When more structure of V is known, for instance when V has a unique non-degenerate minimum in the fundamental domain then one can replace the bound in (1.4) by a full asymptotic expansion – see §5 for a detailed analysis in dimension one. That shows that the error bound in (1.4) is optimal – see Figure 2. We also remark that the spectrum of $P_{\rm c}$ is absolutely continuous while the spectrum of $P_{\rm d}$ may have a very complicated structure depending on the rationality properties of h. In particular, we can see discontinuities in $d(h)$ – see §4.2.1.

2. Localization of spectra of periodic operators

Instead of considering the operators given in (1.2) and (1.3), we will consider operators unitarily equivalent to $P_{\rm d}$ and $P_{\rm c}$ respectively: with $\mathbb{T}^n := \mathbb{R}^n/(2\pi\mathbb{Z})^n$,

$$\begin{aligned} H &:= \sum_{j=1}^n 2(1-\cos x_j) + V(hD_x), \quad x \in \mathbb{T}^n, \quad H : L^2(\mathbb{T}^n) \to L^2(\mathbb{T}^n), \\ P &:= -h^2\Delta + V(x), \quad x \in \mathbb{R}^n, \quad P : H^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n). \end{aligned} \tag{2.1}$$

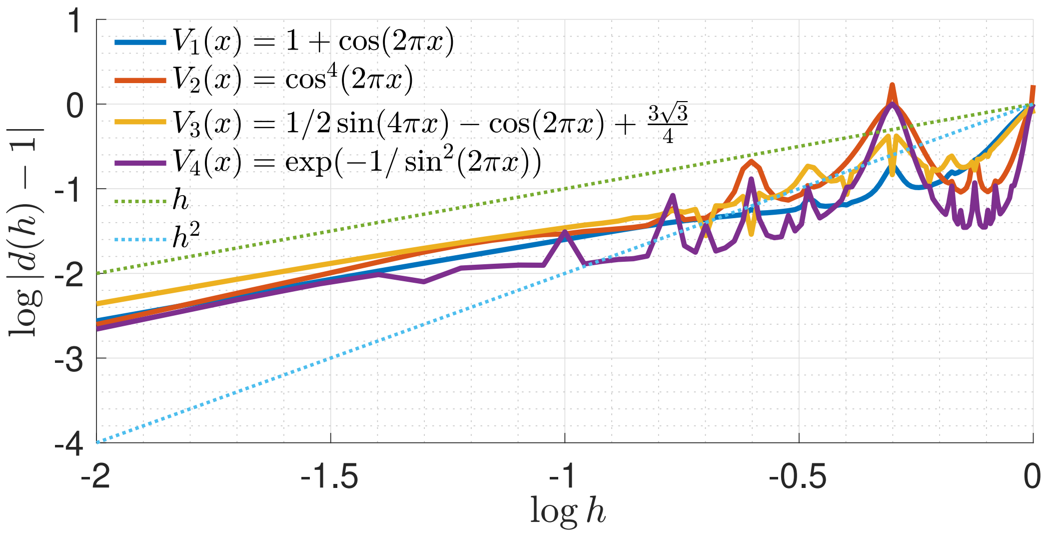

FIGURE 2. The log log plot corresponding to Figure 1 indicating that $\mathcal{O}(h)$ in Theorem 1 is optimal.

Without loss of generality we can assume that $\min V = 0$ and that $\bar{F} = \{x : 0 \leq x_j \leq 1\}$.

Assumption (1.1) implies that we can choose an open subset, $\Omega \Subset \bar{F}$, such that $V|_{\bar{F}\setminus\Omega} > c_0 > 0$. We can also choose an open neighbourhood (in $\mathbb{R}^n$), Γ of ∂F such that $V|_\Gamma > c_0 > 0$. The image of Γ under V (or just Γ) will be called the barrier. This is illustrated in Figure 3.

We will use the following set of localizing functions:

$$\begin{gathered}\chi, \tilde{\chi}, \psi \in C_c^\infty(\mathbb{R}^n; [0,1]), \quad \sum_{\gamma\in\mathbb{Z}^n} \chi(\xi - \gamma) = 1, \quad \chi|_\Omega = 1, \\ \operatorname{supp} \nabla\chi, \operatorname{supp} \nabla\tilde{\chi}, \operatorname{supp} \nabla\psi \subset \Gamma, \quad \tilde{\chi}|_{\operatorname{supp}\chi} = 1, \quad \psi|_{\operatorname{supp}\tilde{\chi}} = 1.\end{gathered} \tag{2.2}$$

We then define

$$V_0(x) := V(x) + 1 - \psi(x), \quad V_0(x) > \min(c_0, 1), \quad x \notin \Omega \tag{2.3}$$

and the corresponding operators

$$\begin{gathered}H_0 := \sum_{j=1}^n 2(1 - \cos x_j) + V_0(hD_x), \quad x \in \mathbb{T}^n, \quad H_0 : L^2(\mathbb{T}^n) \to L^2(\mathbb{T}^n), \\ P_0 := -h^2\Delta + V_0(x), \quad x \in \mathbb{R}^n, \quad P_0 : H^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n).\end{gathered} \tag{2.4}$$

These operators have discrete spectrum in a neighbourhood of 0 (see the proof of Lemma 3 for that standard fact).

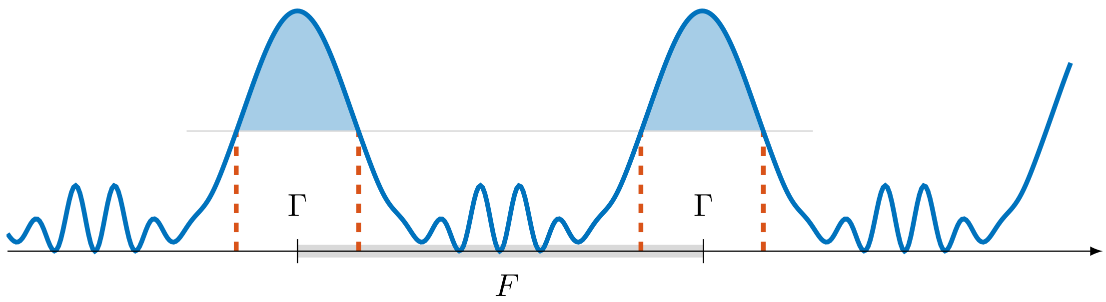

FIGURE 3. Graph of a potential V with a barrier, over a fundamental domain $F \subset \mathbb{R}$ (indicated in grey), showing a neighbourhood Γ of the boundary ∂F such that $V|_\Gamma > \min V$. The barrier $V(\Gamma)$ is shaded blue.

The key result now is given in

Lemma 1. *In the notation of* (2.1) *and* (2.4)

$$\begin{aligned} \operatorname{Spec}(H) \cap [0, c_0/2] &\subset \operatorname{Spec}(H_0) + (-\varepsilon(h), \varepsilon(h)), \\ \operatorname{Spec}(P) \cap [0, c_0/2] &\subset \operatorname{Spec}(P_0) + (-\varepsilon(h), \varepsilon(h)), \end{aligned} \tag{2.5}$$

where $\varepsilon(h) = \mathcal{O}(h^\infty)$.

Proof. We will prove the first assertion in (2.5). The second one can be proved similarly. It is more standard and also follows from Floquet theory and the existence of a barrier. We will use semiclassical pseudodifferential calculus on $\mathbb{T}^n$ – see [Zw12, §5.3.1] for a presentation which allows us to cite results from [Zw12, Chapter 4].

Let $z \in \mathbb{C}$ and set

$$Q := H - z, \quad Q_0 := H_0 - z.$$

Let $r_\gamma : L^2(\mathbb{T}) \to L^2(\mathbb{T})$ be the multiplication operator $r_\gamma u(x) = e^{i\gamma x/h} u(x)$ and $\bullet_\gamma(\xi) = \bullet(\xi - \gamma)$, $\bullet = \chi, \tilde{\chi}, \psi$ (from (2.2)). Then

$$r_\gamma Q = Q r_\gamma, \quad r_\gamma \bullet (hD) = \bullet_\gamma(hD) r_\gamma, \quad \bullet = \chi, \tilde{\chi}, \psi. \tag{2.6}$$

As a candidate for an approximate inverse of Q we introduce

$$F := \sum_{\gamma \in \mathbb{Z}^n} \tilde{\chi}_\gamma(hD)(Q_0^\gamma)^{-1} \chi_\gamma(hD), \quad Q_0^\gamma := r_\gamma Q_0 r_{-\gamma}.$$

Since $\|(Q_0^\gamma)^{-1}\|_{L^2 \to L^2} = d(z, \operatorname{Spec}(H_0))^{-1}$ we have

$$F = \mathcal{O}(d(z, \operatorname{Spec}(H_0))^{-1}).$$

From (2.6), we see that

$$Q\tilde{\chi}_\gamma(hD) = r_\gamma(Q_0 - (1 - \psi(hD)))r_{-\gamma}\tilde{\chi}_\gamma(hD) = (Q_0^\gamma - (1 - \psi_\gamma(hD))\tilde{\chi}_\gamma(hD).$$

The assumptions that $\psi = 1$ on the support of $\tilde{\chi}$, and $\tilde{\chi} = 1$ on the support of χ, and $\sum_\gamma \chi_\gamma = 1$ (see (2.2)) give

$$QF = I + \sum_{\gamma \in \mathbb{Z}^n} [Q_0^\gamma, \tilde{\chi}_\gamma(hD)](Q_0^\gamma)^{-1}\chi_\gamma(hD).$$

We now modify Q_0 to make it invertible without changing it on the support of $\nabla\tilde{\chi}$. To this end, let $\varphi \in C_{\rm c}^\infty(\mathbb{R}^n; [0,1])$ satisfy (in the notation of (2.2))

$$\operatorname{supp}\varphi \subset \Gamma, \quad \varphi|_{\operatorname{supp}\nabla\tilde{\chi}} = 1.$$

We then put

$$H_1 = H_0 + 1 - \varphi(hD), \quad Q_1 = H_1 - z.$$

Since all the terms in the symbol of H_1 (also denoted H_1 for simplicity), are non-negative, and $2 - \psi(\xi) - \varphi(\xi) \geq 2$ for $\xi \notin \Gamma$ and $V|_\Gamma > c_0$, the symbol of H_1 satisfies

$$H_1(x,\xi) = 2\sum_{j=1}^n (1 - \cos(x_j)) + V(\xi) + 1 - \psi(\xi) + 1 - \varphi(\xi) \geq c > 0.$$

Hence, [Zw12, Theorem 4.29] gives the existence of Q_1^{-1} (with a bound independent of h) for $z < c_1$, $c_1 > 0$ and $0 < h < h_0$. Writing $Q_1^\gamma = r_\gamma Q_1 r_{-\gamma}$ we have

$$(Q_0^\gamma)^{-1} = (Q_1^\gamma)^{-1} - (Q_1^\gamma)^{-1}(Q_0^\gamma - Q_1^\gamma)(Q_0^\gamma)^{-1}$$

which gives

$$\begin{aligned} QF = I &+ \sum_{\gamma \in \mathbb{Z}^n} [Q_0^\gamma, \tilde{\chi}_\gamma(hD)](Q_1^\gamma)^{-1}\chi_\gamma(hD) \\ &- \sum_{\gamma \in \mathbb{Z}^n} [Q_0^\gamma, \tilde{\chi}_\gamma(hD)](Q_1^\gamma)^{-1}(Q_0^\gamma - Q_1^\gamma)(Q_0^\gamma)^{-1}\chi_\gamma(hD). \end{aligned}$$

Since the symbol of $[Q_0^\gamma, \tilde{\chi}_\gamma(hD)]$ has support contained in $\operatorname{supp}\nabla\tilde{\chi}_\gamma$ and $Q_0^\gamma = Q_1^\gamma$ there, the second sum is $\mathcal{O}(h^\infty d(z, \operatorname{Spec}(H_0))^{-1})$ since $\sum_\gamma \chi_\gamma = 1$. Hence,

$$QF = I + \sum_{\gamma \in \mathbb{Z}^n} A_\gamma + \mathcal{O}(h^\infty d(z, \operatorname{Spec}(H_0))^{-1})_{L^2 \to L^2},$$

where

$$A_\gamma = [Q_0^\gamma, \tilde{\chi}_\gamma(hD)](Q_1^\gamma)^{-1}\chi_\gamma(hD), \quad Q_j^\gamma = r_\gamma Q_j r_{-\gamma}.$$

To bound the sum of A_γ we will use the Cotlar–Stein Lemma, see [Zw12, Theorem C.5] and for that we need to estimate the norms of $A_\gamma A_\rho^*$ and $A_\gamma^* A_\rho$.

By construction, $\operatorname{supp}\chi_\gamma \cap \operatorname{supp}\chi_\rho = \emptyset$ unless $\rho = \gamma + \sum_{j=1}^n a_j e_j$ with $a_j \in \{-1, 0, 1\}$. In particular, the supports are disjoint if $|\gamma - \rho| > \sqrt{n}$ and hence $\chi_\gamma(hD)\chi_\rho(hD) = 0$ if $|\gamma - \rho| > \sqrt{n}$. Since

$$A_\gamma A_\rho^* = [Q_0^\gamma, \tilde{\chi}_\gamma(hD)](Q_1^\gamma)^{-1}\chi_\gamma(hD)\chi_\rho(hD)(Q_1^\rho)^{-1}[Q_0^\rho, \tilde{\chi}_\rho(hD)]^*$$

(if $z \in \mathbb{R}$, Q_1^ρ is selfadjoint and to keep the notation simple we make that assumption) this means that $A_\gamma A_\rho^* = 0$ if $|\gamma - \rho| > \sqrt{n}$. For $|\gamma - \rho| \leq \sqrt{n}$ we note that modulo terms of size $O(h^\infty)$, the symbol of $[Q_0^\gamma, \tilde{\chi}_\gamma(hD)]$ has support contained in $\operatorname{supp} \nabla \tilde{\chi}_\gamma$ where $\chi_\gamma \equiv 0$ – see [Zw12, Theorem 4.25]. Since Q_1 is invertible we find for fixed γ that

$$\sum_{\rho \in \mathbb{Z}^n} \|A_\gamma A_\rho^*\|^{1/2} = \sum_{|\rho - \gamma| \leq \sqrt{n}} \|A_\gamma A_\rho^*\|^{1/2} = \mathcal{O}(h^\infty),$$

and the bound is uniform in γ. This gives $\sup_\gamma \sum_{\rho \in \mathbb{Z}^n} \|A_\gamma A_\rho^*\|^{1/2} = \mathcal{O}(h^\infty)$.

Next, we consider

$$A_\gamma^* A_\rho = \chi_\gamma(hD)(Q_1^\gamma)^{-1}[Q_0^\gamma, \tilde{\chi}_\gamma(hD)]^*[Q_0^\rho, \tilde{\chi}_\rho(hD)](Q_1^\rho)^{-1}\chi_\rho(hD).$$

We will show that

$$\|A_\gamma^* A_\rho\|^{1/2} = \mathcal{O}(\langle \gamma - \rho \rangle^{-\infty} h^\infty), \tag{2.7}$$

which implies that $\sup_\gamma \sum_{\rho \in \mathbb{Z}^n} \|A_\gamma^* A_\rho\|^{1/2} = \mathcal{O}(h^\infty)$.

To see (2.7), we first consider the case of $|\gamma - \rho| \leq \sqrt{n}$. Then, as in the analysis of $A_\gamma A_\rho^*$, $[Q_0^\rho, \tilde{\chi}_\rho(hD)](Q_1^\rho)^{-1}\chi_\rho(hD) = \mathcal{O}(h^\infty)_{L^2 \to L^2}$, uniformly in ρ, giving (2.7). When $|\gamma - \rho| > \sqrt{n}$, we note that $\chi_\gamma = \mathcal{O}(m_\gamma^{-N})$ for any N, where m_γ is an order function (in the sense of [Zw12, §4.4]) given by $m_\gamma(x, \xi) := (1 + |\xi - \gamma|^2)^{\frac{1}{2}}$. Composition formula for pseudodifferential operators [Zw12, Theorem 4.18] then give $A_\gamma A_\rho^* = B_{\rho\gamma}(x, hD, h)$, $B_{\rho\gamma} \in S(\mathcal{O}(h^\infty) m_\gamma^{-N} m_\rho^{-N})$. Since $\sup_{\xi \in \mathbb{R}^n} m_\gamma^{-N} m_\rho^{-N} \leq 2^{N/2} \langle \rho - \gamma \rangle^{-N}$ (Peetre's inequality), (2.7) follows.

Hence the assumptions of the the Cotlar–Stein Lemma [Zw12, Theorem C.5] are satisfied and we conclude that

$$QF = 1 + R, \quad \|R\|_{L^2 \to L^2} \leq \tfrac{1}{2}\varepsilon(h) d(z, \operatorname{Spec}(H_0))^{-1} \quad \varepsilon(h) = \mathcal{O}(h^\infty).$$

This shows that

$$d(z, \operatorname{Spec}(H_0)) \geq \varepsilon(h) \implies (H - z)^{-1} = Q^{-1} = F(1 + R)^{-1},$$

that is $z \notin \operatorname{Spec}(H)$, proving the first claim in (2.5). $\square$

3. Proof of the comparison result

We will now study the ground states of H_0 and P_0. They are localized to $x = 0$, $\xi \in \Omega$, and $\xi = 0$, $x \in \Omega$, respectively:

Lemma 2. *Suppose that $\chi \in S(\mathbb{R}^{2n}, 1)$ (see [Zw12, §4.4]), $\chi \geq 0$, $\operatorname{supp} \chi \subset \mathbb{R}^n \times B_{\mathbb{R}^n}(0, 1)$, and for some $c_j > 0$, $j = 0, 1$,*

$$V_0(x) < c_0 \text{ and } |\xi| < c_1 \implies \chi(x, \xi) = 1.$$

If

$$(H_0 - \lambda)u_1 = u_0, \quad (P_0 - \lambda)w_1 = w_0, \quad \lambda = \mathcal{O}(h),$$

then, with $R(x,\xi)=(\xi,x)$,

$$\begin{aligned} u_1 &= (R^*\chi)^{\mathrm{w}}(x,hD)u_1 + \mathcal{O}(\|u_1\|h^\infty)_{L^2} + \mathcal{O}(\|u_0\|)_{L^2}, \quad L^2 = L^2(\mathbb{T}^n), \\ w_1 &= \chi^{\mathrm{w}}(x,hD)w_1 + \mathcal{O}(\|w_1\|h^\infty)_{\mathscr{S}} + \mathcal{O}(\|w_0\|)_{L^2}, \quad L^2 = L^2(\mathbb{R}^n), \end{aligned} \tag{3.1}$$

where we identified $B_{\mathbb{R}^n}(0,1)$ *with a subset of* $\mathbb{T}^n := \mathbb{R}^n/(2\pi\mathbb{Z})^n$.

Proof. Let us consider the case of H_0: since $2\sum_{j=1}^n(1-\cos x_j)+V_0(\xi)+R^*\chi(x,\xi) > c_2 > 0$, we see that $H_0 + (R^*\chi)^{\mathrm{w}}(x,hD) - \lambda$ is invertible for h small enough, with bounds independent of h (see [Zw12, Theorem 4.29]). Writing $\chi^{\mathrm{w}} := \chi^{\mathrm{w}}(x,hD)$ we then have $u_1 = u_2 + u_3$, where

$$u_2 = (H_0 + (R^*\chi)^{\mathrm{w}} - \lambda)^{-1}(R^*\chi)^{\mathrm{w}}u_1, \quad u_3 = (H_0 + (R^*\chi)^{\mathrm{w}} - \lambda)^{-1}u_0. \tag{3.2}$$

If $\widetilde{\chi}$ has the same properties as χ and $\widetilde{\chi}=1$ on $\operatorname{supp}\chi$, then the composition formula [Zw12, Theorem 4.18] shows that

$$(1-(R^*\widetilde{\chi})^{\mathrm{w}})(H_0 + (R^*\chi)^{\mathrm{w}} - \lambda)^{-1}(R^*\chi)^{\mathrm{w}} = \mathcal{O}(h^\infty)_{L^2\to L^2},$$

that is, in the notation of (3.2), $(R^*\widetilde{\chi})^{\mathrm{w}}u_2 = u_2 + \mathcal{O}(h^\infty\|u_1\|)_{L^2}$. Hence,

$$\begin{aligned} (R^*\widetilde{\chi})^{\mathrm{w}}u_1 &= (R^*\widetilde{\chi})^{\mathrm{w}}u_2 + (R^*\widetilde{\chi})^{\mathrm{w}}u_3 = u_2 + \mathcal{O}(h^\infty\|u_1\|)_{L^2} + \mathcal{O}(\|u_0\|)_{L^2} \\ &= u_1 + \mathcal{O}(h^\infty\|u_1\|)_{L^2} + \mathcal{O}(\|u_0\|)_{L^2}. \end{aligned}$$

This gives the first statement in (3.1) with χ replaced by $\widetilde{\chi}$. The argument for P_0 is the same. ☐

To compare the spectra it is convenient to make another modification and consider an operator on $\mathbb{R}^n$ whose ground state is within $\mathcal{O}(h^\infty)$ of H_0. We define it as follows: let

$$\begin{gathered} A(\xi) := 2\sum_{j=1}^n (2-\cos\xi_j - \psi_0(\xi_j)), \\ \psi_0 \in C_{\mathrm{c}}^\infty((-1,1);[0,1]), \quad \psi_0|_{(-\frac12,\frac12)} = 1, \quad \psi_0(-t)=\psi_0(t). \end{gathered} \tag{3.3}$$

We then put

$$P_1 := A(hD_x) + V_0(x). \tag{3.4}$$

If w is the ground state of H_0 then Lemma 2 shows that it is localized and hence, after taking the semiclassical Fourier transform, produces a quasimode for P_1 (i.e., a solution to $(P_1-\lambda)u = \mathcal{O}(h^\infty)_{L^2}$, $\|u\|=1$). Similarly, a ground state of P_1 produces a quasimode for H_0 (using an appropriate periodization argument, cf. the proof of [BeWi22, Corollary 1.4]). Hence,

$$\min\operatorname{Spec}(H_0) = \min\operatorname{Spec}(P_1) + \mathcal{O}(h^\infty).$$

To obtain a comparison with $\min\operatorname{Spec}(P_0)$ we record the following lemma:

Lemma 3. *Suppose that $V_0 \in C^\infty(\mathbb{R}^n)$, $\min V_0 = 0$, $V_0(x) > c_0 > 0$ for $|x| \geq R$. Then, there exists C_0 and h_0 such that for $0 < h < h_0$,*

$$\operatorname{Spec}(-h^2\Delta + V_0) \cap [0, C_0 h] = \operatorname{Spec}_{\rm pp}(-h^2\Delta + V_0) \cap [0, C_0 h].$$

If $\lambda(h) := \min \operatorname{Spec}_{\rm pp}(-h^2\Delta + V_0)$ and $(-h^2\Delta + V_0)u = \lambda(h)u$, $\|u\| = 1$, then

$$h^2/C_0 \leq \lambda(h) \leq C_0 h \quad \text{and} \quad \|(hD)^2 u\|^2 \leq C h \lambda(h). \tag{3.5}$$

Proof. The fact that the spectrum near zero is discrete is standard: suppose that $V_1(x) = V_0(x)$ for $|x| \geq R$ and $V_1(x) > c_0$ everywhere. Then $R(\lambda) := (-h^2\Delta + V_1(x) - \lambda)^{-1} : L^2(\mathbb{R}^n) \to H_h^2(\mathbb{R}^n)$ exists for $\operatorname{Re}\lambda < c_0$ if h is small enough: see [Zw12, Theorems 4.29, 7.1]. Then

$$-h^2\Delta + V_0 - \lambda = (-h^2\Delta + V_1 - \lambda)(I + R(\lambda)(V_0 - V_1)). \tag{3.6}$$

Since for $\operatorname{Re}\lambda < c_0$, $R(\lambda)(V_0 - V_1)$ is a compact operator on L^2 (for instance we can consider it as a pseudodifferential operator using [Zw12, §8.1] and then use [Zw12, Theorem 4.28]) it follows from [Zw12, Theorem D.4] that $\lambda \mapsto (I + R(\lambda)(V_0 - V_1))^{-1}$ is meromorphic in $\operatorname{Re}\lambda < c_0$. That means that the resolvent of $-h^2\Delta + V_0$ is meromorphic there and the spectrum is discrete.

That $h^2/C_0 < \lambda(h) \leq C_0 h$ is equally standard. To see the upper bound, suppose that $\psi \in C_c^\infty(B(0,1))$ and $\int_{\mathbb{R}^n} |\psi(x)|^2 dx = 1$. Suppose that $V_0(x_0) = 0 = \min V_0$ and assume without loss of generality that $x_0 = 0$. Then $V_0(x) = \mathcal{O}(|x|^2)$. Define $\psi_h(x) := h^{-\frac{n}{4}}\psi(h^{-\frac12}x)$. Then

$$(-h^2\Delta + V_0(x))\psi_h(x) = h\left(-h^{-\frac{n}{4}}\Delta\psi(h^{-\frac12}x) + h^{-\frac{n}{4}}\mathcal{O}((|h^{-\frac12}x|^2)\psi(h^{-\frac12}x)\right) =: h\widetilde{\psi}_h.$$

Since $\|\psi_h\| = 1$ and $\|\widetilde{\psi}_h\| \leq C_0$ for some constant C_0, this shows $\min_{\|u\|=1}\langle(-h^2\Delta + V_0)u, u\rangle \leq C_0 h$, that is $\lambda(h) \leq C_0 h$.

For the lower bound on $\lambda(h)$, we note that the localization Lemma 1 applies to $-h^2\Delta + V_0(x)$ and hence we can replace u by an approximate mode supported in $|x| < R_0$ and satisfying $(-h^2\Delta + V_0(x) - \lambda(h))u = \mathcal{O}(h^\infty)_{L^2}$. In particular, $\|x_j u\|_{L^2} \leq R_0$. Hence, from the uncertainty principle (see [Zw12, Theorem 3.9]),

$$\|hD_{x_j}u\|_{L^2} \geq \frac{h}{2\|x_j u\|} \geq h/C_1.$$

Together with $V_0 \geq 0$, the equation for (the new) u gives

$$\|hDu\|^2 + \|V_0^{\frac12}u\|_{L^2}^2 = \lambda(h) + \mathcal{O}(h^\infty), \qquad D := \tfrac{1}{i}(\partial_{x_1}, \ldots, \partial_{x_n}), \tag{3.7}$$

and this shows that $\lambda(h) \geq h^2/C_0$ (after replacing C_0 with $\max(C_0, C_1^2)$ if necessary).

To obtain the second part of (3.5), we consider the equation satisfied by $hD_{x_k}u$:

$$-h^2\Delta(hD_{x_k}u) + V_0 hD_{x_k}u + h(D_{x_k}V_0)u = \lambda(h)hD_{x_k}u.$$

Pairing the two sides with $hD_{x_k}u$, integrating by parts in the first term, and then using $|D_{x_k}V_0| \leq CV_0^{\frac{1}{2}}$ and (3.7) gives

$$\begin{aligned}\|hD_{x_k}hDu\|^2 &\leq \lambda(h)\|hD_{x_k}u\|^2 - h\langle (D_{x_k}V_0)u, hD_{x_k}u\rangle \\ &\leq \lambda(h)^2 + Ch\|V_0^{\frac{1}{2}}u\|\|hD_{x_k}u\| \leq \lambda(h)^2 + Ch\lambda(h) \\ &\leq (C+C_0)h\lambda(h),\end{aligned} \tag{3.8}$$

which gives (3.5). □

We also need an analogue of this lemma for P_1 defined in (3.4):

Lemma 4. *Let $A(\xi)$ be given by (3.3) and suppose that $V_0 \in C^\infty(\mathbb{R}^n)$, $\min V_0 = 0$, $V_0(x) > c_0 > 0$ for $|x| \geq R$. Then, there exists C_0 and h_0 such that for $0 < h < h_0$,*

$$\operatorname{Spec}(A(hD) + V_0) \cap [0, C_0h] = \operatorname{Spec}_{\rm pp}(A(hD) + V_0) \cap [0, C_0h].$$

If $\lambda(h) := \min \operatorname{Spec}_{\rm pp}(A(hD) + V_0)$ and $(A(hD) + V_0)u = \lambda(h)u$, $\|u\| = 1$, then

$$h^2/C_0 \leq \lambda(h) \leq C_0h \quad \text{and} \quad \|(hD)^2u\|^2 \leq Ch\lambda(h). \tag{3.9}$$

Proof. We follow the steps in the proof of Lemma 3. As in the beginning of the proof of Lemma 1 we see that there exists $\chi \in C_{\rm c}^\infty(\mathbb{R}^{2n})$ such that $A(hD)+V_0(x)+\chi^{\rm w}(x,hD)-\lambda$, $\lambda = \mathcal{O}(h)$, is invertible. We then have an analogue of (3.6) (with $-h^2\Delta$ replaced by $A(hD)$ and V_1 by $V_0 + \chi^{\rm w}(x,hD)$) which shows that the resolvent of $A(hD) + V_0$ is meromorphic near 0 and the spectrum is discrete there.

To see the upper bound on $\lambda(h)$, suppose that $\psi \in C_{\rm c}^\infty(B(0,1))$ and $\int_{\mathbb{R}^n} |\psi(x)|^2 dx = 1$. Suppose that $V_0(x_0) = 0 = \min V_0$ and assume without loss of generality that $x_0 = 0$. Then $V_0(x) = \mathcal{O}(|x|^2)$. We define $B(t)$ so that $2(2 - \cos t - \psi_0(t)) = t^2 B(t)^2$ and thus

$$\begin{gathered} A(hD) = \sum_{j=1}^n B_j(hD)^2(hD_{x_j})^2, \quad B_j(\xi) = B(\xi_j), \\ B_j \in S(\langle \xi_j \rangle^{-1}), \quad B_j(\xi) \geq \langle \xi_j \rangle^{-1}/C, \quad \xi \in \mathbb{R}^n. \end{gathered} \tag{3.10}$$

For $\psi_h(x) := h^{-\frac{n}{4}}\psi(h^{-\frac{1}{2}}x)$ we have $(A(hD) + V_0)\psi_h = h\widetilde{\psi}_h$, where

$$\widetilde{\psi}_h(x) = h^{-\frac{n}{4}} \sum_{j=1}^n B_j(hD)^2(D_j^2\psi)(h^{-\frac{1}{2}}x) + h^{-\frac{n}{4}}\mathcal{O}((|h^{-\frac{1}{2}}x|^2)\psi(h^{-\frac{1}{2}}x) = \mathcal{O}(1)_{L^2}.$$

This shows that $\lambda(h) \leq C_0h$.

For the lower bound on $\lambda(h)$, we replace u by a quasimode localized using $\chi \in C_{\rm c}^\infty$ (allowed by Lemma 2) to see that a pairing of (3.10) with u gives

$$\sum_{j=1}^n \|B_j(hD)hD_{x_j}u\|^2 + \|V_0^{\frac{1}{2}}u\|^2 = \lambda(h) + \mathcal{O}(h^\infty). \tag{3.11}$$

Since u is localized in ξ and x, and $B_j(hD)$ is elliptic, we can again use the uncertainty principle:

$$\|B_j(hD)hD_{x_j}u\| \geq \|hD_{x_j}u\|/C - \mathcal{O}(h^\infty) \geq h/(2C\|x_j u\|) \geq h/C_1.$$

Combined with (3.11) this gives $\lambda(h) \geq h^2/C_1^2$.

To obtain the second part of (3.9) we again differentiate the equation with hD_{x_k} and pair the result with $hD_{x_k}u$ (see (3.8))

$$\sum_{j=1}^n \|B_j(hD)hD_{x_j}D_{x_k}u\|^2 \leq \lambda(h)\|hD_{x_k}u\|^2 + Ch\|V_0^{\frac{1}{2}}u\|\|hD_{x_k}u\| \leq C_1 h\lambda(h).$$

Since u is localized (by Lemma 2) and B_j's are elliptic (in $S(\langle\xi_j\rangle^{-1})$), we obtain the desired bound. □

Suppose $\varphi \in C_c^\infty(\mathbb{R}^n; [0,1])$ is supported in a small neighbourhood of 0 and equal to 1 near 0. Then u in the statement of Lemma 3 satisfies

$$u = \varphi(hD)u + \mathcal{O}(h^\infty)_{\mathscr{S}}.$$

(This follows from semiclassical ellipticity of $-h^2\Delta + V_0 - \lambda(h)$ for $|\xi| > \delta$ for any $\delta > 0$, see [Zw12, Theorem 4.29].) We make sure to choose φ so that $\psi_0 \equiv 1$ on $\operatorname{supp}\varphi$, where ψ_0 is given by (3.3), and write

$$\sum_{j=1}^n 2(1-\cos\xi_j)\varphi(\xi) = |\xi|^2\varphi(\xi) + \sum_j^n \xi_j^4 a_j(\xi), \quad a_j \in C_c^\infty(\mathbb{R}^n).$$

Then

$$\begin{aligned}\langle P_1 u, u\rangle &= \langle (A(hD)\varphi(hD) + V_0)u, u\rangle + \mathcal{O}(h^\infty) \\ &= \langle(-h^2\Delta + V_0)u, u\rangle + \sum_{j=1}^n \langle a_j(hD)(hD_{x_j})^4 u, u\rangle + \mathcal{O}(h^\infty) \\ &\leq \lambda(h) + C\|(hD)^2u\|^2 + \mathcal{O}(h^\infty) \leq \lambda(h)(1 + C_1 h),\end{aligned}$$

where we used (3.5) to get the last inequality. This shows that

$$\min\operatorname{Spec}(H_0) = \min\operatorname{Spec}(P_1) + \mathcal{O}(h^\infty) \leq \min\operatorname{Spec}(P_0)(1 + \mathcal{O}(h)). \tag{3.12}$$

Similarly we obtain the inequality with H_0 and P_0 replaced (using Lemma 4 instead of Lemma 3):

$$\min\operatorname{Spec}(P_0) \leq \min\operatorname{Spec}(P_1)(1 + \mathcal{O}(h)) = \min\operatorname{Spec}(H_0)(1 + \mathcal{O}(h)). \tag{3.13}$$

The inclusions (2.5) show that

$$\min\operatorname{Spec}(H) \geq \min\operatorname{Spec}(H_0) - \mathcal{O}(h^\infty), \quad \min\operatorname{Spec}(P) \geq \min\operatorname{Spec}(P_0) - \mathcal{O}(h^\infty).$$

Since we can use the ground state eigenfunctions of H_0 and P_0 as test functions for H and P respectively (their localization to Ω is key here), the opposite inequalities follow. Combined with (3.12) and (3.13) this concludes the proof of (1.4).

4. Numerical experiments

Numerical investigation of the spectrum of the discrete operator (1.2) poses some subtle challenges which require review of different aspects of the theory. Our experiments are conducted in 1D and we specialize to that case in this section.

4.1. **Auxiliary family of operators.** Let $V \in C^1(\mathbb{T}^1)$, $\mathbb{T}^1 := \mathbb{R}/\mathbb{Z}$. To study $\mathrm{Spec}(P_{\mathrm{d}}(h))$ for incommensurable h, we introduce an auxiliary family generalizing (1.2)

$$(P_{\mathrm{d}}(h,\theta)v)(\gamma) := 2v(\gamma) - v(\gamma+1) - v(\gamma-1) + V(h\gamma+\theta)v(\gamma), \quad \gamma \in \mathbb{Z}$$

with $h > 0$ and $\theta \in \mathbb{R}/\mathbb{Z}$. In addition, we define

$$\Sigma_h := \bigcup_{\theta\in\mathbb{R}/\mathbb{Z}} \mathrm{Spec}(P_{\mathrm{d}}(h,\theta)). \tag{4.1}$$

We recall the following well-known result.

Lemma 5. [HelSj88, (1.2)] *For $h \notin \mathbb{Q}$ the spectrum of $P(h,\theta)$ does not depend on θ and thus $\Sigma_h = \mathrm{Spec}(P(h,\theta))$ for all $\theta \in \mathbb{R}/\mathbb{Z}$.*

Under the assumption $h = p/q \in \mathbb{Q}$, operators $P_{\mathrm{d}}(h,\theta)$ are periodic and we can describe the spectrum of $P_{\mathrm{d}}(h,\theta)$ using Bloch-Floquet theory with Bloch boundary condition $v_{n+q} = e^{i\theta_1 q}v_n$. This implies that (see [KRL14, Remark 1.10])

$$\mathrm{Spec}(P_{\mathrm{d}}(h,\theta')) = \bigcup_{\theta_1\in\mathbb{R}/\mathbb{Z}} \mathrm{Spec}(M_{(\theta_1,\theta')}) \quad \text{and} \quad \Sigma_h = \bigcup_{\theta\in\mathbb{R}^2/\mathbb{Z}^2} \mathrm{Spec}(M_\theta)$$

with $M_\theta \in \mathbb{C}^{q\times q}$ given by

$$M_\theta := 2I_q - e^{-i\theta_1}K_q^* - e^{i\theta_1}K_q + \sum_{\beta\in\mathbb{Z}} w_\beta e^{i\beta\theta_2}(J_{p,q})^\beta,$$

$$J_{p,q} := \mathrm{diag}(e^{2\pi i(j-1)p/q}), \qquad (K_q)_{ij} := \begin{cases} 1 \text{ if } j = (i+1) \bmod q \\ 0 \text{ otherwise.} \end{cases}$$

It follows that approximating the spectrum of $\mathrm{Spec}(P_{\mathrm{d}}(h))$ for $h \in \mathbb{Q}$ reduces to computing spectra of $M_{\theta_1,0}$ over a fine enough discretisation of θ_1. To study $\mathrm{Spec}(P_{\mathrm{d}}(h))$ for $h \in \mathbb{R}\backslash\mathbb{Q}$, we use that $\Sigma_h = \mathrm{Spec}(P_{\mathrm{d}}(h))$ by Lemma 5 and the following quantitative continuity bound obtained by Avron, v. Mouche and Simon:

Lemma 6. [AMS90, Proposition 7.1] *Let $V \in C^1(\mathbb{R}/\mathbb{Z})$, then the map $\mathbb{R} \ni h \mapsto \Sigma_h$ is 1/2-Hölder continuous in Hausdorff distance d_H. In particular, for $h, h' \in \mathbb{R}$*

$$d_H(\Sigma_h, \Sigma_{h'}) \le C_V |h - h'|^{1/2},$$

This results implies that the spectrum $\operatorname{Spec}(P_{\rm d}(h))$ for irrational h can be well-approximated by computing spectra of M_θ for $\theta \in \mathbb{T}^2$. Thus, in addition to $d(h)$ defined in (1.4), we numerically study

$$D(h) := \frac{\min \Sigma_h}{\min \operatorname{Spec}(P_{\rm c}(h))},$$

where Σ_h was given in (4.1).

The numerical results are shown in Figures 1 and 2 for rational values of h and in Figures 4 and 5 for irrational values (that is, using $D(h)$ above as proxy). The figures show the optimality of Theorem 1 in both cases. For irrational h we have $D(h) = d(h)$. For rational h we have $D(h) \le d(h)$. While $d(h)$ in general is not continuous in h, $D(h)$ is continuous in h.

The experiments are performed for four potential:

(1) $V_1(x) := 1 + \cos(2\pi x)$, the *subcritical* Harper operator with non-degenerate minima.
(2) $V_2(x) := \cos^4(2\pi x)$, a potential with degenerate minima, that is $V^{(k)}(1/4) = 0$, $k < 4$, but $V^{(4)}(1/4) = 24(2\pi)^4$.
(3) $V_3(x) := \frac{1}{2}\sin(4\pi x) - \cos(2\pi x) + \frac{1}{4}3\sqrt{3}$, a potential with asymmetric wells at points $x = \mathbb{Z} - \frac{1}{12}$ with series expansion $V_3(x) = 3\sqrt{3}\pi^2(x + \frac{1}{12})^2 - 2\pi^3(x + \frac{1}{12})^3 - 3\sqrt{3}\pi^4(x + \frac{1}{12})^4 + \mathcal{O}((x + \frac{1}{12})^5)$.
(4) $V_4(x) := \exp(-1/\sin^2(2\pi x))$, a non-analytic C^∞ potential with minima of infinite order at the zeros of the sine function.

We now show that it is in general *not true* that $\mathbb{R} \ni h \mapsto \min \operatorname{Spec}(P_{\rm d}(h))$, let alone $\mathbb{R} \ni h \mapsto \operatorname{Spec}(P_{\rm d}(h))$, is continuous. The maps however are continuous on $\mathbb{R} \setminus \mathbb{Q}$.

4.2. **(Dis)-continuity of spectra.** To explain the discrepancy between Figures 1 and 4, especially close to $h = 1/2$ and $h = 1$, we argue that $\operatorname{Spec}(P_{\rm d}(h))$ and also $\min \operatorname{Spec}(P_{\rm d}(h))$ are in general discontinuous in the parameter $h \in \mathbb{R}$. By Lemma 6, it suffices to show that $\operatorname{Spec}(P_{\rm d}(h)) \ne \Sigma_h$ and $\min \operatorname{Spec}(P_{\rm d}(h)) > \min \Sigma_h$, respectively for suitable choices of h. We illustrate this in Figures 6 and 7, respectively.

4.2.1. *Discontinuities at $h = \frac{1}{2}$.* For $V(x) = 1 + \cos(2\pi x)$ we find

$$M_\theta = \begin{pmatrix} 3 - 2\cos\theta_1 & \cos\theta_2 \\ \cos\theta_2 & 3 - 2\cos(\theta_1 + \pi) \end{pmatrix}.$$

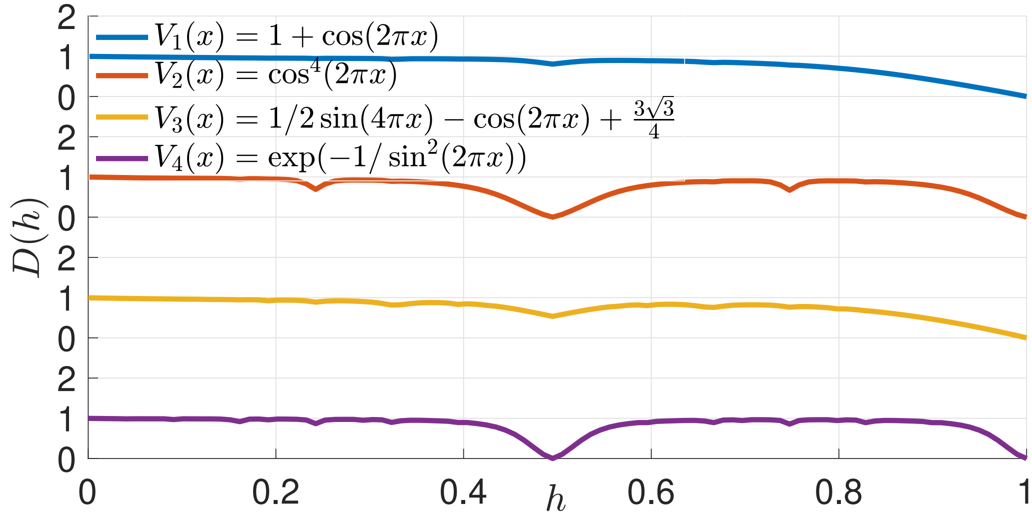

FIGURE 4. Illustration of the limiting quantity $D(h) := \frac{\min \Sigma_h}{\min \operatorname{Spec}(P_c(h))}$ in (1.4) sampled at rational $h \in \mathbb{Q}$ and stacked vertically. Since $D(h)$ is continuous in h and $D(h) = d(h)$ for irrational h this serves as a proxy for the limiting quantity in (1.4) for $h \in \mathbb{R} \setminus \mathbb{Q}$. It follows from [DSS24] that $D(h) \leq 1$ for $h \in \mathbb{R}$.

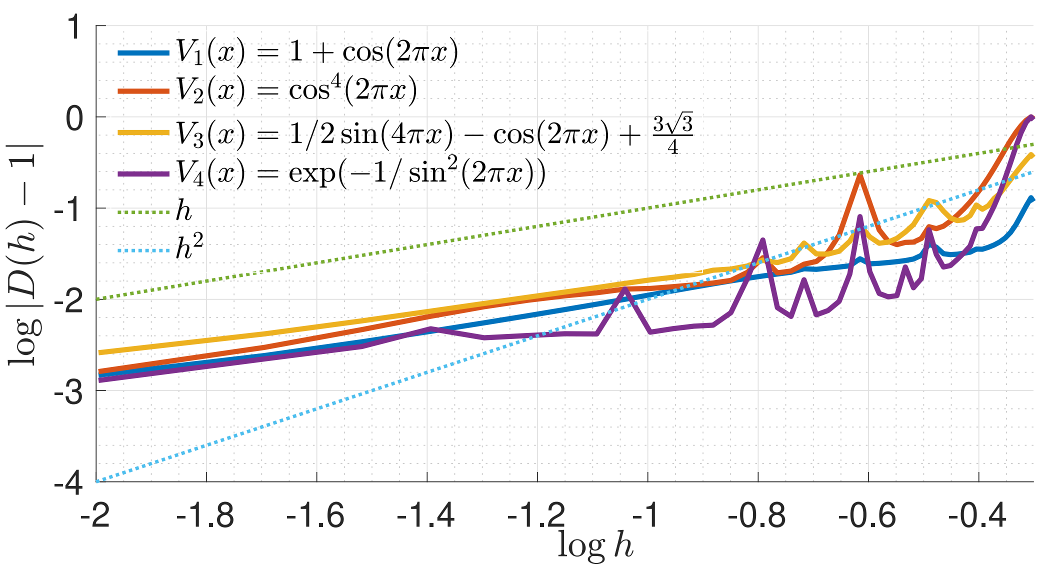

FIGURE 5. log log plot associated with Figure 4 indicating that $|D(h) - 1| = \mathcal{O}(h)$ in Theorem 1 is optimal.

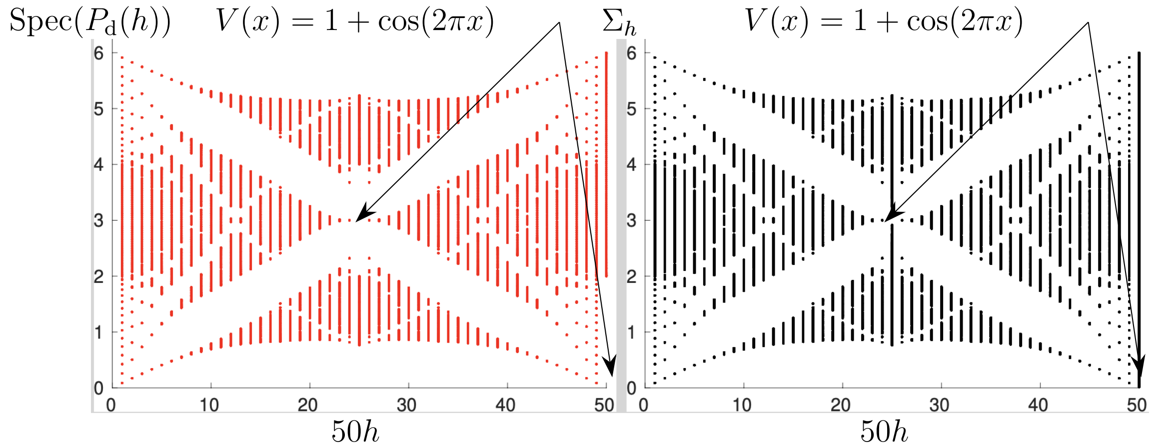

FIGURE 6. Hofstadter butterfly $h = \frac{p}{50} \mapsto \mathrm{Spec}(P_{\mathrm{d}}(h))$ (left) and $h = \frac{p}{50} \mapsto \Sigma_h$ (right) for $V(x) = 1 + \cos(2\pi x)$. Discontinuities at $p = 25, 50$ are clearly visible on the left. Visible discrepancies between the two butterflies are indicated by arrows.

The spectrum of this matrix is given by

$$\mathrm{Spec}(M_\theta) = \left\{ 3 \pm \frac{\sqrt{5 + 4\cos(2\theta_1) + \cos(2\theta_2)}}{\sqrt{2}} \right\}.$$

For $\theta_2 = 0$, we have $\bigcup_{\theta_1 \in \mathbb{R}} \mathrm{Spec}(M_{\theta_1,0}) = [3-\sqrt{5}, 2] \cup [4, 3+\sqrt{5}]$, while $\bigcup_{\theta \in \mathbb{R}^2} \mathrm{Spec}(M_\theta) = [3-\sqrt{5}, 3+\sqrt{5}]$.

Similarly, if $V(x) = \cos^4(2\pi x)$, then

$$M_\theta = \mathrm{diag}(2 - 2\cos(\theta_1) + \cos^4(\theta_2), 2 - 2\cos(\theta_1 + \pi) + \cos^4(\theta_2)),$$

with $\bigcup_{\theta_1 \in \mathbb{R}} \mathrm{Spec}(M_{\theta_1}) = [1, 5]$ while $\bigcup_{\theta \in \mathbb{R}^2} \mathrm{Spec}(M_\theta) = [0, 5]$.

4.2.2. *Discontinuities at $h = 1$.* For $h = 1$ and $V(x) = 1 + \cos(2\pi x)$, we have

$$M_\theta = 3 - 2\cos\theta_1 + \cos\theta_2$$

which implies that $\bigcup_{\theta_1 \in \mathbb{R}} \mathrm{Spec}(M_{\theta_1,0}) = [2, 6]$ while $\bigcup_{\theta \in \mathbb{R}^2} M_\theta = [0, 6]$.

For $V(x) = \cos^4(2\pi x)$ we have

$$M_\theta = 2 - 2\cos\theta_1 + \cos^4\theta_2$$

which implies that $\bigcup_{\theta_1 \in \mathbb{R}} \mathrm{Spec}(M_{\theta_1,0}) = [1, 5]$ while $\bigcup_{\theta \in \mathbb{R}^2} M_\theta = [0, 5]$.

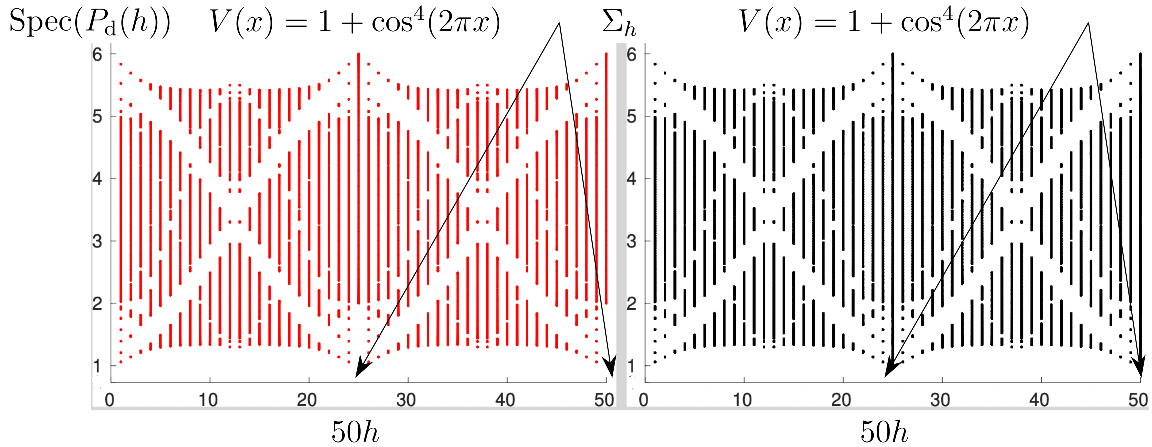

FIGURE 7. Hofstadter butterfly $h = \frac{p}{50} \mapsto \mathrm{Spec}(P_{\mathrm{d}}(h))$ (left) and $h = \frac{p}{50} \mapsto \Sigma_h$ (right) for $V(x) = 1 + \cos^4(2\pi x)$. Discontinuities at $p = 25, 50$ are clearly visible on the left. Visible discrepancies between the two butterflies are indicated by arrows.

5. THE BOHR-SOMMERFELD QUANTIZATION CONDITION

The distribution of eigenvalues of a symbol exhibiting a potential well can be expressed using a Bohr-Sommerfeld quantization condition. A rigorous approach to that condition was developed by Helffer-Robert [HelRob84]. It allows us to compare our numerical computations of the bottom of the spectrum to the analytic expressions obtained from the quantization condition. We let $p^{\mathrm{w}}(x, hD)$ be either

$$p^{\mathrm{w}}(x, hD) = -h^2\Delta + V_0(x) \quad \text{or} \quad p^{\mathrm{w}}(x, hD) = 2(1 - \cos(hD)) + V_0(x) \tag{5.1}$$

(see (3.4)) with V_0 as in (2.3). We use an elegant presentation of higher order Bohr–Sommerfeld rules developed by Colin de Verdière [CdV05],

$$2\pi(n + \tfrac{1}{2})h = S(E_n, h) = \sum_{j=0}^{\infty} h^{2j} S_{2j}(E_n), \quad n \in \mathbb{N}_0. \tag{5.2}$$

It follows from [HelSj88] (see also [HiZw24] for a recent treatment of a more general case) that for analytic potentials V with non-degenerate wells, the Bohr–Sommerfeld rule is also valid for the bottom of the spectrum, $n = 0$. The analyticity assumption is not essential: asymptotic formulas for the ground state in the case of non degenerate minimum hold in all dimensions – see [DiSj99, Theorem 3.6, Theorem 4.23] and references given there. In the analytic case we can use the more computationally tractable Bohr–Sommerfeld rules but the expansions in terms of the potential are ultimately the same.

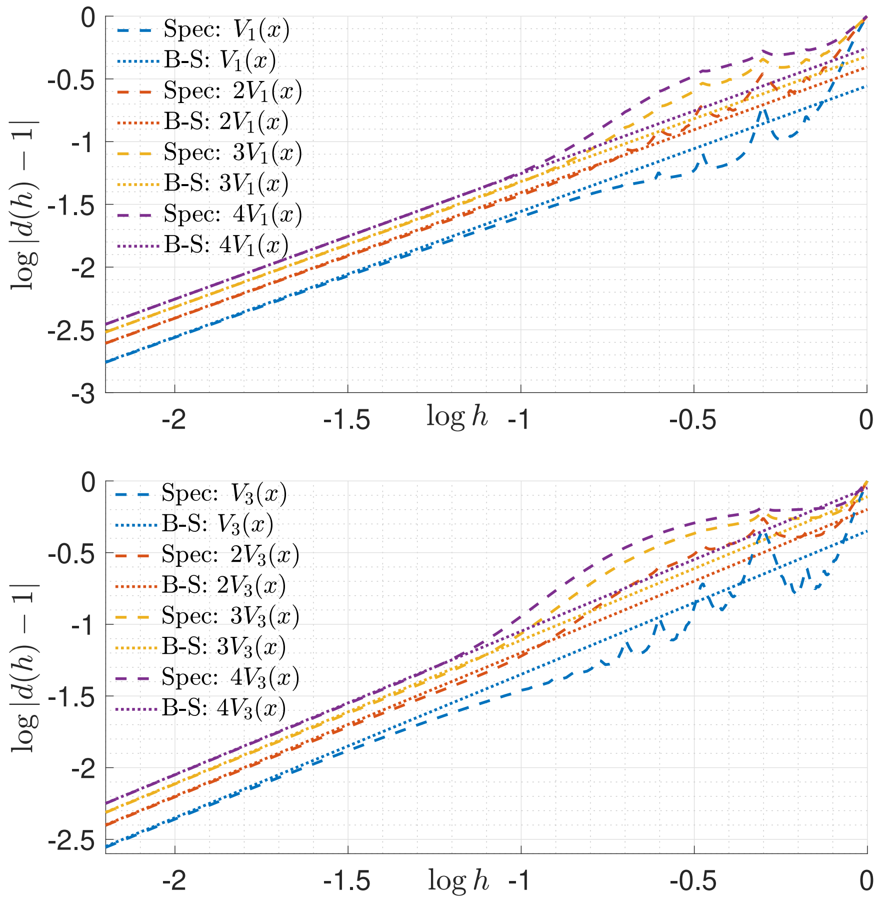

FIGURE 8. Linear convergence rate of $|d(h)-1|$ illustrated by comparison with leading term obtained from Bohr-Sommerfeld quantization condition in (5.6) to spectral computations for various multiples of the potentials V_1 (top) and V_3 (bottom), i.e. operators $p^{\mathrm{w}}(x,hD) = -h^2\Delta + \lambda V_j$ and $p^{\mathrm{w}}(x,hD) = 2(1-\cos(hD)) + \lambda V_j(x)$ and $\lambda \in \{1,2,3,4\}$.

Hence, we restrict ourselves to the two potentials V_1, V_3 described on page 12, as the quantization rule may not apply to V_2 (degenerate well) and V_4 (non-analytic potential with an infinitely degenerate well).

The first two terms in (5.2) are given by

$$S_0(E) = \int_{\{p\le E\}} dx\, d\xi, \quad S_2(E) = -\tfrac{1}{24}\partial_E^2 \int_{\{p\le E\}} \det(p'')\, dx\, d\xi.$$

The first term is the classical action ($dx\, d\xi$ is the Lebesgue measure on $\mathbb{R}^2$). The second one comes from the proof of [CdV05, Theorem 2]. For analytic V_0 such that

$$V_0(x) = a_0x^2 + a_1x^3 + a_2x^4 + \mathcal{O}(x^5) \tag{5.3}$$

Table 1. Coefficients α_i appearing in the asymptotic expansion of the action terms S_0, S_2 in (5.4).

Action coefficients				
Symbol	$\xi^2 + V_1$	$\xi^2 + V_3$	$2(1-\cos(\xi))+V_1$	$2(1-\cos(\xi))+V_3$
a_0	$2\pi^2$	$3\sqrt{3}\pi^2$	$2\pi^2$	$3\sqrt{3}\pi^2$
α_1	$\frac{1}{16\pi\sqrt{2}}$	$\frac{4}{81\pi\cdot 3^{1/4}}$	$\frac{1}{16\pi\sqrt{2}} + \frac{1}{32}a_0^{-1/2}$	$\frac{4}{81\pi\cdot 3^{1/4}} + \frac{1}{32}a_0^{-1/2}$
α_2	$\frac{\pi}{8\sqrt{2}}$	$\frac{11\pi}{27\cdot 3^{3/4}}$	$\frac{\pi}{8\sqrt{2}} + \frac{1}{32}a_0^{1/2}$	$\frac{11\pi}{27\cdot 3^{3/4}} + \frac{1}{32}a_0^{1/2}$

near $x = 0$ with $a_0 > 0$ (which holds for appropriate translations of V_1, V_3 with $a_0 = 2\pi^2$, $a_1 = 0$, $a_2 = -2\pi^4/3$ and $a_0 = 3\sqrt{3}\pi^2$, $a_1 = -2\pi^3$, $a_2 = -3\sqrt{3}\pi^4$, respectively) we have

$$S_0(E) = \pi a_0^{-1/2} E + \pi\alpha_1 E^2 + \mathcal{O}(E^3), \quad S_2(E) = \pi\alpha_2 + \mathcal{O}(E) \tag{5.4}$$

for α_i specified in Table 1 for V_1, V_3 and p in (5.1). Here, we used that the leading term of $S_0(E)$ is given only in terms of the leading order Taylor coefficient of the quadratic well potential. This fact and further details on how to obtain the coefficients can be found in the appendix. From the expansion of the action (5.4) and the quantization condition (5.2), we immediately obtain

$$E_0(h) = a_0^{1/2} h - a_0^{1/2}(a_0\alpha_1 + \alpha_2)h^2 + \mathcal{O}(h^3). \tag{5.5}$$

As seen in Table 1, there is a difference in α_i depending on the choice of p in (5.1). This difference only depends on the leading term in (5.3), and this is true for any such potential, see Lemmas 9 and 10 in the appendix. We can relate this to $d(h)$ in (1.4) by inserting the semiclassical approximation for (5.5) which gives (see the remarks after (5.2))

Proposition 7. *Suppose that $V \in C^\infty(\mathbb{R};\mathbb{R})$ is $\mathbb{Z}$-periodic, V has a single minimum, x_0, in a fundamental domain and $V(x) = a_0(x-x_0)^2 + \mathcal{O}(|x-x_0|^3)$, $a_0 > 0$. Then*

$$d(h) = 1 - \frac{\sqrt{a_0}}{16} h + \mathcal{O}(h^2). \tag{5.6}$$

We illustrate the effectiveness of (5.6) in Figure 8. In Figures 9 and 10, we illustrate the fast convergence of the Bohr-Sommerfeld rule to compute $E_0(h)$ in (5.5). In addition, in Figure 9, we show asymptotics of $\min \operatorname{Spec}(P_{\mathrm{c}}(h))$ and $\min \operatorname{Spec}(P_{\mathrm{d}}(h))$ indicating the $h^{2k/(k+1)}$ behaviour, where $2k$ is the order of vanishing of V at the bottom of the well. (This follows from a simple rescaling argument.) The scaling is visible for relatively large $h > 0$ for analytic potentials V_1, V_2, V_3, but less so for the non-analytic potential V_4.

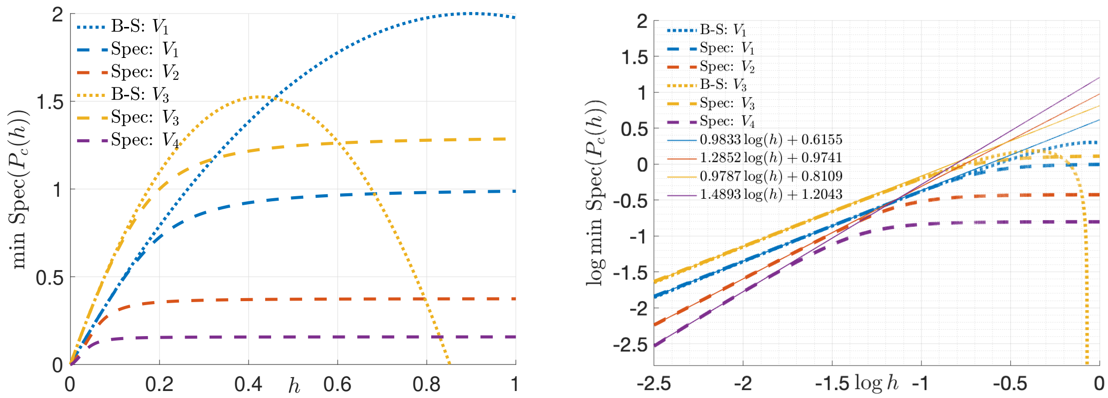

FIGURE 9. Comparison of $\min(\mathrm{Spec}(P_{\mathrm{c}}(h)))$ computed using direct spectral (Spec) computations and using the first two terms of the Bohr-Sommerfeld (B-S) condition, see (5.5), for potentials V_1, V_3. We also include a linear fit at log-scale. It confirms the linear dependence on h for potentials with non-degenerate minima and suggests the expected $h^{\frac{4}{3}}$ behaviour for the potential with the fourth order minimum and $h^{\frac{3}{2}}$ for V_4 (while a larger power is expected from scaling).

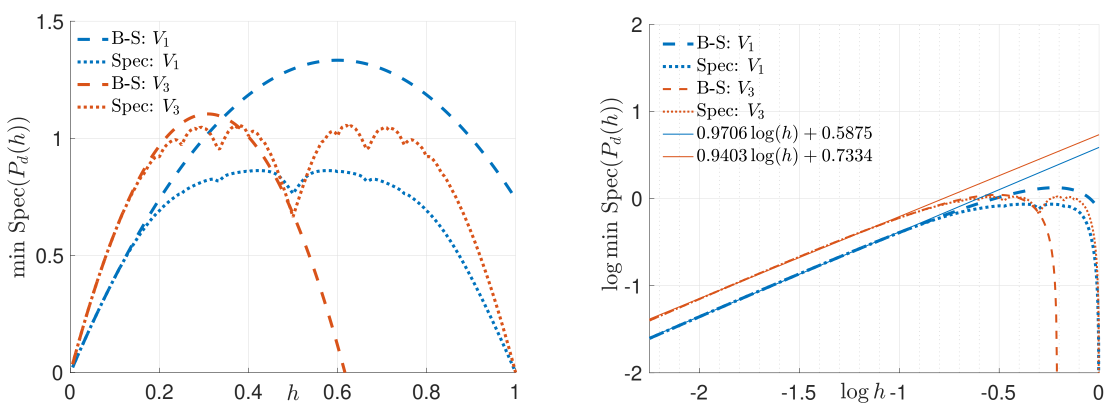

FIGURE 10. Comparison of $\min(\mathrm{Spec}(P_{\mathrm{d}}(h)))$ computed using direct spectral (Spec) computations and using the first two terms of the Bohr-Sommerfeld (B-S) condition, see (5.5), for potentials V_1, V_3 with linear fit at log-scale.

APPENDIX: COMPUTATION OF BOHR-SOMMERFELD COEFFICIENTS

Let $V(x) = \sum_{n\geq 2} a_{n-2}x^n$ with $a_n \in \mathbb{R}$ and $a_0 > 0$. We then solve $V(x(y)) = y^2$ recursively by looking for an asymptotic expansion $x(y) = \sum_{n\geq 1} \beta_n y^n$ with $\beta_1 > 0$ such that $x_m(y) = \sum_{n=1}^{m} \beta_n y^n$ satisfies $|V(x_m(y)) - y^2| = \mathcal{O}(|y|^{m+2})$. One directly verifies $\beta_1 = a_0^{-1/2}$. Assume now that we have found x_m, then for x_{m+1} we find

$$\begin{aligned} V(x_{m+1}(y)) &= \sum_{n\geq 2} a_n(\beta_{m+1}y^{m+1} + x_m(y))^n \\ &= \sum_{n\geq 2} a_n \sum_{k=0}^{n} \binom{n}{k} (\beta_{m+1}y^{m+1})^{n-k} x_m(y)^k \\ &= y^2 + \sum_{n\geq 2} a_n \sum_{k=0}^{n-1} \binom{n}{k} (\beta_{m+1}y^{m+1})^{n-k} x_m(y)^k + \sum_{n\geq m+2} c_{n,m}y^n \end{aligned}$$

for some coefficients $c_{n,m}$, where we used the induction in the last step. For this to satisfy $|V(x_{m+1}(y)) - y^2| = \mathcal{O}(|y|^{m+3})$ we must eliminate the terms of order y^{m+2} on the right-hand side. These are produced in the middle sum when $n = 2$ and $k = 1$, and in the right sum when $n = m+2$, so they are eliminated by setting $\beta_{m+1} := -c_{m+2,m}/\beta_1$. This way we find for the positive branch of $V^{-1}(y^2)$ and asymptotic formula

$$\begin{aligned} V^{-1}(y^2) = a_0^{-1/2} y - \tfrac{1}{2} a_0^{-2} a_1 y^2 + (\tfrac{5}{8} a_0^{-7/2} a_1^2 - \tfrac{1}{2} a_0^{-5/2} a_2) y^3 \\ + (-a_0^{-5} a_1^3 + \tfrac{3}{2} a_0^{-4} a_1 a_2 - \tfrac{1}{2} a_0^{-3} a_3) y^4 + \mathcal{O}(y^5). \end{aligned}$$

From this expression, we readily obtain the following result.

Lemma 8. *Let V be real analytic such that*

$$V(x) = a_0 x^2 + a_1 x^3 + \dots$$

with $a_0 > 0$. For $x > 0$ we set $y^2 = V(x)$ and let V^{-1} denote the positive branch of the inverse such that $x = V^{-1}(y^2)$, $V^{-1}(0) = 0$, and $dx/dy = 2y/V'(V^{-1}(y^2))$. Then

$$\frac{2y}{V'(V^{-1}(y^2))} = b_0 + b_1 y + b_2 y^2 + b_3 y^3 + \mathcal{O}(y^4),$$

where

$$\begin{aligned} b_0 = a_0^{-1/2}, \quad b_1 = -a_0^{-2} a_1, \quad b_2 = \tfrac{15}{8} a_0^{-7/2} a_1^2 - \tfrac{3}{2} a_0^{-5/2} a_2 \\ b_3 = -4 a_0^{-5} a_1^3 + 6 a_0^{-4} a_1 a_2 - 2 a_0^{-3} a_3. \end{aligned}$$

We use this result to compute $S_0(E)$:

Lemma 9. *Let $p(x,\xi) = A(\xi) + V(x)$ with V as in Lemma 8, and $A(\xi) = \xi^2$ or $A(\xi) = 2(1 - \cos\xi)$. Let $S_0(E) = \int_{\{p\leq E\}} dx\, d\xi$. If $A(\xi) = \xi^2$ then*

$$S_0(E) = a_0^{-1/2}\pi E + \tfrac{1}{4}(\tfrac{15}{8} a_0^{-7/2} a_1^2 - \tfrac{3}{2} a_0^{-5/2} a_2)\pi E^2 + \mathcal{O}(E^3). \tag{A.1}$$

If $A(\xi) = 2(1 - \cos\xi)$ then

$$S_0(E) = a_0^{-1/2}\pi E + \tfrac{1}{4}(\tfrac{15}{8} a_0^{-7/2} a_1^2 - \tfrac{3}{2} a_0^{-5/2} a_2 + \tfrac{1}{8} a_0^{-1/2})\pi E^2 + \mathcal{O}(E^3). \tag{A.2}$$

Proof. We start with the case $A(\xi) = \xi^2$. Then

$$S_0(E) = \int_{\{p\le E\}} dx\, d\xi = \int_{\{\xi^2+V(x)\le E,\ x>0\}} dx\, d\xi + \int_{\{\xi^2+V(-x)\le E,\ x>0\}} dx\, d\xi,$$

where the last identity follows by a change of variables. Now apply Lemma 8 to each of the two integrals on the right, noting that $\widetilde{V}(x) := V(-x) = \tilde a_0 x^2 + \tilde a_1 x^3 + \dots$ for $x > 0$ with $\tilde a_{2j} = a_{2j}$ and $\tilde a_{2j+1} = -a_{2j+1}$. Changing variables $y^2 = V(x)$ and $y^2 = \widetilde{V}(x)$, respectively, we obtain

$$S_0(E) = \int_{\{\xi^2+y^2\le E,\ y\ge 0\}} (b_0 + \tilde b_0 + (b_1+\tilde b_1)y + (b_2+\tilde b_2)y^2 + (b_3+\tilde b_3)y^3 + \mathcal{O}(y^4))\, dy\, d\xi$$

with b_j as in the lemma, and with $\tilde b_j$ defined as b_j but with a_j replaced by $\tilde a_j$. Then $b_0 + \tilde b_0 = 2b_0$, $b_2 + \tilde b_2 = 2b_2$, and $b_1 + \tilde b_1 = b_3 + \tilde b_3 = 0$. Changing to polar coordinates we get

$$S_0(E) = \int_0^{E^{1/2}} \int_{-\pi/2}^{\pi/2} (2b_0 r + 2b_2 r^3 \cos^2 t)\, dt\, dr + \mathcal{O}(E^3) = b_0\pi E + \tfrac{1}{4} b_2 \pi E^2 + \mathcal{O}(E^3).$$

Inserting the expressions for b_j from Lemma 8 gives (A.1).

Next, consider the case when $A(\xi) = 2(1-\cos\xi)$. Make the change of variables $\eta^2 = 2(1-\cos\xi)$ so that $\xi = \arccos(1-\eta^2/2)$ for $\xi \ge 0$. This gives $d\xi = (1-\eta^2/4)^{-1/2} d\eta$, so $d\xi = (1 + \eta^2/8 + \mathcal{O}(\eta^4))\, d\eta$ by Taylor's formula. Hence,

$$\begin{aligned} S_0(E) &= \int_{\{\eta^2+y^2\le E,\ y\ge 0\}} (2b_0 + 2b_2 y^2 + \mathcal{O}(y^4))(1 + \eta^2/8 + \mathcal{O}(\eta^4))\, dy\, d\eta \\ &= b_0 \pi E + \tfrac{1}{4}(b_2 + \tfrac{1}{8} b_0)\pi E^2 + \mathcal{O}(E^3). \end{aligned}$$

Inserting the expressions for b_j from Lemma 8 gives (A.2). ∎

Lemma 10. *Let $p(x,\xi) = A(\xi) + V(x)$ with V as in Lemma 8, and $A(\xi) = \xi^2$ or $A(\xi) = 2(1-\cos\xi)$. Let $S_2(E) = -\frac{1}{24}\partial_E^2 \int_{\{p\le E\}} A''(\xi)V''(x)\, dx\, d\xi$. If $A(\xi) = \xi^2$ then*

$$S_2(E) = \tfrac{1}{24}(\tfrac{21}{4} a_0^{-5/2} a_1^2 - 9 a_0^{-3/2} a_2)\pi + \mathcal{O}(E). \tag{A.3}$$

If $A(\xi) = 2(1-\cos\xi)$ then

$$S_2(E) = \tfrac{1}{24}(\tfrac{21}{4} a_0^{-5/2} a_1^2 - 9 a_0^{-3/2} a_2 + \tfrac{3}{4} a_0^{1/2})\pi + \mathcal{O}(E). \tag{A.4}$$

Proof. We start with the case $A(\xi) = \xi^2$. We compute $S_2(E) = -\frac{1}{24}\partial_E^2 I(E)$, where after a change of variable

$$I(E) = \int_{\{\xi^2+V(x)\le E,\ x>0\}} 2V''(x)\, dx\, d\xi + \int_{\{\xi^2+V(-x)\le E,\ x>0\}} 2V''(-x)\, dx\, d\xi.$$

As in the proof of Lemma 9, we change variables $y^2 = V(x)$ and $y^2 = V(-x)$, respectively. Using Lemma 8 and writing $V''(V^{-1}(y^2)) = \sum_{j=0}^{3} c_j y^j + \mathcal{O}(y^4)$, we get

$$c_0 = 2a_0, \quad c_1 = 6a_0^{-1/2}a_1, \quad c_2 = -3a_0^{-2}a_1^2 + 12a_0^{-1}a_2,$$
$$c_3 = \tfrac{30}{8}a_0^{-7/2}a_1^3 - 15a_0^{-5/2}a_1a_2 + 20a_0^{-3/2}a_3,$$

and $I(E) = I_+(E) + I_-(E)$, where

$$I_\pm(E) = \int_{\{\xi^2+y^2\le E,\ y\ge 0\}} 2\Big(\sum_{j=0}^{3}(\pm 1)^j c_j y^j + \mathcal{O}(y^4)\Big)\Big(\sum_{j=0}^{3}(\pm 1)^j b_j y^j + \mathcal{O}(y^4)\Big)\, dy\, d\xi,$$

with b_j as in the lemma. Performing the multiplication and computing $I_+ + I_-$ we get

$$I(E) = \int_{\{\xi^2+y^2\le E,\ y\ge 0\}} (4b_0c_0 + 4(b_0c_2 + b_1c_1 + b_2c_0)y^2 + \mathcal{O}(y^4))\, dy\, d\xi.$$

Changing to polar coordinates gives

$$\begin{aligned} I(E) &= \int_0^{E^{1/2}} \int_{-\pi/2}^{\pi/2} (4b_0c_0r + 4(b_0c_2 + b_1c_1 + b_2c_0)r^3\cos^2 t)\, dt\, dr + \mathcal{O}(E^3) \\ &= 2b_0c_0\pi E + \tfrac{1}{2}(b_0c_2 + b_1c_1 + b_2c_0)\pi E^2 + \mathcal{O}(E^3). \end{aligned}$$

Hence,

$$S_2(E) = -\tfrac{1}{24}I''(E) = -\tfrac{1}{24}(b_0c_2 + b_1c_1 + b_2c_0)\pi + \mathcal{O}(E).$$

Inserting the expressions for b_j and c_j we obtain (A.3).

Next, consider the case when $A(\xi) = 2(1 - \cos\xi)$. Change variables from x to y as above, and then make the change of variables $\eta^2 = 2(1 - \cos\xi)$ so that $\xi = \arccos(1 - \eta^2/2)$ for $\xi \ge 0$, $d\xi = (1 + \eta^2/8 + \mathcal{O}(\eta^4))\, d\eta$, and $A''(\xi) = 2\cos\xi = 2 - \eta^2$. This gives

$$\begin{aligned} I(E) = \int_{\{\eta^2+y^2\le E,\ y\ge 0\}} &\big[2b_0c_0 + 2(b_0c_2 + b_1c_1 + b_2c_0)y^2 + \mathcal{O}(y^4)\big] \\ &\times (2 - \eta^2)(1 + \eta^2/8 + \mathcal{O}(\eta^4))\, dy\, d\eta. \end{aligned}$$

Here, $(2-\eta^2)(1+\eta^2/8+\mathcal{O}(\eta^4)) = 2(1 - \frac{3}{8}\eta^2 + \mathcal{O}(\eta^4))$ so changing to polar coordinates and computing the resulting integrals we obtain

$$I(E) = 2b_0c_0\pi E + \tfrac{1}{2}((b_0c_2 + b_1c_1 + b_2c_0) - \tfrac{3}{8}b_0c_0)\pi E^2 + \mathcal{O}(E^3),$$

and

$$S_2(E) = -\tfrac{1}{24}I''(E) = -\tfrac{1}{24}(b_0c_2 + b_1c_1 + b_2c_0 - \tfrac{3}{8}b_0c_0)\pi + \mathcal{O}(E).$$

Inserting the expressions for b_j and c_j gives (A.4). □

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References

[AMS90] J. Avron, P. v. Mouche, and B. Simon, *On the measure of the spectrum for the almost Mathieu operator*, Communications in Mathematical Physics, 132, no. 1, pp. 103-118. 1990.

[BeWi22] S. Becker and J. Wittsten, *Semiclassical quantization conditions in strained moiré lattices,* arXiv:2206.03349, (2022). To appear in Comm. Math. Phys.

[BeZw19] S. Becker and M. Zworski, *Magnetic oscillations in a model of graphene,* Comm. Math. Phys. **367** (2019), 941–989.

[CdV05] Y. Colin de Verdière, *Bohr-Sommerfeld rules to all orders,* Ann. Henri Poincaré (2005), 925–936.

[DSS24] I. Detherage, Z. Stier and N. Srivastava, *On the ground state energies of discrete and semi-classical Schrödinger operators,* arXiv:2405.05907, (2024).

[DiSj99] M. Dimassi and J. Sjöstrand, *Spectral Asymptotics in the Semi-Classical Limit*, Cambridge U Press, 1999.

[HelRob84] B. Helffer and D. Robert, *Puits de potentiel généralisés et asymptotique semi-classique*, Ann. Inst. H. Poincaré Phys. Théor. 41, 291–331, 1984.

[HelSj88] B. Helffer and J. Sjöstrand, *Analyse semi-classique pour l'équation de Harper (avec application à l'équation de Schrödinger avec champ magnétique)*. Mémoires de la Société Mathématique de France, Serie 2, no. 34 (1988).

[HelSj89b] B. Helffer and J. Sjöstrand, *Semiclassical analysis for Harper's equation.* III. *Cantor structure of the spectrum*, Mem. Soc. Math. France (N.S.) **39** (1989), 1–124.

[HiZw24] M. Hitrik and M. Zworski, *Overdamped QNM for Schwarzschild black holes.*

[KRL14] P. Kerdelhué, and J. Royo-Letelier, *On the low lying spectrum of the magnetic Schrödinger operator with kagome periodicity*, Reviews in Mathematical PhysicsVol. 26, No. 10, 1450020 (2014).

[Zw12] M. Zworski, *Semiclassical Analysis*, Graduate Studies in Mathematics **138**, AMS, 2012.

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