ENDPOINTS OF THE SPECTRUM OF PERIODIC OPERATORS ARE GENERICALLY SIMPLE

FRÉDÉRIC KLOPP AND JAMES RALSTON

Abstract. In this note, we prove that the edges of the spectral bands of a periodic Schrödinger operator are generically simple.

Résumé. Cette note est consacrée à la preuve de ce que, pour un opérateur de Schrödinger périodique générique, les bord de bandes spectrales sont simples.

0. Introduction

In this note, we prove that the edges of the spectral bands of a periodic Schrödinger operator are generically simple.

More precisely, on $\mathbb{R}^n$, consider the Schrödinger operator $H(V) = -\Delta + V$ where V is a real valued, measurable, $\mathbb{Z}^n$-periodic potential. For the sake of simplicity, let us assume that V is bounded. Then it is well known (see e.g. [10, 11]) that the spectrum of $H(V)$ can be constructed in the following way. Let $\mathbb{T}^n$ denote the (flat) n-torus, $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$. In $L^2(\mathbb{T}^n)$ consider the operators

$$H(k, V) = -(\partial + 2\pi ik)^2 + V, \ k \in \mathbb{T}^n,$$

with common domain $H^2(\mathbb{T}^n)$. As V is real-valued and bounded, for each k, $H(k, V)$ is a self-adjoint operator with eigenvalues $\{\lambda_j(k, V)\}_{j=1}^{\infty}$ which we list in ascending order with multiplicities, $\lambda_j(k, V) \leq \lambda_{j+1}(k, V)$. Then, the spectrum of $H(V)$ is given by

$$\sigma(H(V)) = \bigcup_{j=1}^{+\infty} \lambda_j(\mathbb{T}^n, V).$$

Since the spectrum of $H(V)$ is a closed subset of $\mathbb{R}$, its complement in $\mathbb{R}$ is a countable union of disjoint open intervals, called *gaps* in solid state physics. The Floquet eigenvalues $\lambda_j(k, V)$ are continuous in k, and hence their ranges

$$B_j = \{\lambda_j(k, V) : k \in \mathbb{T}^n\}$$

are closed intervals which are called *bands* of the spectrum. In this note we are concerned with the ends of the gaps, i.e. the endpoints of bands which are also endpoints of the spectrum.

Let λ be a point in the spectrum of $H(V)$. We say that λ is *simple* if there exists a single Floquet eigenvalue that assumes the value λ, i.e. there exists a unique $j \geq 1$ such that for some $k \in \mathbb{T}^n$, $\lambda_j(k, V) = \lambda$. Note that, since the Floquet eigenvalues are continuous with respect to

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k and the torus $\mathbb{T}^n$ is compact, if λ is simple, in a neighborhood of λ, energies either do not belong the $\sigma(H(V))$ or are simple. Moreover, if they are simple, they are assumed by the same Floquet eigenvalue.

Let $\mathcal{V}_k$ denote the set of bounded $\mathbb{Z}^n$-periodic potentials, V, for which the spectrum of the Schrödinger operator $H(V)$ has at least k open gaps. This is open in the topology of $L^\infty(\mathbb{T}^n)$. Our main result then states

Theorem 0.1. *The set of potentials V for which the endpoints of at least k gaps in the spectrum of $H(V)$ are simple is a dense, open subset of $\mathcal{V}_k$ in the topology of $L^\infty(\mathbb{T}^n)$.*

The assumptions on the potential used in this note were chosen for the sake of technical simplicity; they are not optimal and may be relaxed (see e.g. [10]).

In dimension 1 i.e. if $n = 1$, Theorem 0.1 is well known; endpoints are *always* simple Floquet eigenvalues (see e.g [6]). In dimension larger than 1 it was known that the lower end of the lowest band, i.e. the bottom of the spectrum, is simple (see [1, 3]), and that the Floquet eigenvalue assuming this value has a non degenerate minimum at that value. As far as we know, without any further assumptions, the structure of the higher bands is unknown.

Simplicity of spectral endpoints plays an important role in many problems on periodic and perturbations of periodic Schrödinger operators. We give some references concerning the scattering theory ([2, 5]), the theory of resonances ([7]), and the study of the counting functions for eigenvalues in a gap ([9, 4]) for perturbations of periodic Schrödinger operators.

1. The proofs

We keep the notation of section 0. Consider now λ_0, the upper endpoint of a gap for $\sigma(H(V_0))$. Hence, there exists $m \in \mathbb{N}$ and $\varepsilon > 0$ such that

$$\lambda_m(k, V_0) \leq \lambda_0 - \varepsilon < \lambda_0 \leq \lambda_{m+1}(k, V_0)$$

for all $k \in \mathbb{T}^n$. Then Theorem 0.1 is a consequence of the following.

Theorem 1.1. *There is a continuous curve, $V(t)$, in $L^\infty(\mathbb{T}^n)$ with $V(0) = V_0$ such that for $0 < t < \epsilon$ the eigenvalue $\lambda_{m+1}(k,t)$ of $H(k, V(t))$ is simple whenever $\lambda_{m+1}(k,t)$ is sufficiently close to $\min_{k\in\mathbb{T}^n} \lambda_{m+1}(k,t)$.*

Of course, an analogue of Theorem 1.1 holds for the lower ends of gaps. Now assume Theorem 1.1 is proven. By the continuity of the Floquet eigenvalues of $H(V)$, the simplicity of a band edge is stable under small perturbations. Starting from a potential V_0, one can then first perturb it so as to make its first gap endpoint simple, then its second gap endpoint and so on for k of the open gaps for V_0 , proving Theorem 0.1.

Proof of Theorem 1.1. We begin by noting that comparison with

$$-(\partial + 2\pi i k)^2 + \min_{\mathbb{T}^n} V_0(x)$$

shows that there is an M such that $\lambda_M(k, V_0) > \lambda_0 + 1$ for all $k \in \mathbb{T}^n$. For each $k_0 \in \mathbb{T}^n$ we choose a simple, closed contour in the complex plane, $C(k_0)$, enclosing $\{\lambda_j(k_0, V_0)\}_{j=m+1}^{M}$, which crosses the real axis between $\lambda_m(k_0, V_0)$ and $\lambda_{m+1}(k_0, V_0)$ and between eigenvalues of $H(k_0, V_0)$

above $\lambda_M(k_0,V_0)$. Then for $|k-k_0|$ and $\|V-V_0\|_\infty$ sufficiently small, the orthogonal projection

$$P_{k_0}(k,V)=\frac{1}{2\pi i}\int_{C(k_0)}(H(k,V)-zI)^{-1}dz$$

is real analytic in k and V. Hence, we can choose an orthonormal basis $\{\phi_{m+1}^{(k_0)},\ldots,\phi_{R(k_0)}^{(k_0)}\}$ for the range of $P(k,V)$ which is real analytic in (k,V) on a neighborhood of (k_0,V_0). Here and elsewhere we use neighborhoods in $\mathbb{T}^n$, and $|p-p_0|$ stands for the Euclidean distance between p_0 and the closest conjugate of p under $\mathbb{Z}^n$. Thus we have a cover of $\mathbb{T}^n$ by open sets, and, selecting a finite sub-cover, we have open sets $\mathcal{O}_1,\ldots,\mathcal{O}_P$ with the following properties:

1. for each $\mathcal{O}_i$ we have an orthonormal set $\{\phi_{m+1}^{(i)}(k,V),\ldots,\phi_{R_i}^{(i)}(k,V)\}$ such that the ϕ's are analytic in (k,V) on $\overline{\mathcal{O}}_i\times\{\|V-V_0\|<\delta\}$, and
2. the span of $\{\phi_{m+1}^{(i)}(k,V),\ldots,\phi_{R_i}^{(i)}(k,V)\}$ contains all eigenfunctions of $H(k,V)$ belonging to eigenvalues greater than or equal $\lambda_{m+1}(k,V)$ and less than or equal to λ_0+1.

Next we choose $\hat{k}$ and ϕ_0, $\|\phi_0\|=1$, such that $H(\hat{k},V_0)\phi_0=\lambda_0\phi_0$. Since $\|\phi_0\|=1$, we can choose $x_0\in\mathbb{T}^n$ such that $|\phi_0(x_0)|\geq 1$. The idea behind this proof is to set $V(t)=V_0-tV'$, where V' is an approximate delta function at x_0. It requires a little work to show that $V(t)$ will have the desired properties. To simplify notation we will suppress the index $i=1,\ldots,P$ which specifies the open set $\mathcal{O}_i$ until the final steps of the proof. We will assume that $k\in\mathcal{O}$, one of the $\mathcal{O}_i$, with the understanding that all estimates which involve k hold for all i, and that all constructions are done for each i.

First, we need the estimate

$$\sum_{j=m+1}^{R}|\phi_j(x,k,V_0)-\phi_j(x_0,k,V_0)|^2<1/3 \tag{1}$$

for $k\in\overline{\mathcal{O}}$ when $|x-x_0|<\epsilon_0$. Since the ϕ_j's are finite linear combinations of eigenfunctions of H, and multiplying these eigenfunctions by $\exp(-2\pi ik\cdot x)$ makes them eigenfunctions of $-\Delta+V$, standard results on elliptic regularity (see, e.g. [8], Chapter 3, Section 14) imply that the C^α-norms of the ϕ_j's are uniformly bounded in k, giving (1). This would hold for $V_0\in L^p(\mathbb{T}^n)$ for any $p>n/2$. We assume that ϵ_0 is also small enough that $|\phi_0(x)|^2>2/3$ for $|x-x_0|<\epsilon_0$. We choose $V_1\in C_0^\infty(|x-x_0|<\epsilon_0)$ such that $V_1(x)\geq 0$ and $\int V_1dx=1$, and set $V(t)=V_0-tV_1$.

To see that the lowest eigenvalues of $H(k,V(t))$ above the gap have the desired behavior we will use the variational characterization (Max-Min Principle). This requires some careful choices. First we will modify $\{\phi_{m+1}(k,V(t)),\ldots,\phi_R(k,V(t))\}$ so that

$$\frac{d}{dt}\langle\phi_i(k,V(t)),H(k,V(t))\phi_j(k,V(t))\rangle=\langle\phi_i(k,V(t)),\frac{d}{dt}H(k,V(t))\phi_j(k,V(t))\rangle \tag{2}$$

for all choices of i and j. Letting $\dot{f}$ denote df/dt, we see that (2) will hold if $\langle\dot{\phi}_i,\phi_j\rangle=0$ for all i and j. Setting $\tilde{\phi}_i=\sum_j u_{ij}\phi_j$, we have

$$\langle\dot{\tilde{\phi}}_r,\tilde{\phi}_s\rangle=\sum_j\overline{\dot{u}_{rj}}u_{sj}+\sum_{i,j}\overline{u_{ri}}u_{sj}\langle\dot{\phi}_i,\phi_j\rangle.$$

Hence, setting U equal to the matrix with entries u_{ij} and A equal to the matrix with entries $-\langle \phi_i, \dot{\phi}_j \rangle$, (2) will hold when the ϕ_i's are replaced by the $\tilde{\phi}_i$'s provided that

$$\dot{U} = UA. \tag{3}$$

We solve (3) with $U(0) = I$. Note that $U(t)$ is unitary because the orthonormality of the ϕ_i's makes A skew-symmetric, and it depends analytically on k on $\overline{\mathcal{O}}$ Hence, assuming that the ϕ's are the $\tilde{\phi}$'s just constructed, both (1) and (2) hold for $V = V(t)$ when t is sufficiently small. The analytic dependence of the ϕ_i's on V implies that all derivatives of $\langle \phi_i(k, V(t)), H(k, V(t))\phi_j(k, V(t)) \rangle$ with respect to t are uniformly bounded in k for t sufficiently small. Fixing an $\mathcal{O}_i$ containing $\hat{k}$, we can write ϕ_0 in terms of the ϕ_j's associated with this $\mathcal{O}_i$, $\phi_0 = \sum_j c_j \phi_j(\hat{k}, V_0)$, and then define $\phi_0(t) = \sum_j c_j \phi_j(\hat{k}, V(t))$. Then by construction

$$\frac{d}{dt}\langle \phi_0(t), H(\hat{k}, V(t))\phi_0(t) \rangle|_{t=0} = -\langle \phi_0(0), V_1 \phi_0(0) \rangle \leq -2/3.$$

Hence

$$\langle \phi_0(t), H(\hat{k}, V(t))\phi_0(t) \rangle \leq \lambda_0 - 2t/3 + O(t^2). \tag{4}$$

On each $\mathcal{O}_i$, define

$$\phi_*^{(i)}(k,t) = \sum_j \overline{\phi_j^{(i)}(x_0, k, V_0)}\phi_j^{(i)}(k, V(t)).$$

Given $\phi(k,t) = \sum_j a_j \phi_j^{(i)}(k, V(t))$, we have $\langle \phi(k,t), \phi_*^{(i)}(k,t) \rangle = 0$ if and only if

$$\sum_j a_j \phi_j^{(i)}(x_0, k, V_0) = 0. \tag{5}$$

Assuming (5) and $\|\phi\| = 1$, we have for $k \in \overline{\mathcal{O}_i}$

$$\begin{aligned}
\frac{d}{dt}\langle \phi(k,t), H(k, V(t))\phi(k,t) \rangle|_{t=0} &= -\langle \phi(k,0), V_1 \phi(k,0) \rangle \\
&= -\int_{|x-x_0|<\epsilon_0} |\sum_j a_j (\phi_j^{(i)}(x,k,V_0) - \phi_j^{(i)}(x_0,k,V_0))|^2 V_1(x) dx \\
&\geq -1/3.
\end{aligned}$$

Hence for $k \in \overline{\mathcal{O}_i}$

$$\langle \phi(k,t), H(k, V(t))\phi(k,t) \rangle \geq \lambda_0 - t/3 + O(t^2), \tag{6}$$

where the $O(t^2)$ is uniform in both k and ϕ for $\|\phi\| = 1$. In view of the variational characterization of the eigenvalues of $H(k, V(t))$ the estimate (4) implies that

$$\lambda_{m+1}(\hat{k}, V(t)) < \lambda_0 - t/2$$

for $0 < t < \epsilon$ with ϵ sufficiently small, and, since (6) bounds the minimum over the subspace defined by (4) from below,

$$\lambda_{m+2}(k, V(t)) > \lambda_0 - t/2$$

for $0 < t < \epsilon$, where ϵ is independent of k. Thus we have the desired result. This completes the proof of Theorem 1.1.

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(Frédéric Klopp) Département de Mathématique, Institut Galilée, U.R.A 742 C.N.R.S, Université de Paris-Nord, Avenue J.-B. Clément, F-93430 Villetaneuse, France

E-mail address: klopp@math.univ-paris13.fr

(James Ralston) Department of Mathematics, U.C.L.A., 6363 Math Sciences, 405 Hilgard Avenue, Box 951555, Los Angeles, CA 90095-1555

E-mail address: ralston@math.ucla.edu