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On the spectrum of $p^2+V(x)+\epsilon x$, with V periodic and ϵ complex

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Abstract. It is shown that $-\mathrm{d}^2/\mathrm{d}x^2+V(x)+\epsilon x$, with $V(x)$ periodic and $\mathrm{Im}\,\epsilon\neq 0$, has a spectrum in the form of a ladder for $|\epsilon|$ small.

A recent important paper by Herbst (1979) shows, among other things, that the one-dimensional Schrödinger Hamiltonian

$$H_0=-\mathrm{d}^2/\mathrm{d}x^2+\epsilon x, \tag{1}$$

$\mathrm{D}(H_0)=\mathrm{D}(p^2)\cap\mathrm{D}(x)$, $\mathrm{Im}\,\epsilon\neq 0$ has a compact resolvent and an empty spectrum. H_0 has a compact resolvent by a quadratic estimate (Herbst 1979),

$$\|H_0\psi\|^2+a\|\psi\|^2\geqslant b(\|p^2\psi\|^2+\|x\psi\|^2), \tag{2}$$

with ϵ dependent on a and b. The fact that H_0 has an empty spectrum follows from the invariance of the spectrum under translations:

$$\sigma(H_0+\epsilon\alpha)=\sigma(H_0), \qquad \alpha\in\mathbb{R}. \tag{3}$$

Since $\sigma(H_0)$ is countable, $\sigma(H_0)=\varnothing$. Relation (3) follows from

$$U_\alpha H_0 U_\alpha^{-1}=H_0+\epsilon\alpha, \tag{4}$$

where $(U_\alpha f)(x)=f(x+\alpha)$.

We shall prove:

Theorem 1. Let $V(x)$ be piecewise continuous, $V(x+1)=V(x)$, real and $V(x)\neq$ constant. Fix $0<\theta<\pi$, $\epsilon=|\epsilon|\mathrm{e}^{\mathrm{i}\theta}$. Let

$$H=H_0+V(x), \tag{5}$$

with $\mathrm{D}(H)=\mathrm{D}(H_0)$. Then:

(i) H is closed and has a compact resolvent.

(ii) For $0<|\epsilon|<\epsilon_0$, the spectrum $\sigma(H)$ is not empty, is purely discrete (by(i)) and is invariant under translation by ϵ.

(i) is the easy part of the theorem and is the subject of proposition 1 and corollary 1 below. The rest of the paper is devoted to proving the non-emptiness of the spectrum. To this end we shall use the periodicity of the spectrum to prove stability.

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Remarks.

(i) Theorem 1 is relevant to the theory of semiconductors: it is associated with the 'Stark ladder' controversy (Avron 1976, Wannier 1960, 1962, 1969, Zak 1968, 1969).

(ii) Although we make no claim for real ϵ, we note that Bentosela (1979) showed that for ϵ real there are long-lived states constructed from a subspace with a 'fixed band index'.

(iii) Zak (1968, 1969) postulates that the ladder corresponds to distinct atomic states.

(iv) For ϵ real the spectrum of the self-adjoint extension of H has no discrete eigenvalues:

$$\sigma[H(\epsilon \neq 0)] = (-\infty, \infty) \tag{6}$$

and

$$\sigma[H(\epsilon = 0)] = [\lambda_0, \lambda_1] \cup [\lambda_2, \lambda_3] \cup \ldots, \qquad -\infty < \lambda_0 < \lambda_1 \leqslant \lambda_2 < \lambda_3 \leqslant \lambda_4 \ldots \tag{7}$$

(see Avron *et al* 1977a, Reed and Simon 1978).

(v) $V \neq$ constant comes into the theorem through the existence of at least one (instability) gap in the band spectrum (Reed and Simon 1978), $(\epsilon = 0)$, i.e. at least one of the $\leqslant$ in (7) is $<$.

(vi) In fact, not only is $R(\lambda) = [H - \lambda]^{-1}$ compact but also $\mathcal{J}_p$, $p > 3/2$, i.e. the singular values of R are in l^p (see Reed and Simon 1978). This follows from the Weyl estimate of the distribution of eigenvalues of $p^2 + |x|$ and a perturbative argument analogous to those in Avron *et al* (1977b) and Avron and Simon (1978). This seems to indicate a 1–1 correspondence between the 'bands' and the 'Stark ladders'.

Proposition 1. Let A have a compact resolvent with a numerical range contained in a strip $\Theta(A)$ (a half-plane is allowed); then

$$\|[A - \lambda]^{-1}\| \leqslant \{\mathrm{dist}[\lambda, \Theta(A)]\}^{-1}. \tag{8}$$

Proof. A is closed and has no proper extensions. Hence m-accretiveness follows from accretiveness. By multiplying A by a phase and shift it can be made accretive. A standard result (Phillips 1959) on m-accretives gives (8). □

From this and theorem II.1 of Herbst (1979) follows:

Corollary 1. Let $V(x) \in L^2_{\mathrm{LOC}}$ and be periodic. Then V is bounded by zero relative to H_0.

Proof. By the quadratic estimate (2),

$$b\|xR_0(\lambda)\|^2 \leqslant (1 + a\|R_0(\lambda)\|^2). \tag{9}$$

Now

$$\|V[H_0 - \lambda]^{-1}\| \leqslant \|V[p^2 - \lambda]^{-1}\|(1 + |\epsilon|\,\|xR_0(\lambda)\|). \tag{10}$$

V is bounded by zero relative to p^2 (Phillips 1959). By (9) and proposition 1, λ can be chosen so that the RHS of (10) is arbitrarily small. □

This proves part (i) of theorem 1.

The proof $\sigma(H)\neq\varnothing$ is a rigorous version of the 'single band approximation' (Avron *et al* 1977a, Wannier 1960, 1962, 1969, Zak 1968, 1969). In the first step, corollary 2, we prove that a restriction of the Hamiltonian to a subspace of a single band has a spectrum (a Stark ladder). This also holds for the Hamiltonian with no 'interband interaction'. The second step is a proof of the global stability of the spectrum under the 'interband interaction'.

Equation (8) will help us to control the displacement of the Stark ladder eigenvalues in a direction (in the complex plane) perpendicular to ϵ. Although we have no control on the displacement of the Stark ladder eigenvalues in the direction parallel to ϵ, the periodicity of the spectrum in this direction, together with a standard theorem on the upper semi-continuity of the spectrum, gives the global stability (without self-adjointness of the unperturbed operator!).

We collect here results from the theory of Bloch Hamiltonians which are needed in what follows; see Avron *et al* (1977b), Avron and Simon (1978), Blount (1962), Kohn (1959) and Reed and Simon (1978) for details.

The reduced Bloch functions $\psi_{nk}(\cdot)\in l^1(2\pi\mathbb{Z}+k)\subset l^2(2\pi\mathbb{Z}+k)$,

$$|\psi_{nk}(p)|\leqslant C_{nk}(1+p^2)^{-1}. \tag{11}$$

ψ_{nk} can be chosen to be real and analytic in k (Avron *et al* 1977b, Avron and Simon 1978), and for isolated bands can be chosen to be periodic (Kohn 1959): $\psi_{n,k+2\pi}=\psi_{n,k}$. (An isolated band is one with non-vanishing intervals of instability.) Moreover, $\psi_{n,k}$ may be chosen so that (Blount 1962)

$$\sum_{a\in 2\pi\mathbb{Z}+k}\bar{\psi}_{nk}(a)\frac{\mathrm{d}}{\mathrm{d}k}\psi_{nk}(a)=0.$$

Bloch functions which satisfy the above properties are a basis in L^2. This basis is known as the crystal momentum representation:

$$\hat{f}(n,k)=\sum_{a\in 2\pi\mathbb{Z}+k}\bar{\psi}_{nk}(a)f(a+k). \tag{12}$$

For an isolated band n and $f\in L^2\cap L^\infty$, equation (12) is absolutely convergent and $\hat{f}(n,k+2\pi)=\hat{f}(n,k)$.

Let E_n denote the orthogonal projection on the nth band. Then (Blount 1962)

$$(E_n\hat{x}E_nf)(n,k)=\mathrm{i}(\mathrm{d}/\mathrm{d}k)\hat{f}(n,k), \qquad f\in \mathrm{D}(H). \tag{13}$$

Now $\mathrm{d}/\mathrm{d}k$, where

$$\mathrm{D}\left(\frac{\mathrm{d}}{\mathrm{d}k}\right)==\left\{f|f\in AC[-\pi,\pi];f(-\pi)=f(\pi);f,\frac{\mathrm{d}f}{\mathrm{d}k}\in L^2(-\pi,\pi)\right\},$$

has a pure point spectrum (see example III.2.7 in Kato 1966). This extends to $\mathrm{d}/\mathrm{d}k+g(k)$ with g measurable, since

$$\frac{\mathrm{d}}{\mathrm{d}k}+g=\exp\left(-\int_{-\pi}^{k}g(t)\,\mathrm{d}t\right)\frac{\mathrm{d}}{\mathrm{d}k}\exp\left(\int_{\pi}^{k}g(\tau)\,\mathrm{d}\tau\right). \tag{14}$$

Consequently:

Corollary 2. Let $A_n=E_nHE_n$ be the restriction of H to an isolated band n. Then A_n has a pure point spectrum. In fact,

$$\sigma(A_n)=\left\{\lambda\,|\,\lambda=m\epsilon+\frac{1}{2\pi}\int_{-\pi}^{\pi}\epsilon_n(k)\,\mathrm{d}k,\ m\in\mathbb{Z}\right\},\tag{15}$$

where $\epsilon_n(k)$ is the dispersion of the band.

Proof. We shall prove

$$\mathrm{D}(A_n)=\mathrm{D}(\mathrm{d}/\mathrm{d}k)=\mathrm{D}(\mathrm{d}/\mathrm{d}k+\epsilon_n(k)).$$

Since $\epsilon_n(k)$ is analytic, the RHS is immediate. First note that, for an isolated band n, $[x, E_n]$ is bounded:

$$[x,E_n]=-\frac{1}{\pi}\int_{\Gamma_n}(p^2+V-\xi)^{-1}p(p^2+V-\xi)^{-1}\,\mathrm{d}\xi.\tag{16}$$

Γ_n is a (finite) contour around the spectrum of the nth band, and the integrand in (16) is bounded.

Let $f\in\mathrm{D}(x)\cap\mathrm{D}(p^2)$; then $(\widehat{E_nxf})(n,k)\in L^2(-\pi,\pi)$. By (16), $\{E_n\widehat{[x,E_n]}f\}(n,k)\in L^2(-\pi,\pi)$. Hence $(\widehat{E_nxE_nf})=\mathrm{i}(\mathrm{d}/\mathrm{d}k)\hat{f}(n,k)\in L^2(-\pi,\pi)$. The converse is also true. Let $\hat{f}(k)$, $\hat{f}'(k)\in L^2(-\pi,\pi)$. By the converse of (12), $f(p)=\psi_{nk}(p)\hat{f}(k)$. But

$$\|f'(p)\|_{L^2(-\infty,\infty)}\leqslant\left\{\int_{-\pi}^{\pi}\|\psi'_{nk}\|^2_{l^2_k}|f(k)|^2\,\mathrm{d}k\right\}^{1/2}+\|\hat{f}'\|_{L^2(-\pi,\pi)}<\infty.$$

The periodicity of f in k follows from (12). □

Lemma 1. Let E_n be the orthogonal projection on the isolated nth-band subspace, $E'_n+E_n=1$. Let $W_n=E_nxE'_n+E'_nxE_n$. W_n is the 'interband interaction'. Then

(*a*) W_n is bounded and invariant under the discrete translations U_α, $\alpha\in\mathbb{Z}$.

(*b*) The numerical range of $E_nHE_n\restriction_{E_nL^2(\mathrm{d}x)}$ is contained in the strip

$$\Theta(E_nHE_n)\subseteq\{z\,|\,z=\epsilon_n(k)+\epsilon\alpha,\ \alpha\in\mathbb{R},\ k\in[-\pi,\pi]\}.$$

(*c*) The numerical range of $E'_nHE'_n\restriction_{E'_nL^2(\mathrm{d}x)}$ is contained in the half-plane

$$\Theta(E'_nHE'_n)\subseteq\{z\,|\,z=\epsilon_m(k)+\alpha\epsilon+\beta,\ \alpha\in\mathbb{R},\ \beta>0,\ m\neq n\}.$$

Proof.

$$E'_nxE_n=E'_n[x,E_n].\tag{17}$$

The RHS is bounded by (16). Translation invariance follows from $[U_\alpha, E_n]=0$, $\alpha\in\mathbb{Z}$. (*b*) and (*c*) follow by arguments identical to those in Blount (1962). □

By proposition 1, W_n is bounded by zero relative to H. Let

$$\tilde{H}(\beta)=H-\beta\epsilon W_n.\tag{18}$$

It is easy to see that $\tilde{H}(\beta)$ enjoys the properties of H in part (i) of theorem 1 and has a numerical range contained in a half-plane lying to the right of a straight line in the ϵ direction. By corollary 2 and lemma 1, the boundedness of W_n, there is a neighbourhood of 1 such that, for β close to 1, $\sigma[\tilde{H}(\beta)]\neq\varnothing$. For such β, $\tilde{H}(\beta)$ also satisfies part (ii) of theorem 1. We shall now prove that, for all $0\leqslant\beta\leqslant1$, $\sigma[\tilde{H}(\beta)]$ has eigenvalues in a strip about the nth band, stretched in the ϵ direction.

Proof. For simplicity consider ϵ imaginary, $\theta = \pi/2$ and n the lowest (isolated) band. $\sigma[\tilde{H}(1)]$ has eigenvalues on the line

$$\mathrm{Re}\, z = \frac{1}{2\pi} \int_{-\pi}^{\pi} \epsilon_n(k)\, \mathrm{d}k$$

which intersects the real axis at $l(1)$. Let $l(\beta)$ denote the intersect as β decreases towards zero. Since $\tilde{H}(\beta)$ has a numerical range in a half-plane extending to the right, $l(\beta) \geqslant -M$. Choose m in the gap. By proposition 1,

$$\|[\tilde{H}(1) - m]^{-1}\| \leqslant F(\theta = \pi/2) < \infty. \tag{19}$$

Choose $\epsilon_0 > 0$ such that $\epsilon_0 \|W_n\| F(\theta) < 1$, and let S be the strip bounded by the lines $\mathrm{Re}\, z = -M$ and $\mathrm{Re}\, z = m$. By the second resolvent equation, ∂S belongs to the resolvent set of $\tilde{H}(\beta)$, $0 \leqslant \beta \leqslant 1$. Let $\beta_0 \in [0, 1)$ be the largest β such that $\sigma[\tilde{H}(\beta)] \cap S = \varnothing$. Consider the compact set $S_0 = \{z | z \in S, -\epsilon_0 \leqslant \mathrm{Im}\, z \leqslant \epsilon_0\}$. By the upper semicontinuity of the spectrum (Kato 1966), there is a neighbourhood of β_0 such that S_0 belongs to the resolvent set of $\tilde{H}(\beta)$. Thus there is no such β_0. Suppose now β_0 is the smallest β such that $\tilde{H}(\beta)$ has a spectrum in S. By the invariance of the spectrum under shifts by ϵ, and the fact that ∂S belongs to the resolvent set of $\tilde{H}(\beta)$ for all β, $\tilde{H}(\beta_0)$ has at least one eigenvalue in the interior of S_0. By a standard perturbation argument there is a neighbourhood of β_0 such that S_0 contains an eigenvalue of $\tilde{H}(\beta)$. Thus there is no such smallest $\beta_0 \in [0, 1]$. □

We conclude with a speculative remark. The quasi-nil-potency of H_0 is expected to be unstable under perturbations by a local potential function. If so, Hamiltonians with 'generic' V's in equation (5) would have a point spectrum even if there is no spectrum for such V's for $\epsilon = 0$. If the complex field behaviour of the spectrum is relevant to the real field behaviour, one would speculate enhanced binding in homogeneous fields!

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