THE ESSENTIAL SPECTRUM
OF SCHRÖDINGER, JACOBI, AND CMV OPERATORS

By

YORAM LAST*‡ AND BARRY SIMON†‡

Abstract. We provide a very general result which identifies the essential spectrum of broad classes of operators as exactly equal to the closure of the union of the spectra of suitable limits at infinity. Included is a new result on the essential spectra when potentials are asymptotic to isospectral tori. We also recover within a unified framework the HVZ Theorem and Krein's results on orthogonal polynomials with finite essential spectra.

1 Introduction

One of the simplest but also most powerful ideas in spectral theory is Weyl's theorem, of which a typical application is

Theorem 1.1. *If V, W are bounded functions on $\mathbb{R}^\nu$ and*

$$\lim_{|x|\to\infty} [V(x) - W(x)] = 0,$$

then

$$\sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta + W)\,. \tag{1.1}$$

(In this Introduction, in order to avoid technicalities, we take potentials bounded.) Our goal in this paper is to find a generalization of this result which allows "slippage" near infinity. Typical of our results are the following.

Theorem 1.2. *Let V be a bounded periodic function on $(-\infty, \infty)$ and H_V the operator $-d^2/dx^2 + V(x)$ on $L^2(\mathbb{R})$. For $x > 0$, define $W(x) = V(x + \sqrt{x})$ and let*

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H_W be $-d^2/dx^2 + W(x)$ on $L^2(0,\infty)$ with some selfadjoint boundary conditions at zero. Then

$$\sigma_{\text{ess}}(H_W) = \sigma(H_V). \tag{1.2}$$

Theorem 1.3. *Let α be irrational and let H be the discrete Schrödinger operator on $\ell^2(\mathbb{Z})$ with potential $\lambda\cos(\alpha n)$. Let $\widetilde{H}$ be the discrete Schrödinger operator on $\ell^2(\{0,1,2,\dots\})$ with potential $\lambda\cos(\alpha n + \sqrt{n})$. Then*

$$\sigma_{\text{ess}}(\widetilde{H}) = \sigma(H). \tag{1.3}$$

Our original motivation in this work was extending a theorem of Barrios–López [9] in the theory of orthogonal polynomials on the unit circle (OPUC); see [77, 78].

Theorem 1.4 (see Example 4.3.10 of [77]). *Let $\{\alpha_n\}_{n=0}^\infty$ be a sequence of Verblunsky coefficients such that for some $a \in (0,1)$, one has*

$$\lim_{n\to\infty} |\alpha_n| = a, \qquad \lim_{n\to\infty} \frac{\alpha_{n+1}}{\alpha_n} = 1. \tag{1.4}$$

Then the CMV matrix for α_n has essential spectrum identical to the case $\alpha_n \equiv a$.

This goes beyond Weyl's theorem in that α_n may not approach a: rather $|\alpha_n| \to a$, but the phase is slowly varying and may not have a limit. The way to understand this result is to realize that $\alpha_n \equiv a$ is a periodic set of Verblunsky coefficients. For each $\lambda \in \partial\mathbb{D}$ ($\mathbb{D} = \{z : |z| < 1\}$), the set of periodic coefficients with the same essential spectrum is the constant sequence $\alpha_n = \lambda a$. Note that (1.4) says in a precise sense that the given α_n approach this isospectral torus. Our aim was to prove the following result.

Theorem 1.5. *If a set of Verblunsky coefficients or Jacobi parameters is asymptotic to an isospectral torus, then the essential spectrum of the corresponding CMV or Jacobi matrix is identical to the common essential spectrum of the isospectral torus.*

In Section 5, we make precise what we mean by "asymptotic to an isospectral torus." Theorem 1.5 gives a positive answer to Conjecture 12.2.3 of [78].

In the end, we found an extremely general result. To describe it, we recall some ideas in our earlier paper [49]. We first consider Jacobi matrices ($b_n \in \mathbb{R}$, $a_n > 0$)

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \cdots \\ a_1 & b_2 & a_2 & \cdots \\ 0 & a_2 & b_3 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix} \tag{1.5}$$

where, in line with our convention to deal with the simplest cases in this Introduction, we suppose there exists $K \in (0, \infty)$ such that

$$\sup_n |b_n| + \sup_n |a_n| + \sup_n |a_n|^{-1} \leq K. \tag{1.6}$$

A right limit point of J is a double-sided Jacobi matrix $J^{(r)}$ with parameters $\{a_n^{(r)}, b_n^{(r)}\}_{n=-\infty}^{\infty}$ so that there is a subsequence n_j with

$$a_{n_j+\ell} \to a_\ell^{(r)}, \qquad b_{n_j+\ell} \to b_\ell^{(r)} \tag{1.7}$$

as $j \to \infty$ for each fixed $\ell = 0, \pm 1, \pm 2, \dots$. In [49], we noted that

Proposition 1.6. *For each right limit point,* $\sigma(J^{(r)}) \subset \sigma_{\text{ess}}(J)$.

This is a basic result which many, ourselves included, regard as immediate. For if $\lambda \in \sigma(J^{(r)})$ and $\varphi^{(m)}$ is a sequence of unit trial functions with $\|(J^{(r)} - \lambda)\varphi^{(m)}\| \to 0$, then for any $j(m) \to \infty$, $\|(J - \lambda)\varphi^{(m)}(\cdot + n_{j(m)})\| \to 0$; and if $j(m)$ is chosen going to infinity fast enough, then $\varphi^{(m)}(\cdot - n_{j(m)}) \to 0$ weakly, so $\lambda \in \sigma_{\text{ess}}(J)$.

Let $\mathcal{R}$ be the set of right limit points. Clearly, Proposition 1.6 says that

$$\overline{\bigcup_{r \in \mathcal{R}} \sigma(J^{(r)})} \subset \sigma_{\text{ess}}(J). \tag{1.8}$$

Our new realization here for this example is

Theorem 1.7. *If* (1.6) *holds, then*

$$\overline{\bigcup_{r \in \mathcal{R}} \sigma(J^{(r)})} = \sigma_{\text{ess}}(J). \tag{1.9}$$

Remark. It is an interesting question whether anything is gained in (1.9) by taking the closure—that is, whether the union is already closed. In every example we can analyze, the union is closed. V. Georgescu has informed us that the methods of [27] imply that the union is always closed and that the details of the proof of this fact are the object of a paper in preparation.

Surprisingly, the proof is a rather simple trial function argument. The difficulty with such an argument tried naively is the following. To say that $J^{(r)}$ is a right limit point means that there exist $L_m \to \infty$ so that $J \restriction [n_{j(m)} - L_m, n_{j(m)} + L_m]$ shifted to $[-L_m, L_m]$ converges uniformly to $J^{(r)} \restriction [-L_m, L_m]$. But L_m might grow very slowly with m. Weyl's criterion says that if $\lambda \in \sigma_{\text{ess}}(J)$, there are trial functions φ_k supported on $[n_k - \tilde{L}_k, n_k + \tilde{L}_k]$ such that $\|(J - \lambda)\varphi_k\| \to 0$. By a compactness argument, one can suppose the n_k are actually $n_{j(m)}$'s for some right limit. The difficulty is that $\tilde{L}_m$ might grow much faster than L_m, so translated φ_k's are not good trial functions for $J^{(r)}$.

The key to overcoming this difficulty is to prove that one can localize trial functions in some interval of fixed size L, making a localization error of $O(L^{-1})$. This is what we do in Section 2. In this idea, we were motivated by arguments in Avron et al. [6], although to handle the continuum case, we need to work harder.

The use of localization ideas to understand essential spectrum, an implementation using double commutators, is not new—it goes back to Enss [23] and was raised to high art by Sigal [74]. Enss and Sigal, and also Agmon [1] and Gårding [25], later used these ideas and positivity inequalities to locate $\inf \sigma_{\text{ess}}(H)$, which suffices for the HVZ Theorem but not for some of our applications.

What distinguishes our approach and allows stronger results is that, first, we use trial functions exclusively and, second, as noted above, we study all of σ_{ess} rather than only its infimum. Third, and most significantly, we do not limit ourselves to sets that are cones near infinity but instead take balls. This gives us small operator errors rather than compact operator errors (although one can modify our arguments and take ball sizes that go to infinity slowly, and so get a compact localization error). This makes the method much more flexible.

While this paper is lengthy because of many different applications, the underlying idea is captured by the mantra "localization plus compactness." Here compactness means that resolvents restricted to balls of fixed size translated to zero lie in compact sets. We have in mind the topology of norm convergence once resolvents are multiplied by the characteristic functions of arbitrary fixed balls.

Because we need to control $\|(A-\lambda)\varphi\|^2$ and not just $\langle\varphi, (A-\lambda)\varphi\rangle$, if we used double commutators, we would need to control $[j, [j, (A-\lambda)^2]]$; so, in the continuum case, we get unbounded operators and the double commutator is complicated. For this reason, following [6] and [36], we use single commutators and settle for an inequality rather than the equality one gets from double commutators.

After we completed this paper and released a preprint, we learned of some related work using C^*-algebra techniques to compute $\sigma_{\text{ess}}(H)$ as the closure of a union of spectra of asymptotic Hamiltonians at infinity; see Georgescu–Iftimovici [27] and Măntoiu [56]. Further work is in [4, 26, 28, 29, 57, 71]. We also learned of very recent work of Rabinovich [67], based in part on [48, 62, 65, 66, 68, 69], using the theory of Fredholm operators to obtain results on the essential spectrum as a union of spectra of suitable limits at infinity.

Thus, the notion that in great generality the essential spectra is a union of spectra of limits at infinity is not new. Our contributions are twofold. First, some may find our direct proof via trial functions more palatable than arguments relying on considerable machinery. Second, the examples of Section 4, Section 5, and Section 7(b), (c) are (so far as we know) new, although it is certainly true that the methods of [27, 56, 67] can analyze some or even all these examples. In particular, we settle Conjecture 12.2.3 of [78].

There is obviously considerable overlap in philosophies (which, after all, both extend the ideas of the HVZ Theorem) and results in these papers. The techniques seem to be rather different, although we suspect a translation of the C^*-algebra machinery to more prosaic terms may reveal similarities that are, for now, not clear to us.

The paper [28] has results stated without reference to C^*-algebras (although the proofs use them); our Theorems 3.7 and 3.12 are special cases of Theorem 1.1 of [28].

We present the localization lemmas in Section 2 and prove our main results in Section 3. Section 4 discusses an interesting phenomena involving Schrödinger operators with severe oscillations at infinity. Section 5 has the applications to potentials asymptotic to isospectral tori and includes results stronger than Theorems 1.2, 1.3, and 1.5. In particular, we settle positively Conjecture 12.2.3 of [78]. Section 6 discusses the HVZ Theorem, and Section 7 other applications. Section 8 discusses magnetic fields.

We can handle the common Schrödinger operators associated to quantum theory with or without magnetic fields as well as orthogonal polynomials on the real line (OPRL) and unit circle (OPUC).

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2 Localization estimates

Here we use localization formulae but with partitions of unity concentrated on balls of fixed size in place of the previous applications which typically take j's homogeneous of degree zero near infinity. Also, we use single commutators.

Let $\mathcal{H}$ be a separable Hilbert space and A a selfadjoint operator on $\mathcal{H}$. Let $\{j_\alpha\}$ be a set of bounded selfadjoint operators indexed by either a discrete set S, like $\mathbb{Z}^\nu$, or by $\alpha \in \mathbb{R}^\nu$. In the latter case, we suppose that j_α is measurable and uniformly bounded in α. We assume that $\{j_\alpha\}$ is a partition of unity, namely,

$$\sum_{\alpha\in S} j_\alpha^2 = 1 \qquad \text{or} \qquad \int_{\alpha\in\mathbb{R}^\nu} j_\alpha^2 \, d^\nu\alpha = 1 \tag{2.1}$$

where the convergence of the sum or the meaning of the integral is in the weak operator topology sense. Two examples which often arise are $\mathcal{H} = \ell^2(\mathbb{Z}^\nu)$, $\psi \in \ell^2(\mathbb{Z}^\nu)$ real-valued with $\sum_n \psi(n)^2 = 1$, and $\{j_m\}_{m\in\mathbb{Z}^\nu}$ is multiplication by $\psi(\cdot - m)$, or $\mathcal{H} = L^2(\mathbb{R}^\nu, d^\nu x)$, $\psi \in L^2(\mathbb{R}^\nu, d^\nu x) \cap L^\infty(\mathbb{R}^\nu, d^\nu x)$ real-valued with $\int \psi(x)^2 \, d^\nu x = 1$, and $\{j_y\}_{y\in\mathbb{R}^\nu}$ is multiplication by $\psi(\cdot - y)$.

Assume that for each α, j_α maps the domain of A to itself and let φ be a vector in the domain of A. Observe that

$$\begin{aligned} \|Aj_\alpha\varphi\|^2 &= \|(j_\alpha A + [A, j_\alpha])\varphi\|^2 \\ &\le 2\|j_\alpha A\varphi\|^2 + 2\|[A, j_\alpha]\varphi\|^2. \end{aligned} \tag{2.2}$$

Thus

Proposition 2.1.

$$\sum_\alpha \|Aj_\alpha\varphi\|^2 \le 2\|A\varphi\|^2 + \langle\varphi, C\varphi\rangle \tag{2.3}$$

where

$$C = 2\sum_\alpha -[A, j_\alpha]^2. \tag{2.4}$$

Remark. Since $[A, j_\alpha]$ is skew-adjoint, $-[A, j_\alpha]^2 = [j_\alpha, A]^*[j_\alpha, A] \ge 0$.

Proof. (2.3) is immediate from (2.2) since

$$\sum_\alpha \|j_\alpha A\varphi\|^2 = \sum_\alpha \langle A\varphi, j_\alpha^2 A\varphi\rangle = \|A\varphi\|^2 \tag{2.5}$$

and

$$\|[A, j_\alpha]\varphi\|^2 = -\langle\varphi, [A, j_\alpha]^2\varphi\rangle. \tag{2.6}$$

□

Theorem 2.2. *There exists α such that $j_\alpha\varphi \ne 0$ and*

$$\|Aj_\alpha\varphi\|^2 \le \left\{2\left(\frac{\|A\varphi\|}{\|\varphi\|}\right)^2 + \|C\|\right\}\|j_\alpha\varphi\|^2. \tag{2.7}$$

Proof. Denote the quantity in brackets in (2.7) by d. Then, since $\|\varphi\|^2 = \sum_\alpha \|j_\alpha\varphi\|^2$, (2.3) implies

$$\sum_\alpha [\|Aj_\alpha\varphi\|^2 - d\|j_\alpha\varphi\|^2] \leq 0,$$

so at least one term with $\|j_\alpha\varphi\| \neq 0$ is nonpositive. □

To deal with unbounded A's, we suppose that $\sqrt{C}$ is A-bounded.

Theorem 2.3. *Suppose A is unbounded and*

$$\langle\varphi, C\varphi\rangle \leq \delta(\|A\varphi\|^2 + \|\varphi\|^2). \tag{2.8}$$

Then there exists an α with $j_\alpha\varphi \neq 0$ such that

$$\|Aj_\alpha\varphi\|^2 \leq \left\{(2+\delta)\frac{\|A\varphi\|^2}{\|\varphi\|^2} + \delta\right\}\|j_\alpha\varphi\|^2. \tag{2.9}$$

Proof. By (2.3) and (2.8), we have

$$\sum_\alpha \|Aj_\alpha\varphi\|^2 \leq (2+\delta)\|A\varphi\|^2 + \delta\|\varphi\|^2.$$

As before, (2.9) follows. □

3 The essential spectrum

This is the central part of this paper. We begin with Theorem 1.7, the simplest of our results.

Proof of Theorem 1.7. We have already proved (1.8) in the remarks after Proposition 1.6, so suppose $\lambda \in \sigma_{\text{ess}}(J)$. Recall Weyl's criterion, $\lambda \in \sigma_{\text{ess}}(J)$ if and only if there exist unit vectors $\varphi_m \xrightarrow{w} 0$ with $\|(J-\lambda)\varphi_m\| \to 0$.

Given ε, pick a trial sequence $\{\varphi_m\}$ such that each φ_m is supported in $\{n : n > m\}$ and

$$\|(J-\lambda)\varphi_m\|^2 \leq \tfrac{1}{3}\varepsilon^2\|\varphi_m\|^2; \tag{3.1}$$

we can do this by Weyl's criterion, since $f_j \xrightarrow{w} 0$ implies $\sum_{n<m}|f_j(n)|^2 \to 0$ for each m.

For $L = 1, 2, 3, \ldots$, let

$$\psi_L(n) = \begin{cases} \frac{n-1}{L}, & n = 1, 2, \ldots, L \\ \frac{2L-1-n}{L}, & n = L, L+1, \ldots, 2L-1 \\ 0, & n \geq 2L-1 \end{cases} \tag{3.2}$$

and let

$$c_L^2 = \sum_n |\psi_L(n)|^2, \tag{3.3}$$

so that $c_L \sim L^{1/2}$ in the sense that for some $0 < a \le b < \infty$,

$$aL^{1/2} \le c_L \le bL^{1/2}. \tag{3.4}$$

For $\alpha = 1, 2, \dots$, let

$$j_{\alpha,L}(n) = c_L^{-1}\psi_L(n+\alpha). \tag{3.5}$$

Then, by (3.3),

$$\sum_\alpha j_{\alpha,L}^2 \equiv 1. \tag{3.6}$$

Since $|\psi_L(n+1) - \psi_L(n)| \le L^{-1}$, we have

(3.7)

$$|\langle \delta_n, [j_{\alpha,L}, J]\delta_m\rangle| = \begin{cases} \sup_n |a_n|\, c_L^{-1}L^{-1} & \text{if } |n-m| = 1 \text{ and } |n-\alpha-L| \le L, \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, $C \equiv \sum_\alpha 2[j_{\alpha,L}, J]^2$ is a 5-diagonal matrix with matrix elements bounded by

$$2 \cdot 2(2L)c_L^{-2}L^{-2}\big(\sup_n |a_n|\big)^2, \tag{3.8}$$

where the second two comes from the number of k's which make a nonzero contribution to $\langle \delta_n, [j_{\alpha,L}, J]\delta_k\rangle\langle \delta_k, [j_{\alpha,L}, J]\delta_m\rangle$. By (3.4), there is a constant K depending on $\sup_n|a_n|$ such that

$$\|C\| \le KL^{-2}. \tag{3.9}$$

Picking L so that $KL^{-2} < \varepsilon^2/3$, we see by Theorem 2.2 that there exists j_{α_m} such that $\|j_{\alpha_m}\varphi_m\| \neq 0$ and

$$\|(J-\lambda)j_{\alpha_m}\varphi_m\| \le \varepsilon\|j_{\alpha_m}\varphi_m\|. \tag{3.10}$$

The intervals

$$I_m = [\alpha_m + 1, \alpha_m + 2L - 1]$$

which support $j_{\alpha_m}\varphi_m$ have fixed size and move out to infinity since $I_m \subset \{n : n \ge m - L\}$. Since the set of real numbers with $|b| + |a| + |a|^{-1} \le K$ is compact and L is finite, we can find a right limit point $J^{(r)}$ such that a subsequence of $J \restriction I_m$ translated by $\alpha_m + L$ converges to $J^{(r)} \restriction [1-L, L-1]$. Using translations of the trial functions $j_{\alpha_m}\varphi_m$, we find ψ_m such that

$$\lim_{m\to\infty} \frac{\|(J^{(r)} - \lambda)\psi_m\|}{\|\psi_m\|} \leq \varepsilon, \tag{3.11}$$

which means

$$\operatorname{dist}(\lambda, \sigma(J^{(r)})) \leq \varepsilon. \tag{3.12}$$

Since ε is arbitrary, we have $\lambda \in \overline{\bigcup \sigma(J^{(r)})}$. □

We have been pedantically careful in the proof above so that below we can be much briefer and just relate to this idea as "localization plus compactness" and not provide details.

We turn next to the CMV matrices defined by a sequence of Verblunsky coefficients $\{\alpha_j\}_{j=0}^\infty$ with $\alpha_j \in \mathbb{D}$. We define the unitary 2×2 matrix $\Theta(\alpha) = \left(\begin{smallmatrix} \overline{\alpha} & \rho \\ \rho & -\alpha \end{smallmatrix}\right)$, where $\rho = (1-|\alpha|^2)^{1/2}$, and $\mathcal{L} = \Theta_0 \oplus \Theta_2 \oplus \Theta_4 \oplus \cdots$, $\mathcal{M} = 1 \oplus \Theta_1 \oplus \Theta_3 + \cdots$, where 1 is a 1×1 matrix and $\Theta_j = \Theta(\alpha_j)$. Then the CMV matrix is the unitary matrix $\mathcal{C} = \mathcal{L}\mathcal{M}$. Given a two-sided sequence $\{\alpha_j\}_{j=-\infty}^\infty$, we define $\tilde{\mathcal{L}} = \cdots \Theta_{-2} \oplus \Theta_0 \oplus \Theta_2$ and $\widetilde{\mathcal{M}} = \Theta_{-1} \oplus \Theta_1 \oplus \Theta_3 \oplus \cdots$ on $\ell^2(\mathbb{Z})$, where Θ_j acts on the span of δ_j and δ_{j+1}. We set $\tilde{\mathcal{C}} = \tilde{\mathcal{L}}\widetilde{\mathcal{M}}$. See [77, 78] for a discussion of the connection of CMV and extended CMV matrices to OPUC.

Note that in [77, 78], the symbol $\tilde{\mathcal{C}}$ is used for the very different purpose of denoting transpose of $\mathcal{C}$ (alternate CMV matrix).

If $\{\alpha_j\}_{j=0}^\infty$ is a set of Verblunsky coefficients with

$$\sup_j |\alpha_j| < 1, \tag{3.13}$$

we call $\{\beta_j\}_{j=-\infty}^\infty$ a right limit point if there is a sequence m_j so that for $\ell = 0, \pm 1, \dots,$

$$\lim_{j\to\infty} \alpha_{m_j+\ell} = \beta_\ell, \tag{3.14}$$

and we call $\tilde{\mathcal{C}}(\beta)$ a right limit of $\mathcal{C}(\alpha)$.

Theorem 3.1. *Let $\mathcal{C}(\alpha)$ be the CMV matrix of a sequence obeying* (3.13). *Let $\mathcal{R}$ be the set of right limit extended CMV matrices. Then*

$$\sigma_{\text{ess}}(\mathcal{C}(\alpha)) = \overline{\bigcup_{\mathcal{R}} \tilde{\mathcal{C}}(\beta)}. \tag{3.15}$$

Proof. The arguments of Section 2 extend to unitary A if $-[j_\alpha, A]^2$ is replaced by $[j_\alpha, A]^*[j_\alpha, A]$. Matrix elements of $[j_\alpha, \mathcal{C}]$ are bounded by $\sup_{n,|k|\leq 2}|j_\alpha(n+k) - j_\alpha(n)|$ since $\mathcal{C}$ has matrix elements bounded by 1 and is 5-diagonal. Thus, C is 9-diagonal; otherwise, the argument extends with no change since $\{\alpha : |\alpha| \leq \sup_j |\alpha_j|\}$ is a compact subset of $\mathbb{D}$. □

Next, we remove the condition that $\sup|\alpha_j| < 1$ in the OPUC case and the conditions $\sup|b_j| < \infty$ and $\inf|a_j| > 0$ in the OPRL case. The key, of course, is to preserve compactness, that is, existence of limit points; to do that, we need only extend the notion of right limit.

If $\{\alpha_j\}_{j=-\infty}^{\infty}$ is a two-sided sequence in $\overline{\mathbb{D}}$, one can still define $\tilde{\mathcal{C}}(\alpha_j)$ since $\Theta(\alpha_j)$ makes sense. If $|\alpha_j| = 1$, then $\rho_j = 0$ and $\Theta(\alpha_j) = \begin{pmatrix} \overline{\alpha}_j & 0 \\ 0 & -\alpha_j \end{pmatrix}$ is a direct sum in such a way $\mathcal{L}$ and $\mathcal{M}$ both decouple into direct sums on $\ell^2(-\infty, j] \oplus \ell^2[j+1, \infty)$, so $\mathcal{C}$ decouples. If a single α_j has $|\alpha_j| = 1$, we decouple into two semi-infinite matrices (both related by unitary transforms to ordinary CMV matrices), but if more than one α_j has $|\alpha_j| = 1$, there are finite direct summands.

In any event, we can define $\tilde{\mathcal{C}}(\alpha_j)$ for $\{\alpha_j\} \in \times_{j=-\infty}^{\infty} \overline{\mathbb{D}}$ and define right limit points of $\mathcal{C}(\alpha_j)$ even if $\sup|\alpha_j| = 1$. Since matrix elements of $\mathcal{C}$ are still bounded by 1, $\mathcal{C}$ is still 5-diagonal and $\times_{j=-\infty}^{\infty} \overline{\mathbb{D}}$ is compact, we immediately have

Theorem 3.2. *With the extended notion of $\tilde{\mathcal{C}}$, Theorem 3.1 holds even if* (3.13) *fails.*

For bounded Jacobi matrices, we still want $\sup(|a_n| + |b_n|) < \infty$, but we do not need $\inf|a_n| > 0$. Again, the key is to allow two-sided Jacobi matrices J_r with some $a_n = 0$, in which case J_r decouples on $\ell^2(-\infty, n] \oplus \ell^2[n+1, \infty)$. If a single $a_n = 0$, there are two semi-infinite matrices. If more than one $a_n = 0$, there are finite Jacobi summands. Again, with no change in proof except for the change in the meaning of right limits to allow some $a_n^{(r)} = 0$, we have

Theorem 3.3. *Theorem 1.7 remains true if* (1.6) *is replaced by*

$$\sup_n \, (|a_n| + |b_n|) < \infty \tag{3.16}$$

so long as $J^{(r)}$ are allowed with some $a_n^{(r)} = 0$.

In Section 7, we use Theorems 3.2 and 3.3 to complement the analysis of Krein (which appeared in Akhiezer–Krein [3]) for bounded Jacobi matrices with finite essential spectrum and of Golinskii [30] for OPUC with finite derived sets.

Our commutator argument requires that $|a_n|$ is bounded, but one can also handle $\limsup|b_n| = \infty$. It is useful to make the following

Definition. Let A be a possibly unbounded selfadjoint operator. We say that $+\infty$ lies in $\sigma_{\text{ess}}(A)$ if $\sigma(A)$ is not bounded above, and $-\infty$ lies in $\sigma_{\text{ess}}(A)$ if $\sigma(A)$ is not bounded below.

We now allow two-sided Jacobi matrices, $\tilde{J}$, with $b_n = +\infty$ and/or $b_n = -\infty$ (and also $a_n = 0$). If $|b_n| = \infty$, we decouple into $\ell^2(-\infty, n-1] \oplus \ell^2[n+1, \infty)$ and place b_n in "$\sigma_{\text{ess}}(\tilde{J})$." With this extended definition, we still have compactness, that is, for any intervals in $\mathbb{Z}_+$, $I_1, I_2, \dots$ of fixed finite size ℓ with $\ell^{-1} \sum_{j \in I_n} j \to \infty$, there is a subsequence converging to a set of Jacobi parameters with possibly $b_n = +\infty$ or $b_n = -\infty$. We therefore have

Theorem 3.4. *Theorem 1.7 remains true if* (1.6) *is replaced by*

$$\sup_n |a_n| < \infty \tag{3.17}$$

so long as $J^{(r)}$ are allowed to have some $a_n^{(r)} = 0$ and/or some $b_n^{(r)} = \pm\infty$.

Remarks. 1. This includes the conventions on when $\pm\infty$ lies in $\sigma_{\text{ess}}(J)$. To prove this requires a simple separate argument. Namely, $\langle \delta_n, J\delta_n \rangle = b_n$, so $b_n \in$ numerical range of $J =$ convex hull of $\sigma(J)$. Thus, if $b_{n_j} \to \pm\infty$, then $\pm\infty \in \sigma(J)$.

2. If $\sup_n |a_n| = \infty$, σ_{ess} can be very subtle; see [43, 44].

Next, we turn to Jacobi matrices on $\mathbb{Z}^\nu$ (including $\nu = 1$), that is, J acts on $\ell^2(\mathbb{Z}^\nu)$ via

$$(Ju)(n) = \sum_{|m-n|=1} a_{(n,m)} u(m) + \sum_n b_n u(n), \tag{3.18}$$

where the b_n's are indexed by $n \in \mathbb{Z}^\nu$ and the $a_{(n,m)}$'s by bonds $\{m, n\}$ (unordered pairs) with $|m - n| = 1$. For simplicity of exposition, we suppose

$$\sup_{|m-n|=1} \left(|a_{(n,m)}| + |a_{(n,m)}|^{-1}\right) + \sup_n |b_n| < \infty, \tag{3.19}$$

although we can, as above, also handle some limits with $a_{(n,m)} = 0$ or some $|b_n| = \infty$. With no change, one can also control finite-range off-diagonal terms; and with some effort on controlling $[j_\alpha, J]$, it should be possible to control infinite-range off-diagonal terms with sufficiently rapid off-diagonal decay.

Let us call $\tilde{J}$ a limit point of J at infinity if and only if there are points $n_j \in \mathbb{Z}^\nu$ with $n_j \to \infty$ so that for every finite k, ℓ,

$$b_{n_j+\ell} \to \tilde{b}_\ell, \qquad a_{(n_j+\ell, n_j+k)} \to \tilde{a}_{(k,\ell)}. \tag{3.20}$$

Let $\mathcal{L}$ denote the set of limits $\tilde{J}$.

Theorem 3.5. *Let J be a Jacobi matrix of the form* (3.18) *on* $\ell^2(\mathbb{Z}^\nu)$. *Suppose* (3.19) *holds. Then,*

$$\sigma_{\rm ess}(J) = \overline{\bigcup_{\tilde{J}\in\mathcal{L}} \sigma(\tilde{J})}. \tag{3.21}$$

Proof. We can define partitions of unity $j_{\alpha,L}$ indexed by $\alpha \in \mathbb{Z}^\nu$ with $j_\alpha(n) \neq 0$ only if $|n-\alpha| \leq L$ and with $-\sum_\alpha [j_\alpha, J]^2$ bounded by $O(L^{-2})$. With this, the proof is the same as in the one-dimensional case. □

It is often comforting to consider only limit points in a single direction. Because the sphere is compact, this is easy.

Definition. Let $e \in S^{\nu-1}$, the unit sphere in $\mathbb{R}^\nu$. We say $\tilde{J}$ is a limit point in direction e if the n_j in (3.20) obey $n_j/|n_j| \to e$. We denote the limit points in direction e by $\mathcal{L}_e$.

Suppose $\tilde{J}$ is a limit point for J with sequence n_j. Since $S^{\nu-1}$ is compact, we can find a subsequence $n_{j(k)}$ so $n_{j(k)}/|n_{j(k)}| \to e_0$ for some e_0. The subsequence also converges to $\tilde{J}$, so $\tilde{J}$ is a limit point for direction e_0. Thus,

Theorem 3.6. *Let J be a Jacobi matrix of the form* (3.18) *on* $\ell^2(\mathbb{R}^\nu)$. *Suppose* (3.19) *holds. Then*

$$\sigma_{\rm ess}(J) = \overline{\bigcup_{e\in S^{\nu-1}} \bigcup_{\tilde{J}\in\mathcal{L}_e} \sigma(\tilde{J})}. \tag{3.22}$$

For example, if $\nu = 1$, we can consider left and right limit points.

Finally, we turn to Schrödinger operators. Here we need some kind of compactness condition of the $-\Delta + V$ that prevents V from oscillating wildly at infinity (but see the next section). We begin with a warmup case that is the core of our general case.

Theorem 3.7. *Let V be a bounded, uniformly continuous function on $\mathbb{R}^\nu$. For each $e \in S^\nu$, call W a limit of V in direction e if and only if there exists $x_j \in \mathbb{R}^\nu$ with $|x_j| \to \infty$ and $x_j/|x_j| \to e$ so that $V(x_j + y) \to W(y)$. Then, with $\mathcal{L}_e$ the limits in direction e,*

$$\sigma_{\rm ess}(-\Delta + V) = \overline{\bigcup_{e} \bigcup_{W\in\mathcal{L}_e} \sigma(-\Delta + W)}. \tag{3.23}$$

Remarks. 1. While we have not stated it explicitly, there is a result for half-line operators.

2. Uniform continuity means $\forall\varepsilon, \exists\delta$, so $|x-y| < \delta \Rightarrow |V(x) - V(y)| < \varepsilon$. It is not hard to see this is equivalent to $\{V(\cdot + y)\}_{y\in\mathbb{Z}^\nu}$ being equicontinuous.

3. This result appears in a more abstract formulation in Georgescu–Iftimovici [28].

Proof. As noted, uniform continuity implies uniform equicontinuity so, by the Arzela–Ascoli theorem (see [70]), given any sequence of balls $\{x : |x - y_j| \le L\}$, there exist e and W in $\mathcal{L}_e$ such that $V(\cdot + y_j) \to W(\cdot)$ uniformly on $\{x : |x| \le L\}$. This is the compactness needed for our argument.

To handle localization, pick any nonnegative rotation invariant C^∞ function ψ supported on $\{x : |x| \le 1\}$ with $\int \psi(x)^2 \, d^\nu x = 1$. Define $j_{x,L}$ as the operator of multiplication by the function

$$j_{x,L}(y) = L^{-\nu/2}\psi(L^{-1}(y - x))$$

and note that

$$\int j_{x,L}^2 \, d^\nu x = 1.$$

With $A = (-\Delta + V - \lambda)$ and $C = 2\int -[A, j_{x,L}]^2 \, d^\nu x$, we have (2.8) with $\delta = O(L^{-2})$, since $C = L^{-2}(c_1\Delta + c_2)$ for constants c_1 and c_2 (for C is translation and rotation invariant and scale covariant).

Now (3.23) follows in the usual way. □

Our final result in this section concerns Schrödinger operators with potentially singular V's. As in the last case, we suppose regularity at infinity. In the next section, we show how to deal with irregular oscillations near infinity. Recall the Kato class and norm [2, 20] is defined as follows.

Definition. $V : \mathbb{R}^\nu \to \mathbb{R}$ is said to live in the Kato class K_ν if and only if

$$\lim_{\alpha \downarrow 0} \left[\sup_x \int_{|x-y| \le \alpha} . |x - y|^{2-\nu} |V(y)| \, d^\nu y \right] = 0. \tag{3.24}$$

(If $\nu = 1, 2$, the definition is different. If $\nu = 2$, $|x-y|^{2-\nu}$ is replaced by $\log[|x-y|^{-1}]$, and if $\nu = 1$, we require $\sup_x \int_{|x-y|\le 1} |V(y)| \, dy < \infty$.) The K_ν norm is defined by

$$\|V\|_{K_\nu} = \sup_x \int_{|x-y| \le 1} |x - y|^{2-\nu} |V(y)| \, d^\nu y. \tag{3.25}$$

We introduce here the

Definition. $V : \mathbb{R}^\nu \to \mathbb{R}$ is called uniformly Kato if and only if $V \in K_\nu$ and

$$\lim_{y \downarrow 0} \|V - V(\cdot - y)\|_{K_\nu} = 0. \tag{3.26}$$

Example 3.8. Let

$$V(x) = \sin(x_1^2). \tag{3.27}$$

Then $V \in K_\nu$, but for $(x_0)_1$ large and $y = (\pi/2(x_0)_1, y_2, \dots)$, $[(x_0 + y)_1]^2 = (x_0)_1^2 + \pi + O(1/(x_0)_1)$; so for x near x_0, $V(x) - V(x-y) \sim 2V(x)$, and because of the $|V(\cdot)|$ in (3.25), we do not have (3.26). We discuss this further in the next section.

Example 3.9. We say p is canonical for $\mathbb{R}^\mu$ if $p = \mu/2$ where $\mu \geq 3$, $p > 2$ if $\mu = 2$, and $p = 1$ if $\mu = 1$. If

$$\sup_x \int_{|x-y|\leq 1} |V(y)|^p \, d^\mu y < \infty, \tag{3.28}$$

then $V \in K_\mu$ (see [20]). Moreover, if

$$\lim_{|x|\to\infty} \int_{|x-y|\leq 1} |V(y)|^p \, d^\mu y = 0, \tag{3.29}$$

it is easy to see that (3.26) holds because V is small at infinity, and (3.26) holds for L^p norm if $V \in L^p$.

Example 3.10. If $\pi \colon \mathbb{R}^\nu \to \mathbb{R}^\mu$ is a linear map onto $\mathbb{R}^\mu$ and $W \in K_\mu$, then $V(x) = W(\pi x)$ is in K_ν, and the K_ν norm of V is bounded by a π-dependent constant times the K_μ norm of W. If W obeys (3.26), so does V.

We combine Examples 3.9 and 3.10 in our study of the HVZ theorem.

Proposition 3.11. *Let V be a uniformly Kato potential on $\mathbb{R}^\nu$ and let $H_x = -\Delta + (\cdot - x)$. Then for any sequence $x_k \to \infty$, there is a subsequence $x_{k(m)}$ and a selfadjoint operator H_∞ such that if $z \in \mathbb{C}\backslash[a,\infty)$ for some $a \in \mathbb{R}$, then*

$$\|[(H_{x_{k(m)}} - z)^{-1} - (H_\infty - z)^{-1}]\chi_S\| \to 0, \tag{3.30}$$

where χ_S is the characteristic function of an arbitrary bounded set.

Remark. Formally, H_∞ is a Schrödinger operator of the form $H_0 + V_\infty$, but V_∞, as constructed, is only in the completion of K_ν, which is known to include some distributions (see [31, 55]).

Proof. It is known that if $W \in K_\nu$, then W is $-\Delta$ form bounded with relative bound zero with bounds depending only on K_ν norms (see [20]). Thus, since all V_x's have the same K_ν norm, we can find a such that $H_x \geq a$ for all x. It also means that for each $z \in \mathbb{C}\backslash[a,\infty)$, we can bound $\||W|^{1/2}(H_x - z)^{-1}\Delta^{1/2}\|$ by $c\|W\|_{K_\nu}$ with c only z-dependent and $\|V\|_{K_\nu}$-dependent.

Let φ be a C^∞ function of compact support and note (constants are z- or $\|V\|_{K_\nu}$-dependent)

$$\begin{aligned}\||W|^{1/2}[(H-z)^{-1},\varphi]\| &\le \|W^{1/2}(H-z)^{-1}[\Delta,\varphi](H-z)^{-1}\| \\ &\le c\|W^{1/2}(H-z)^{-1}\Delta^{1/2}\|\,\|\nabla\varphi\|.\end{aligned}$$

This in turn implies that if S_1 is a ball of radius r fixed about x_0 and S_2 a ball of radius $R > r$, then

$$\|W^{1/2}(1-\chi_{S_2})(H-z)^{-1}\chi_{S_1}\| \to 0$$

as $R \to \infty$. So, if $\|(W_n - W)\chi_S\|_{K_\nu} \to 0$ for all balls and $\sup_n \|W_n\|_{K_\nu} < \infty$, then

$$\|((-\Delta + W_n - z)^{-1} - (-\Delta + W - z)^{-1})\chi_S\| \to 0$$

for all S.

In this way, we see that if V is uniformly Kato and $V_{x_n} \to V_\infty$ in K_ν uniformly on all balls, then

$$\|[(H_{x_n} - z)^{-1} - (H_\infty - z)]^{-1}\chi_S\| \to 0. \tag{3.31}$$

The condition that V is uniformly Kato means convolutions of V with a C^∞ approximate identity converge to V in K_ν norm. Call the approximations $V^{(m)}$. Each is C^∞ with bounded derivatives and so, by the equicontinuity argument in Theorem 3.7, we can find $x_{j_m(n)}$ and $V_\infty^{(m)}$ such that

$$\|[(-\Delta + V^{(m)}_{x_{j_m(n)}} - z)^{-1} - (-\Delta + V^{(m)}_\infty - z)^{-1}]\chi_S\| \to 0.$$

Since $V_x^{(m)} \to V_x$ uniformly in x, a standard $\varepsilon/3$ argument (see [70]) shows that one can find $x_{j(m)}$ such that $\|[(H_{x_m} - z)^{-1} - (H_{x_{m'}} - z)^{-1}]\chi_S\|$ is small for each S as $m, m' \to \infty$. In this way, we obtain the necessary limit operator. □

Given V uniformly Kato, the limits constructed by Proposition 3.11 where $x_n/|x_n| \to e$ are called limits of H in direction e. Again, the next result appears in a more abstract setting in Georgescu–Iftimovici [28].

Theorem 3.12. *Let V be uniformly Kato. Let $\mathcal{L}_e$ denote the limits of H in direction e. Then*

$$\sigma_{\text{ess}}(H) = \overline{\bigcup_e \bigcup_{H_\infty \in \mathcal{L}_e} \sigma(H_\infty)}. \tag{3.32}$$

The papers that use C^*-algebras [27, 56] study $h(p) + V$ in place of $-\Delta + V$. These papers only required that $h(p) \to \infty$ as $p \to \infty$. It seems likely that for many such h's, our methods will work. The condition $h(p) \to \infty$ as $p \to \infty$ is critical in our approach to ensure that if $\varphi_n \to 0$ weakly and $\|(H - E)\varphi_n\| \to 0$, then $\chi_{\{x:|x|<R\}}\varphi_n \to 0$.

It is likely that one can develop a theory for $h(p) + V(x)$ without supposing $h(p) \to \infty$ or even $f(p, x)$, but one would need to consider limits at infinity in phase space, not just on configuration space.

Proof. We pick a so that $H_x \geq a$ for all x. Pick $z \in (-\infty, a)$ and let $\tilde{A}_x = (H_x - z)^{-1}$. As above, $\|[\tilde{A}_x, j_\alpha]\| \leq c\|\nabla j_\alpha\|$ for any j_α in C_0^∞. For $\lambda \in \sigma_{\text{ess}}(H)$, let $A = (H_x - z)^{-1} - (\lambda - z)^{-1}$. Theorem 2.2 provides the necessary localization estimate. Proposition 3.11 provides the necessary compactness. Then (3.32) is proved in the same way as earlier theorems. □

4 Schrödinger operators with severe oscillations at infinity

This section is an aside to note that the lack of uniformity at infinity which can occur if V is merely K_ν is irrelevant to essential spectrum. We begin with Example 3.8, the canonical example of severe oscillations at infinity.

Proposition 4.1. *Let*

$$W(x) = \sin(x^2) \tag{4.1}$$

on $(0, \infty)$ *and let* $H_0 = -d^2/dx^2$ *with* $u(0) = 0$ *boundary conditions. Then*

(1) $W(H_0 + 1)^{-1}$ *is not compact;*

(2) $(H_0 + 1)^{-1/2} W (H_0 - 1)^{-1/2}$ *is compact.*

Remarks. 1. Our proof of (1) shows that $Wf(H_0)$ is noncompact for any continuous $f \not\equiv 0$ on $(0, \infty)$.

2. Consideration of $W = \vec{\nabla} \cdot \vec{Q}$ potentials goes back to the 1970's; (see [8, 12, 13, 17, 18, 21, 40, 41, 58, 72, 73, 79]).

Proof. (1) Let φ be a nonzero $C_0^\infty(0, \infty)$ function in L^2 and let

$$\psi_n(x) = [(H_0 + 1)\varphi](x - n). \tag{4.2}$$

Then

$$\|W(H_0 + 1)^{-1}\psi_n\|^2 = \int W(x)^2 \varphi(x - n)^2 \, dx$$

$$= \tfrac{1}{2} \int \varphi(x)^2 \, dx - \tfrac{1}{2} \int \cos(2x^2) \varphi(x-n)^2 \, dx$$

$$\to \tfrac{1}{2} \int \varphi(x)^2 \, dx \neq 0 \tag{4.3}$$

by an integration by parts. Since $\psi_n \xrightarrow{w} 0$, this shows that $W(H_0 - 1)^{-1}$ is not compact.

(2) Since $\frac{d}{dx}[-\frac{1}{2x}\cos(x^2)] = \sin(x^2) + O(x^{-2})$, we see that

$$Q(x) = \lim_{y \to \infty} - \int_x^y W(z) \, dz$$

exists and

$$|Q(x)| \leq c(x+1)^{-1}. \tag{4.4}$$

Thus $W = [\frac{d}{dx}, Q]$, so

$$(H_0 + 1)^{-1/2} W (H_0 + 1)^{-1/2} = \Big((H_0 + 1)^{-1/2} \, d/dx \Big) (Q(H_0 + 1)^{-1/2}) + cc,$$

where cc stands for the adjoint of the first theorem. Since $(H_0 + 1)^{-1/2} d/dx$ is bounded and $Q(H_0 - 1)^{-1/2}$ is compact (by (4.4)), $(H_0 + 1)^{-1/2} W (H_0 + 1)^{-1/2}$ is compact. □

Thus, oscillations at infinity are irrelevant for the essential spectrum! While the slick argument above somewhat obscures the underlying physics, the reason such oscillations do not matter has to do with the fact that $\sigma_{\text{ess}}(H)$ involves fixed energy, and oscillations only matter at high energy. Our proof below implements this strategy more directly.

We begin by noting that the proof of Proposition 3.11 implies the following.

Theorem 4.2. *Suppose that V_n is a sequence of multiplicative operators satisfying*

(i) *for any $\varepsilon > 0$, there is C_ε such that*

$$\langle \varphi, |V_n| \varphi \rangle \leq \varepsilon \|\nabla \varphi\|^2 + C_\varepsilon \|\varphi\|^2 \tag{4.5}$$

for any n and all $\varphi \in Q(-\Delta)$;

(ii) *for any ball S about zero,*

$$\|(-\Delta + 1)^{-1/2} \chi_S (V_n - V_m)(-\Delta + 1)^{-1/2}\| \to 0 \tag{4.6}$$

as $n, m \to \infty$.

Then for any ball and $z \in \mathbb{C}\backslash[a, \infty)$,

$$\|[(-\Delta + V_n - z)^{-1} - (-\Delta + V_m - z)^{-1}]\chi_S\| \to 0. \tag{4.7}$$

Moreover, if (4.6) *holds as* $n \to \infty$ *with* V_m *replaced by some* V_∞, *then*

$$\lim_{n\to\infty} \|[(-\Delta + V_n - z)^{-1} - (-\Delta + V_\infty - z)^{-1}]\chi_S\| = 0. \tag{4.8}$$

As an immediate corollary, we obtain

Theorem 4.3. *Let* $V \in K_\nu$ *obey*

$$\lim_{R\to\infty} \sup_{|x|\geq R} \int_{|x-y|\leq 1} |x-y|^{-(\nu-2)}|V(y)|\, d^\nu y = 0. \tag{4.9}$$

Then

$$\sigma_{\text{ess}}(-\Delta + V) = [0, \infty). \tag{4.10}$$

Remark. If (4.9) holds, we say that V is K_ν small at infinity.

Proof. By Theorem 4.2, if $x_n \to \infty$,

$$\|[(-\Delta + V(\cdot - x_n) - z)^{-1} - (-\Delta - z)^{-1}]\chi_S\| \to 0; \tag{4.11}$$

so, in a sense, $-\Delta$ is the unique limit point at infinity. The standard localization argument proves (4.10). □

Here is the key to studying general $V \in K_\nu$ with no uniformity at infinity.

Proposition 4.4. *Let* V_n *be a sequence of functions supported in a fixed ball* $\{x : |x| \leq R\}$. *Suppose that*

$$\lim_{\alpha\downarrow 0} \sup_{n,x} \int_{|x-y|\leq\alpha} |x-y|^{-(\nu-2)}|V_n(y)|\, d^\nu y = 0. \tag{4.12}$$

Then there is a subsequence $V_{n(j)}$ *such that*

$$\lim_{j,k\to\infty} \|(-\Delta + 1)^{-1/2}(V_{n(j)} - V_{n(k)})(-\Delta + 1)^{-1/2}\| = 0. \tag{4.13}$$

Proof. Given K, let P_K be the projection in momentum space onto $|p| \leq K$ and $Q_K = 1 - P_K$. Then (4.12) implies that for any $\varepsilon > 0$,

$$\langle \varphi, |V_n|\varphi\rangle \leq \varepsilon\|\nabla\varphi\|^2 + C_\varepsilon\|\varphi\|^2 \tag{4.14}$$

for a fixed C_ε and all n. This implies that

$$\||V_n|^{1/2}(-\Delta + 1)^{-1/2}Q_K\|^2 \leq \varepsilon + C_\varepsilon(K^2 + 1)^{-1/2}, \tag{4.15}$$

so

$$\lim_{K\to\infty} \sup_n \||V_n|^{1/2}(-\Delta+1)^{-1/2}Q_K\| = 0. \tag{4.16}$$

Thus, by a standard diagonalization argument, it suffices to show that for each K, there is a subsequence such that

$$\lim_{j,k\to\infty} \|(-\Delta+1)^{-1/2}P_K(V_{n(j)} - V_{n(k)})P_K(-\Delta+1)^{-1/2}\| = 0. \tag{4.17}$$

In momentum space,

$$Q_n = (-\Delta+1)^{-1/2}P_K V_n P_K(-\Delta+1)^{-1/2} \tag{4.18}$$

has an integral kernel

$$Q_n(p,q) = \chi_{|p|\le K}(p)(p^2+1)^{-1/2}\widehat{V}_n(p-q)\chi_{|q|\le K}(q)(q^2+1)^{1/2}. \tag{4.19}$$

By (4.12) and the fixed support hypothesis, we have

$$\sup_n (\|V_n\|_{L_1} + \|\vec{x}V_n\|_{L^1}) < \infty, \tag{4.20}$$

so that

$$\sup_n (|\widehat{V}_n(k)| + |\nabla\widehat{V}_n(k)|) < \infty. \tag{4.21}$$

This means $\{V_n(k) : |k| \le 2K\}$ is a uniformly equicontinuous family, so we can find a subsequence such that

$$\lim_{j,k\to\infty} \sup_{|k|\le 2K} |\widehat{V}_{n(j)}(k) - \widehat{V}_{n(\ell)}(k)| = 0. \tag{4.22}$$

It follows from (4.19) that

$$\int |Q_{n(j)}(p,q) - Q_{n(\ell)}(p,q)|^2\, dpdq \to 0, \tag{4.23}$$

so (4.17) holds since the Hilbert–Schmidt norm dominates the operator norm. □

Given $V \in K_\nu$, we say that $\widetilde{H}$ is a limit point at infinity in direction e if there exist $x_n \to \infty$ with $x_n/|x_n| \to e$ such that for the characteristic function of any ball and $z \in \mathbb{C}\backslash[a,\infty)$, we have

$$\lim_{n\to\infty} \|[(-\Delta + V(x-x_n) - z)^{-1} - (\widetilde{H} - z)^{-1}]\chi_S\| = 0. \tag{4.24}$$

Let $\mathcal{L}_e$ denote the set of limit points in direction e. Our standard argument using Theorem 4.2 and Proposition 4.4 to get compactness implies

Theorem 4.5. *Let $V \in K_\nu$. Then*

$$\sigma_{\text{ess}}(-\Delta+V) = \overline{\bigcup_e \bigcup_{\widetilde{H}\in\mathcal{L}_e} \sigma(\widetilde{H})}. \tag{4.25}$$

5 Potentials asymptotic to isospectral tori

As a warmup, we prove the following result, which includes Theorem 1.2 as a special case. We consider functions $f\colon \mathbb{R}^\nu \to \mathbb{R}^\nu$ such that

$$\lim_{|x|\to\infty} \sup_{|y|\le L} |f(x) - f(x+y)| = 0 \tag{5.1}$$

for each L. For example, if f is C^1 outside some ball and $|\nabla f(x)| \to 0$ (e.g., $f(x) = \sqrt{x}(x/|x|)$), then (5.1) holds.

Theorem 5.1. *Let V be a function on $\mathbb{R}^\nu$, periodic in ν independent directions such that V is uniformly Kato (e.g., $V \in L^p_{\mathrm{loc}}$ with p a canonical value for $\mathbb{R}^\nu$). Suppose that either V is bounded or $|f(x) - f(y)| \le (1-\varepsilon)|x-y|$ for some $\varepsilon > 0$. Let f obey* (5.1)*. Let $W(x) = V(x + f(x))$. Then*

$$\sigma_{\mathrm{ess}}(-\Delta + W) = \sigma(-\Delta + V). \tag{5.2}$$

Remark. The condition that V is bounded or f is globally Lifschitz is needed to ensure that W is locally L^1. We thank V. Georgescu for pointing out to us the need for this condition, which was missing in our original preprint.

Proof. Let L be the integral lattice generated by some set of periods so that $V(x+\ell) = V(x)$ if $\ell \in L$. Let $\pi\colon \mathbb{R}^\nu \to \mathbb{R}^\nu/L$ be the canonical projection. If $x_j \in \mathbb{R}^\nu$, since $\mathbb{R}^\nu/L$ is compact, we can find a subsequence $m(j)$ such that $\pi((x_{m(j)}) + f(x_{m(j)})) \to x_\infty$. Then

$$-\Delta + W(\cdot - x_{m(j)}) \to -\Delta + V(x - x_\infty),$$

so the limits are translates of $-\Delta + V$, which all have the same essential spectrum. Now (5.2) is immediate from Theorem 3.12. □

Our next result includes Theorem 1.3.

Theorem 5.2. *Let $W\colon \mathbb{R}^d \to \mathbb{R}$ be bounded and continuous and satisfy*

$$W(x+a) = W(x) \tag{5.3}$$

for $a \in \mathbb{Z}^d$. Let $(\alpha_1, \dots, \alpha_d)$ be such that $\{(\alpha_1 n, \alpha_2 n, \dots, \alpha_d n) : n \in \mathbb{Z}\}$ is dense in $\mathbb{R}^d/\mathbb{Z}^d$ (i.e., $1, \alpha_1, \dots, \alpha_d$ are rationally independent). Let $f\colon \mathbb{Z} \to \mathbb{R}^d$ be such that

$$\lim_{n\to\infty} \sup_{|m|\le L} |f(n) - f(n+m)| = 0$$

for each L. Set $V_0(n) = W(\alpha n)$ and

$$V(n) = W(\alpha n + f(n)). \tag{5.4}$$

On $\ell^2(\mathbb{Z})$, *let* $(h_0 u)(n) = u(n+1) + u(n-1)$. *Then*

$$\sigma_{\text{ess}}(h_0 + V) = \sigma(h_0 + V_0). \tag{5.5}$$

Proof. For each $x \in \mathbb{R}^d/\mathbb{Z}^d$, define

$$V_x(n) = W(\alpha n + x). \tag{5.6}$$

Then a theorem of Avron–Simon [7] (see [20]) shows that $\sigma(h_0 + V_x)$ is independent of x (and purely essential). Given any sequence n_j, find a sequence $n_{j(m)}$ such that $f(n_{j(m)}) \to x_\infty$ in $\mathbb{R}^d/\mathbb{Z}^d$. Then $V(n + n_{j(m)}) \to V_{x_\infty}(n)$, so by Theorem 1.7,

$$\sigma_{\text{ess}}(h_0 + V) = \overline{\bigcup_x \sigma(h_0 + V_x)} = \sigma(h_0 + V_0).$$

□

Next, we turn to Theorem 1.5 in the OPUC case. Any set of periodic Verblunsky coefficients $\{\alpha_n\}_{n=0}^\infty$ with

$$\alpha_{n+p} = \alpha_n \tag{5.7}$$

for some p defines a natural function on $\mathbb{C}\backslash\{0\}$, $\Delta(z) = z^{-p/2}\text{Tr}(T_p(z))$, where T_p is a transfer matrix; see Section 11.1 of [78]. (If p is odd, Δ is double-valued; see Chapter 11 of [78] for how to handle odd p.) The function Δ is real on $\partial\mathbb{D}$, and $\sigma_{\text{ess}}(\mathcal{C}(\alpha))$ is a union of ℓ disjoint intervals, where $\ell \leq p$ (generically, $\ell = p$). As proved in Chapter 11 of [78],

$$\{\beta \in \mathbb{D}^p : \Delta(z; \{\beta_{n \bmod p}\}_{n=0}^\infty) = \Delta(z; \alpha)\} \equiv T_\alpha \tag{5.8}$$

is an ℓ-dimensional torus, called the isospectral torus. Moreover, the two-sided CMV matrix, defined by requiring (5.8) for all $n \in \mathbb{Z}$, has

$$\sigma(\tilde{\mathcal{C}}(\beta)) = \sigma_{\text{ess}}(\mathcal{C}(\alpha)) \tag{5.9}$$

for any $\beta \in T_\alpha$.

Given two sequences $\{\kappa_n\}_{n=0}^\infty$ and $\{\lambda_n\}_{n=0}^\infty$ in $\mathbb{D}^p$, define

$$d(\kappa, \lambda) \equiv \sum_{n=0}^\infty e^{-n}|\kappa_n - \lambda_n|. \tag{5.10}$$

Convergence in d-norm is the same as sequential convergence. We define

$$d(\kappa, T_\alpha) = \inf_{\beta \in T_\alpha} d(\kappa, \beta).$$

A sequence γ_n is called asymptotic to T_α if

$$\lim_{m\to\infty} d(\{\gamma_{n+m}\}_{n=0}^\infty, T_\alpha) = 0. \tag{5.11}$$

Then the OPUC case of Theorem 1.5 (settling Conjecture 12.2.3 of [78]) asserts the following.

Theorem 5.3. *Let* (5.11) *hold. Then*

$$\sigma_{\mathrm{ess}}(\mathcal{C}(\{\gamma_n\}_{n=0}^\infty)) = \sigma_{\mathrm{ess}}(\mathcal{C}(\{\alpha_n\}_{n=0}^\infty)). \tag{5.12}$$

Proof. The right limit points are a subset of

$$\{\tilde{\mathcal{C}}(\{\beta_{n \bmod p}\}_{n=-\infty}^\infty) : \{\beta\}_{n=0}^{p-1} \in T_\alpha\},$$

so by Theorem 3.1 and (5.9), (5.12) holds. □

By the same argument using isospectral tori for periodic Jacobi matrices [24, 46, 47, 83] and for Schrödinger operators [22, 52, 59], one has

Theorem 5.4. *If T is the isospectral torus of a given periodic Jacobi matrix, $\tilde{J}$, and J has Jacobi parameters satisfying*

$$\lim_{n\to\infty} \min_{\tilde{a},\tilde{b}\in T} \sum_{\ell=1}^\infty [|a_{n+\ell} - \tilde{a}_\ell| + |b_{n+\ell} - \tilde{b}_\ell|]e^{-\ell} = 0, \tag{5.13}$$

then

$$\sigma_{\mathrm{ess}}(J) = \sigma(\tilde{J}). \tag{5.14}$$

Theorem 5.5. *Let T be the isospectral torus of a periodic potential V_0 on $\mathbb{R}$ and V on $[0,\infty)$ in K_1 and suppose that*

$$\lim_{|x|\to\infty} \inf_{W\in T} \int_0^\infty |V(y+x) - W(y)|e^{-|y|}\, dy = 0. \tag{5.15}$$

Then

$$\sigma_{\mathrm{ess}}\left(-\frac{d^2}{dx^2} + V\right) = \sigma\left(-\frac{d^2}{dx^2} + V_0\right), \tag{5.16}$$

where $-d^2/dx^2 + V$ is defined on $L^2(0,\infty)$ with $u(0) = 0$ boundary conditions and $-d^2/dx^2 + V_0$ is defined on $L^2(\mathbb{R}, dx)$.

The following provides an alternate proof of Theorem 4.3.8 of [77].

Theorem 5.6. *Let $\{\alpha_j\}_{j=0}^\infty$ and $\{\beta_j\}_{j=0}^\infty$ be two sequences of Verblunsky coefficients. Suppose there exist $\lambda_j \in \partial\mathbb{D}$ such that*

$$\text{(i)} \qquad \beta_j\lambda_j - \alpha_j \to 0; \tag{5.17}$$

$$\text{(ii)} \qquad \lambda_{j+1}\bar{\lambda}_j \to 1. \tag{5.18}$$

Then

$$\sigma_{\mathrm{ess}}(\mathcal{C}(\{\alpha_j\}_{j=0}^\infty)) = \sigma_{\mathrm{ess}}(\mathcal{C}(\{\beta_j\}_{j=0}^\infty)). \tag{5.19}$$

Proof. Let $\{\gamma_j\}_{j=-\infty}^{\infty}$ be a right limit of $\{\beta_j\}_{j=0}^{\infty}$, that is, $\beta_{\ell+n_k} \to \gamma_\ell$ for some n_k. By passing to a subsequence, we can suppose $\lambda_{n_j} \to \lambda_\infty$, in which case (5.18) implies $\lambda_{n_j+\ell} \to \lambda_\infty$ for each ℓ fixed. By (5.17), $\{\lambda_\infty \gamma_j\}_{j=-\infty}^{\infty}$ is a right limit of $\{\alpha_j\}_{j=0}^{\infty}$. Since $\sigma(\tilde{C}(\{\lambda\gamma_j\}_{j=-\infty}^{\infty}))$ is λ-independent, (5.19) follows from (3.15). □

6 The HVZ Theorem

For simplicity of exposition, we begin with a case with an infinitely-heavy particle; eventually we consider a situation even more general than arbitrary N-body systems. Thus, H acts on $L^2(\mathbb{R}^{\mu(N-1)}, dx)$ with

(6.1) $$H = -\sum_{j=1}^{N-1} (2m_j)^{-1}\Delta_{x_j} + \sum_{j=1}^{N-1} V_{0j}(x_j) + \sum_{1\le i<j\le N-1} V_{ij}(x_j - x_i)$$

where $x = (x_1, \ldots, x_{N-1})$ with $x_j \in \mathbb{R}^\mu$. Here the V's are in K_μ with K_μ vanishing at infinity. Let a denote a partition $(C_1, \ldots, C_\ell)$ of $\{0, \ldots, N-1\}$ onto $\ell \ge 2$ clusters. We say $(ij) \subset a$ if i, j are in the same cluster $C \in a$, and $(ij) \not\subset a$ if $i \in C_k$ and $j \in C_m$ with $k \neq m$. Let

(6.2) $$H(a) = H - \sum_{\substack{ij\not\subset a\\ i<j}} V_{ij}(x_j - x_i)$$

with $x_0 \equiv 0$. The HVZ Theorem says that

Theorem 6.1. *If each V_{ij} is in K_μ, K_μ vanishing at infinity, then*

(6.3) $$\sigma_{\text{ess}}(H) = \overline{\bigcup_a \sigma(H(a))}.$$

Since $H(a)$ commutes with translations of clusters, H has the form $H(a) = T^a \otimes 1 + 1 \otimes H_a$, where T^a is a Laplacian on $\mathbb{R}^{\mu(\ell-1)}$. Thus, if $\Sigma(a) = \inf \sigma(H_a)$, then $\sigma(H(a)) = [\Sigma(a), \infty)$. So (6.3) says

(6.4) $$\sigma_{\text{ess}}(H) = [\Sigma, \infty), \qquad \Sigma \equiv \inf_a \Sigma(a).$$

This result is, of course, well-known, going back to Hunziker [37], van Winter [84], and Zhislin [88], with geometric proofs by Enss [23], Simon [75], Sigal [74], and Gårding [25]. Until Gårding [25], all proofs involved some kind of combinatorial argument if only the existence of a Ruelle–Simon partition of unity. Like Gårding [25], we are totally geometric with a straightforward proof exploiting our general machine. C^*-algebra proofs can be found in Georgescu–Iftimovici [27, 28] and have a spirit close to our proof below. Rabinovich [67] has a proof of

HVZ using his notion of invertibility at infinity, which also has overlap with our philosophy.

There is one subtlety to mention. Consider the case $\mu = 1$, $N = 3$, so $\mathbb{R}^{\mu(N-1)} = \mathbb{R}^2 = \{(x_1, x_2) : x_1, x_2 \in \mathbb{R}\}$. There are then clearly six special directions: $\pm(1,0)$, $\pm(0,1)$, and $\pm(1/\sqrt{2}, 1/\sqrt{2})$. For any other direction $\hat{e}$, if $x_n/|x_n| \to \hat{e}$, $V \to 0$, and the limit in that direction is $H_0 = H(\{0\},\{1\},\{2\})$.

For $e = \pm(1,0)$, $|(x_n)_1| \to \infty$ and $|(x_n)_1 - (x_n)_2| \to \infty$, so the only limit at infinity would appear to be $H(\{0,2\},\{1\})$. But this is wrong! To say x_n has limit $\pm(1,0)$ says $x_n/|x_n| \to \pm(1,0)$, so $(x_n)_1 \to \pm\infty$. But it does not say $(x_n)_2 \to 0$, only $(x_n)_2/(x_n)_1 \to 0$. For example, if $(x_n)_2 \to \infty$, the limit is H_0. As we see (it is obvious!), the limits are precisely H_0 and translates of $H(\{0,2\},\{1\})$. This still proves (6.3), but with a bit of extra thought needed.

We want to note a general form for extending HVZ, due to Agmon [1]. We consider linear surjections $\pi_j : \mathbb{R}^\nu \to \mathbb{R}^{\mu_j}$ with $\mu_j \le \nu$. Let $V_j : \mathbb{R}^{\mu_j} \to \mathbb{R}$ be in K_{μ_j} vanishing in K_{μ_j} sense at infinity. Then

$$H = -\Delta + \sum_j V_j(\pi_j x) \tag{6.5}$$

is called an Agmon Hamiltonian.

Given $e \in S^{\nu-1}$, define

$$H_e = -\Delta + \sum_{\{j:\pi_j e = 0\}} V_j(\pi_j x) \equiv -\Delta + V_e. \tag{6.6}$$

Note that since H_e commutes with $x \to x + \lambda e$, H_e has the form $H_e = -\Delta_e \otimes 1 + 1 \otimes (-\Delta_{e^\perp} + V_e)$, so $\sigma(H_e) = [\Sigma_e, \infty)$, with $\Sigma_e = \inf \operatorname{spec}(H_e)$.

In general, if $\bigcap_j \ker(\pi_j) \neq \{0\}$, H has some translation invariant degrees of freedom and can, and should, be reduced; but the HVZ Theorem holds for the unreduced case (as well as for the reduced case, since the reduced H which acts on $\mathbb{R}^\nu / \bigcap_j \ker(\pi_j)$ has the form (6.5)). So we do not consider reduction in detail.

By using π_j to write $V_{ij}(x_i - x_j)$ in terms of mass scaled reduced coordinates, any N-body Hamiltonian has the form (6.5), and (6.5) allows many-body forces. For the case of Theorem 6.1, if e is given, define a to be the partition with $(ij) \subset a$ if and only if $e_i = e_j$ (with $e_0 \equiv 0$). Then $H_e = H(a)$ and (6.7) below is (6.3).

Theorem 6.2. *For any Agmon Hamiltonian,*

$$\sigma_{\text{ess}}(H) = \overline{\bigcup_{e \in S^{\nu-1}} \sigma(H_e)}. \tag{6.7}$$

Proof. If $x_n/|x_n| \to e$, we can pass to a subsequence where each $\pi_j x_n$ has a finite limit or else has $|\pi_j x_n| \to \infty$. It follows that the limit at infinity for x_n is a translation (by $\lim \pi_j x_n$) of H_e or of a limit at infinity of H_e. Thus, for any $\widetilde{H}$ in $\mathcal{L}_e$, the set of limits in direction e,

$$\sigma(\widetilde{H}) \subset \sigma(H_e),$$

and so

$$\overline{\bigcup_{\widetilde{H} \in \mathcal{L}_e} \sigma(\widetilde{H})} = \sigma(H_e).$$

Thus (6.7) is (4.25). □

Remark. It is not hard to see that as e runs through $S^{\nu-1}$, $\sigma(H_e)$ has only finitely many distinct values, so the closure in (6.7) is superfluous.

Because we control $\sigma_{\text{ess}}(H)$ directly and do not rely on the a priori fact that one has only to locate $\inf \sigma_{\text{ess}}(H)$ properly (as do all the proofs quoted above, except the original HVZ proofs and Simon [75]), we can obtain results on N-body interactions in which the particles move in a fixed background periodic potential with gaps that can produce gaps in $\sigma_{\text{ess}}(H)$.

7 Additional applications

We turn to some additional applications of our machinery which shed light on earlier works.

(a) Sparse bumps, already considered by Klaus [45] using Birman–Schwinger techniques, by Cycon et al. [20] using geometric methods, and by Hundertmark–Kirsch [36] using methods which are essentially the same as the specialization of our argument to this example. Georgescu–Iftimovici [28] also have a discussion of sparse potentials that overlaps our discussion.

(b) Jacobi matrices with $a_n \to 0$ and CMV matrices with $|\alpha_n| \to 1$, already studied by Maki [54], Chihara [14] (Jacobi), and by Golinskii [30] (CMV).

(c) Bounded Jacobi matrices and CMV matrices with finite essential spectrum, already studied by Krein (in [3]) and Chihara [15] (Jacobi case), and by Golinskii [30] (CMV case).

(d) Find the essential spectrum of a CMV matrix if $\alpha_{j+1}/\alpha_j \to 1$, strengthening results of Barrios–López [9] and Cantero–Moral–Velázquez [11].

Remark. Golinskii [30] for (b) and (c) did not explicitly use CMV matrices but rather studied measures on $\partial\mathbb{D}$, but his results are equivalent to statements about CMV matrices.

Here is the sparse potentials result.

Theorem 7.1 ([45, 20]). *Let W be an L^1 potential of compact support on $\mathbb{R}$. Let $x_0 < x_1 < \cdots < x_n < \cdots$ so $x_{n+1} - x_n \to \infty$. Let*

$$V(x) = \sum_{j=0}^{\infty} W(x - x_j). \tag{7.1}$$

Then

$$\sigma_{\text{ess}}\left(-\frac{d^2}{dx^2} + V(x)\right) = \sigma\left(-\frac{d^2}{dx^2} + W\right). \tag{7.2}$$

Remarks. 1. That W has compact support is not needed. $W(x) \to 0$ sufficiently fast (e.g., bounded by $x^{-1-\varepsilon}$) will do with no change in proof.

2. Discrete eigenvalues of $-d^2/dx^2 + W$ are limit points of eigenvalues for $-d^2/dx^2 + V$.

3. There is a higher-dimensional version of this argument; see [36].

Proof. The limits at infinity are $-d^2/dx^2$ and $-d^2/dx^2 + W(x-a)$. Now use Theorem 3.12 or Theorem 4.5. □

Remark. This example is important because it shows that one needs $\sigma(\widetilde{H})$ and not just $\sigma_{\text{ess}}(\widetilde{H})$.

As for $a_n \to 0$:

Theorem 7.2 ([14]). *Let J be a bounded Jacobi matrix with $a_n \to 0$. Let S be the limit points of $\{b_n\}_{n=1}^{\infty}$. Then*

$$\sigma_{\text{ess}}(J) = S. \tag{7.3}$$

Proof. The limit points at infinity are diagonal matrices with diagonal matrix elements in S; and by a compactness argument, every $s \in S$ is a diagonal matrix element of some limit. Theorem 3.3 implies (7.3). □

Theorem 7.3 ([30]). *Let $\mathcal{C}(\{\alpha_n\}_{n=0}^{\infty})$ be a CMV matrix of a sequence of Verblunsky coefficients with*

$$\lim_{n\to\infty} |\alpha_n| = 1. \tag{7.4}$$

Let S be the set of limit points of $\{-\bar{\alpha}_{j+1}\alpha_j\}$. Then

$$\sigma_{\text{ess}}(\mathcal{C}(\{\alpha_j\}_{j=1}^{\infty})) = S. \tag{7.5}$$

Proof. By compactness of $\partial\mathbb{D}$, if $s \in S$, there is a sequence n_j such that $\alpha_{n_j+\ell}$ has a limit β_ℓ for all ℓ and $s = -\bar\beta_1\beta_0$. The limiting CMV matrices have $|\beta_\ell| = 1$ by (7.4), so are diagonal with matrix elements $-\bar\beta_{\ell+1}\beta_\ell$. Thus, the spectra of limits lie in S; and by the first sentence, any such $s \in S$ is in the spectrum of a limit. Now use Theorem 3.2. □

Next, we turn to the case of finite essential spectrum, first for Jacobi matrices.

Theorem 7.4. *Let $x_1, \dots, x_\ell \in \mathbb{R}$ be distinct. A bounded Jacobi matrix J has*

$$\sigma_{\text{ess}}(J) = \{x_1, \dots, x_\ell\} \tag{7.6}$$

if and only if

(i)

$$\lim_{n\to\infty} a_n a_{n+1} \cdots a_{n+\ell-1} = 0. \tag{7.7}$$

(ii) *If $k \le l$ and n_j is such that*

$$a_{n_j} \to 0, \qquad a_{n_j+k} \to 0, \tag{7.8}$$

$$a_{n_j+m} \to \tilde a_m \neq 0, \qquad m = 1, 2, \dots, k-1, \tag{7.9}$$

$$b_{n_j+m} \to \tilde b_m, \qquad m = 1, 2, \dots, k, \tag{7.10}$$

then the finite $k \times k$ matrix

$$\tilde J = \begin{pmatrix} \tilde b_1 & \tilde a_1 & & & \\ \tilde a_1 & \tilde b_2 & \tilde a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \tilde a_k \\ & & & \tilde a_{k-1} & \tilde b_k \end{pmatrix} \tag{7.11}$$

has spectrum a k-element subset of $\{x_1, \dots, x_\ell\}$.

(iii) *Each x_j occurs in at least one limit of the form* (7.11)

Proof. By Theorem 3.3, (7.6) holds if and only if the limiting $\tilde J$'s have spectrum in $\{x_1, \dots, x_\ell\}$ and there is at least one $\tilde J$ with each x_j in the spectrum. Now $\tilde J$ is a direct sum of finite and/or semi-infinite and/or infinite pieces. The semi-infinite pieces correspond to Jacobi matrices with nontrivial measures which have infinite spectrum. The two-sided infinite pieces also have infinite spectrum. Finite pieces of length m, which have a's nonzero, have m points in their spectrum, so no limit can have a direct summand of length $\ell + 1$ or more. Thus, by compactness, (7.7) holds, that is, any set of ℓ a's in the limit must have at least one zero. Then (ii) is the assertion that the limits have spectrum in $\{x_1, \dots, x_\ell\}$, and (iii) says that each x_j occurs. □

Theorem 7.5. (a) *J obeys*

$$\sigma_{\text{ess}}(J) \subset \{x_1, \dots, x_\ell\} \tag{7.12}$$

if and only if every right limit $\tilde{J}$ satisfies

$$\prod_{j=1}^{\ell} (\tilde{J} - x_j) \equiv P(\tilde{J}) = 0. \tag{7.13}$$

(b) *J satisfies* (7.12) *if and only if $P(J)$ is compact.*

Proof. (a) Since (7.13) holds if and only if $\sigma(\tilde{J}) \subset \{x_1, \dots, x_\ell\}$, this follows from Theorem 3.3.

(b) Since $P(J)$ has finite width, it is compact if and only if all matrix elements go to zero, which is true (by compactness of translates of J) if and only if (7.13) holds for all limits. □

We have now come full circle—for Theorem 7.5(b) is precisely Krein's criterion (stated in [3]), whose proof is immediate by the spectral mapping theorem and the analysis of the spectrum of compact selfadjoint operators. However, our Theorem 7.4 gives an equivalent, but subtly distinct, way to look at the limits. To see this, consider the case $\ell = 2$, that is, two limiting eigenvalues x_1 and x_2.

This has been computed by Chihara [16], who found that necessary and sufficient conditions for $\sigma_{\text{ess}}(J) = \{x_1, x_2\}$ are

$$\lim_{n\to\infty} (a_n^2 + a_{n-1}^2 + (b_n - x_1)(b_n - x_2)) = 0, \tag{7.14}$$

$$\lim_{n\to\infty} (a_n(b_n + b_{n+1} - x_1 - x_2)) = 0, \tag{7.15}$$

$$\lim_{n\to\infty} (a_n a_{n+1}) = 0. \tag{7.16}$$

(There is a typo in [16]: where we give $(b_n - x_1)(b_n - x_2)$ in (7.14), he gives, after changing to our notation, $(b_n - x_1)(b_{n+1} - x_2)$.) To see this from the point of view of $(J - x_1)(J - x_2)$, note that

$$\langle \delta_n, (J - x_1)(J - x_2)\delta_n \rangle = a_n^2 + a_{n-1}^2 + (b_n - x_1)(b_n - x_2), \tag{7.17}$$

$$\langle \delta_{n+1}, (J - x_1)(J - x_2)\delta_n \rangle = a_n(b_n - x_2) + a_n(b_{n+1} - x_1), \tag{7.18}$$

$$\langle \delta_{n+2}, (J - x_1)(J - x_n)\delta_n \rangle = a_n a_{n+1}. \tag{7.19}$$

If we think in terms of limit points, we get a different-looking set of equations. Consider limits, $\tilde{J}$. Of course, (7.16) is just

$$\tilde{a}_n \tilde{a}_{n+1} = 0; \tag{7.20}$$

but the conditions on summands of $\tilde{J}$ become

$$\tilde{a}_n = \tilde{a}_{n-1} = 0 \Rightarrow \tilde{b}_n = x_1 \quad \text{or} \quad \tilde{b}_n = x_2, \tag{7.21}$$

$$\tilde{a}_n \neq 0 \Rightarrow \tilde{b}_{n+1} + \tilde{b}_n = x_1 + x_2 \quad \text{and} \quad \tilde{b}_n \tilde{b}_{n+1} - \tilde{a}_n^2 = x_1 x_2. \tag{7.22}$$

Indeed, (7.21) is the result for 1×1 blocks, and (7.22) says 2×2 blocks have eigenvalues x_1 and x_2. It is an interesting exercise to see that (7.20)–(7.22) are equivalent to

$$\tilde{a}_n^2 + \tilde{a}_{n+1}^2 + (\tilde{b}_n - x_1)(\tilde{b}_n - x_2) = 0, \tag{7.23}$$

$$\tilde{a}_n(\tilde{b}_n + \tilde{b}_{n+1} - x_1 - x_2) = 0, \tag{7.24}$$

$$\tilde{a}_n \tilde{a}_{n+1} = 0. \tag{7.25}$$

One can analyze CMV matrices in a way similar to the above analysis. The analogue of Theorem 7.4 is

Theorem 7.6. *Let $\lambda_1, \dots, \lambda_\ell \in \partial\mathbb{D}$ be distinct. A CMV matrix $\mathcal{C}$ has*

$$\sigma_{\text{ess}}(\mathcal{C}) = \{\lambda_1, \dots, \lambda_\ell\} \tag{7.26}$$

if and only if

(i)

$$\lim_{n\to\infty} \rho_n \rho_{n+1} \cdots \rho_{n+\ell-1} = 0; \tag{7.27}$$

(ii) *if $k \leq \ell$ and n_j is such that*

$$\begin{aligned} &\rho_{n_j} \to 0, && \rho_{n_j+k} \to 0, \\ &\alpha_{n_j+m} \to \tilde{\alpha}_m, && m = 0, 1, 2, \dots, k-1, k, \end{aligned} \tag{7.28}$$

with $|\tilde{\alpha}_m| \neq 1$, $m = 1, \dots, k-1$ (by (7.28), $|\tilde{\alpha}_0| = |\tilde{\alpha}_k| = 1$), then the matrix ($\mathbf{1} = 1 \times 1$ unit matrix),

$$\tilde{\mathcal{C}} = [\Theta(\tilde{\alpha}_1) \oplus \cdots \oplus \Theta(\tilde{\alpha}_{k-1})][-\tilde{\alpha}_0 \mathbf{1} \oplus \Theta(\tilde{\alpha}_2) \oplus \cdots \oplus \Theta(\tilde{\alpha}_{k-2}) \oplus \bar{\tilde{\alpha}}_k \mathbf{1}] \tag{7.29}$$

if k is even and

$$\tilde{\mathcal{C}} = [\Theta(\tilde{\alpha}_1) \oplus \cdots \oplus \Theta(\tilde{\alpha}_{k-2}) \oplus \bar{\tilde{\alpha}}_k \mathbf{1}][-\tilde{\alpha}_0 \mathbf{1} \oplus \Theta(\tilde{\alpha}_2) \oplus \cdots \oplus \Theta(\tilde{\alpha}_{k-1})] \tag{7.30}$$

if k is odd, has eigenvalues k elements among $\lambda_1, \dots, \lambda_\ell$;

(iii) *each of* $\lambda_1, \dots, \lambda_\ell$ *occurs as an eigenvalue of some* $\tilde{\mathcal{C}}$.

Proof. Same as Theorem 7.4. □

The analogue of Theorem 7.5 is

Theorem 7.7. *Let* $\lambda_1, \dots, \lambda_\ell \in \partial\mathbb{D}$ *be distinct. Then*

(a) $\mathcal{C}$ *satisfies*

$$\sigma_{\text{ess}}(\mathcal{C}) \subset \{\lambda_j, \dots, \lambda_\ell\} \tag{7.31}$$

if and only if every right limit $\tilde{\mathcal{C}}$ *obeys*

$$\prod_{j=1}^{\ell} (\tilde{\mathcal{C}} - \lambda_j) \equiv P(\tilde{\mathcal{C}}) = 0; \tag{7.32}$$

(b) $\mathcal{C}$ *satisfies* (7.31) *if and only if* $P(\mathcal{C})$ *is compact.*

Proof. Same as Theorem 7.5. □

We have come to Golinskii's OPUC analogue of Krein's theorem [30]. Again, it is illuminating to consider the case $\ell = 2$. We deal directly with limits of α_j; call them $\tilde{\alpha}_j$. The Theorem 7.6 view of things is

$$\tilde{\rho}_n \tilde{\rho}_{n+1} = 0, \tag{7.33}$$

$$\tilde{\rho}_n = \tilde{\rho}_{n+1} = 0 \Rightarrow -\bar{\tilde{\alpha}}_{n+1}\tilde{\alpha}_n = \lambda_1 \quad \text{or} \quad -\bar{\tilde{\alpha}}_{n+1}\tilde{\alpha}_n = \lambda_2, \tag{7.34}$$

$$\tilde{\rho}_n \neq 0 \Rightarrow -\bar{\tilde{\alpha}}_n\tilde{\alpha}_{n-1} - \bar{\tilde{\alpha}}_{n+1}\tilde{\alpha}_n = \lambda_1 + \lambda_2 \quad \text{and} \quad \tilde{\alpha}_{n-1}\bar{\tilde{\alpha}}_{n+1} = \lambda_1\lambda_2. \tag{7.35}$$

Equation (7.35) comes from the fact that the matrix $\mathcal{C}$ of (7.29) is

$$\begin{pmatrix} \bar{\tilde{\alpha}}_n & \tilde{\rho}_n \\ \rho_n & -\tilde{\alpha}_n \end{pmatrix} \begin{pmatrix} -\tilde{\alpha}_{n-1} & 0 \\ 0 & \bar{\tilde{\alpha}}_{n+1} \end{pmatrix} \tag{7.36}$$

where the determinant is $\tilde{\alpha}_{n-1}\bar{\tilde{\alpha}}_{n+1}$ and the trace is $-\bar{\tilde{\alpha}}_n\tilde{\alpha}_{n-1} - \tilde{\alpha}_n\bar{\tilde{\alpha}}_{n+1}$.

From the point of view of Theorem 7.7, using the CMV matrix is complicated since $(\mathcal{C} - \lambda_1)(\mathcal{C} - \lambda_2)$ is, in general, 9-diagonal! As noted by Golinskii [30], it is easier to use the GGT matrix (see Section 4.1 of [77]), since it immediately implies

$$\tilde{\rho}_n\tilde{\rho}_{n+1} = \langle \delta_{n+2}, \mathcal{G}^2\delta_n \rangle = 0; \tag{7.37}$$

and once that holds, $\mathcal{G}$ becomes tridiagonal! Thus, one gets from $\langle \delta_{n+1}, (\mathcal{G} - \lambda_1)(\mathcal{G} - \lambda_2)\delta_n \rangle = 0$ that

$$\tilde{\rho}_n(-\bar{\tilde{\alpha}}_n\tilde{\alpha}_{n-1} - \bar{\tilde{\alpha}}_{n+1}\tilde{\alpha}_n - \lambda_1 - \lambda_2) = 0, \tag{7.38}$$

and from $\langle \delta_n, (\mathcal{G} - \lambda_1)(\mathcal{G} - \lambda_2)\delta_n \rangle = 0$ that

$$(7.39)\quad (-\bar{\tilde{\alpha}}_{n+1}\tilde{\alpha}_n - \lambda_1)(-\bar{\tilde{\alpha}}_n\tilde{\alpha}_{n-1} - \lambda_2) - \tilde{\rho}_n^2\bar{\tilde{\alpha}}_{n+1}\tilde{\alpha}_{n-1} - \rho_{n+1}^2\bar{\tilde{\alpha}}_{n-2}\tilde{\alpha}_{n+1} = 0.$$

Again, it is an interesting exercise to show that (7.33)–(7.35) are equivalent to (7.37)–(7.39).

Finally, we turn to some cases of CMV matrices recently studied by Cantero, Moral, and Velázquez [11]. In [9], Barrios–López proved that if

$$(7.40)\qquad \frac{\alpha_{j+1}}{\alpha_j} \to 1 \quad \text{and} \quad |\alpha_j| \to a,$$

then

$$(7.41)\qquad \sigma_{\text{ess}}(\mathcal{C}) = \Delta_a \equiv \{z \in \partial\mathbb{D} : |\arg z| \geq 2\arcsin(a)\}.$$

Of course, they stated their result in terms of the essential support of the underlying measure, since $\mathcal{C}$ had not yet been introduced when they wrote their paper!

We can strengthen their result considerably.

Theorem 7.8. *If*

$$(7.42)\qquad \frac{\alpha_{j+1}}{\alpha_j} \to 1 \quad \textit{and} \quad \liminf|\alpha_j| = a,$$

then (7.41) *holds.*

Remark. In [11], which motivated our looking at this example, it is proven that $\sigma_{\text{ess}}(\mathcal{C}) \subset \Delta_a$.

Proof. Since $\alpha_{j+1}/\alpha_j \to 1$, every limit has the form $(\dots, \beta, \beta, \beta, \dots)$; and it is known (see Example 1.6.12 of [77]) that such a $\mathcal{C}_\beta$ has

$$\sigma(\mathcal{C}_\beta) = \Delta_{|\beta|}.$$

Since $a' > a$ implies $\Delta_{a'} \subset \Delta_a$, (7.41) follows from Theorem 3.1. □

One can also use our results here to streamline some of the results contained in Section 3 of [11].

8 Magnetic fields

A magnetic Hamiltonian acts on $\mathbb{R}^\nu$ via

$$(8.1)\qquad H(a, V) = -\sum_{j=1}^{\nu} (\partial_j - ia_j)^2 + V,$$

where a is vector-valued. The magnetic field is the two-form defined by

(8.2) $$B_{jk} = \partial_j a_k - \partial_k a_j.$$

If λ is a scalar function, then

(8.3) $$\tilde{a} = a + \nabla\lambda$$

produces the same B, and one has gauge covariance

(8.4) $$H(\tilde{a}, V) = e^{i\lambda} H(a, V) e^{-i\lambda}.$$

While the mathematically "natural" conditions on a are either $a \in L^4_{\text{loc}}$, $\nabla \cdot a \in L^2_{\text{loc}}$, or $a \in L^2_{\text{loc}}$ (see [20, 51, 76]), for simplicity, we suppose here that B is bounded and uniformly Hölder continuous, that is, for some $\delta > 0$,

(8.5) $$\sup_{x,j,k} |B_{jk}(x)| < \infty, \qquad \sup_{j,k,|x-y|\leq 1} |x-y|^{-\delta} |B_{jk}(x) - B_{jk}(y)| < \infty.$$

It is certainly true that one can allow suitable local singularities. We discuss later what (8.5) implies about choices of a. With this kind of regularity on B, it is easy to prove that for a shift between different gauges of the type we consider below, the formal gauge covariance (8.4) is mathematically valid. Indeed, more singular gauge changes can be justified (see Leinfelder [50]).

If $a_j \to 0$ at infinity, it is easy to implement the ideas of Sections 3 and 4 with no change in the meaning of limit point at infinity; the limits all have no magnetic field. But, as is well known, $a_j \to 0$ requires (very roughly speaking) that B go to zero at least as fast as $|x|^{-1-\varepsilon}$; so this does not even capture all situations where $B_{ij} \to 0$ at infinity. Miller [60] (see also [20, 61]) noted that in two and three dimensions, the way to control $B \to 0$ at infinity is to make suitable gauge changes in Weyl sequences—and that is also the key to what we do here.

We settle for stating a very general limit theorem and make no attempt to apply this theorem to recover the rather extensive literature on HVZ theorems and on essential spectra in periodic magnetic fields [5, 10, 19, 32, 33, 34, 35, 38, 39, 42, 63, 64, 82, 85, 86, 87, 89, 90, 91, 92]. We are confident that can be done and that the ideas below will be useful in future studies. It should also be possible to extend Theorem 5.1 with "slipped periodic" magnetic fields.

Definition. A set of gauges, a_x, depending on x is said to be "regular at infinity" if and only if for every R, we have for some $\delta > 0$,

(8.6) $$\sup_{|x-y|\leq R} |a_x(y)| < \infty, \qquad \sup_{\substack{x,y,z \\ |y-z|<1 \\ |x-y|<R}} |y-z|^{-\delta} |a_x(y) - a_x(z)| < \infty.$$

Proposition 8.1. *If* (8.5) *holds, there exists a set of gauges regular at infinity.*

Proof. The transverse gauge, $\vec{a}_{x_0}$, based at x_0 is defined by

$$a_{x_0;j}(x_0+y)=\sum_k\left[\int_0^1 sB_{kj}(x_0+sy)\,ds\right]y_k. \tag{8.7}$$

That this is a gauge is known (see below). Clearly, if $|x_0-y|\le R$,

$$|\vec{a}_{x_0}(y)|\le \tfrac{1}{2}R\sup_x\|B(x)\|;$$

and if $|y-z|<1$ and $|x_0-y|<R$,

$$|\vec{a}_{x_0}(y)-\vec{a}_{x_0}(z)|\le\tfrac{1}{2}\left\{\sup_x\|B(x)\|+(R-1)\sup_{|y-z|\le1}\left[|y-z|^{-\delta}\|B(y)-B(z)\|\right]\right\}.$$

□

Remarks. 1. We call the choice (8.7) the local transverse gauge.

2. Transverse gauges go back at least to Uhlenbeck [81], who calls them exponential gauges. They have been used extensively by Loss–Thaller [53] (see also Thaller [80]) to study scattering.

3. To see that (8.7) is a gauge is a messy calculation if done directly, but there is a lovely indirect argument of Uhlenbeck [81]. Without loss, take $x_0=0$. Call a gauge transverse if $\vec{a}(0)=0$ and $\vec{x}\cdot\vec{a}=0$. Transverse gauges exist, for if $\vec{a}_0$ is any gauge and

$$\varphi(\vec{x})=-\int_0^1\vec{x}\cdot a_0(s\vec{x})\,ds, \tag{8.8}$$

then $\vec{x}\cdot\nabla\varphi=r\frac{\partial}{\partial r}\varphi=-\vec{x}\cdot a_0(x)$, so $a=a_0+\nabla\varphi$ is transverse. Next, note that if $\vec{a}$ is a transverse gauge, then

$$\begin{aligned}\sum x_kB_{kj}&=(x\cdot\nabla)a_j-\vec{\nabla}_j(x\cdot a)+a_j\\&=\frac{\partial}{\partial r}ra_j.\end{aligned}\tag{8.9}$$

Integrating (8.9) shows (8.7) with $y=0$ is not only a gauge but the unique transverse gauge.

If a_x is a set of gauges regular at infinity, we say $\widetilde{H}$ is a limit at infinity of $H(a,V)$ in direction $\hat{e}$ if and only if with

$$(U_x\varphi)(y)=\varphi(y-x) \tag{8.10}$$

we have that for some sequence x_n, $|x_n| \to \infty$, $x_n/|x_n| \to e$, and for each $R < \infty$ and $z \in \mathbb{C}\backslash[\alpha, \infty)$,

$$U_{x_n}((H(a_{x_n}, V) - z)^{-1})U_{x_n}^{-1}\chi_R \to (\widetilde{H} - z)^{-1}\chi_R \tag{8.11}$$

where χ_R is the characteristic function of a ball of radius R about 0. As usual, $\mathcal{L}_e$ denotes the limits at infinity in direction e.

Theorem 8.2. *If $V \in K_\nu$ and B satisfies* (8.5), *then*

$$\sigma_{\text{ess}}(H(a, V)) = \overline{\bigcup_{e \in S^{\nu-1}} \bigcup_{\widetilde{H} \in \mathcal{L}_e} \sigma(\widetilde{H})}. \tag{8.12}$$

In (8.12), we get the same union if, instead of all regular gauges at infinity, we take only the local transverse gauges.

Proof. By using gauge-transformed Weyl sequences as in [20], it is easy to see that the right side of (8.12) is contained in $\sigma_{\text{ess}}(H(a, V))$. To complete the proof, we need only show that the right side, restricted to local transverse gauges, contains $\sigma_{\text{ess}}(H(a, V))$.

Localization extends effortlessly, since

$$[j, H(a, V)] = \vec{\nabla} j \cdot (\vec{\nabla} - i\vec{a}) + (\vec{\nabla} - i\vec{a}) \cdot \vec{\nabla} j$$

and $\|(\vec{\nabla} - i\vec{a})\varphi\|^2$ is controlled by $H(a, V)$. Thus, we only need compactness of the gauge-transformed operators. Since (8.6) says that the a_x's translated to 0 are uniformly equicontinuous, compactness of the a's is immediate. V's are handled as in Section 4. □

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Yoram Last
INSTITUTE OF MATHEMATICS
THE HEBREW UNIVERSITY OF JERUSALEM
JERUSALEM 91904, ISRAEL
email: ylast@math.huji.ac.il

Barry Simon
MATHEMATICS 253-37
CALIFORNIA INSTITUTE OF TECHNOLOGY
PASADENA, CA 91125, USA
email: bsimon@caltech.edu

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