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COMMENT

On the spectrum of one-electron Hamiltonians with impurities

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Abstract. We study the modifications introduced in the spectrum of a one-electron Hamiltonian with a locally square integrable periodic potential by a class of perturbations, including finite sums of Coulomb potentials. We also remark on some qualitative differences with respect to the spectrum associated with trace class perturbations considered by J Avron.

The analysis of doped insulators or semiconductors has shown that the presence of defects or impurities may lead to the introduction of discrete energy levels in the forbidden energy bands (see Bassani *et al* (1974) for a nice review). The simplest model used to describe such a system is a one-electron Hamiltonian with a locally square integrable periodic potential, to which an element of a large class of long-range order potentials, including Coulomb interactions with a (finite) number of impurity centres, is added. The main purpose of this note is to prove that under these conditions the perturbation introduces at most *isolated point eigenvalues of finite multiplicities* in the forbidden energy bands, which may accumulate at most at an extreme point of a band. The proof is a very simple adaptation of Hunziker's classic argument (1966), together with a remark of Thomas (1973), but because of its relevance to the models, it seems useful to present it here.

In the so-called crystal momentum representation (Blount 1963), neglecting interband transitions, there exists a similar result under the assumption that the perturbation is of trace class (Avron 1977, theorem 2). We comment on some qualitative differences between the spectrum in this approximation and in the less restrictive model considered above.

Let L be a lattice in $\mathbb{R}^3$ and V a potential with

$$V(x+t)=V(x) \qquad x\in\mathbb{R}^3 \qquad t\in L. \tag{1}$$

Let

$$H_0=-\Delta+V \tag{2}$$

as an operator on $\mathscr{H}=L^2(\mathbb{R}^3, \mathrm{d}^3x)$. If $\tilde{L}$ is the lattice dual to L (reciprocal lattice), let $H_0(k)$ be the operator on $l^2(\tilde{L}_k)$, $\tilde{L}_k$ being the coset corresponding to $k\in\mathbb{R}^3/\tilde{L}$ (Avron

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et al 1974), given by

$$H_0(k) = T(k) + V$$

$$(T(k)\Psi)(p) = (p+k)^2\Psi(p) \qquad p \in \tilde{L} \qquad k \in \mathbb{R}^3/\tilde{L}$$

$$(V\Psi)(p) = \sum_{q\in\tilde{L}} \tilde{V}(q)\Psi(p-q)$$

$$\tilde{V}(q) = |\Lambda|^{-1} \int_\Lambda \exp(-\mathrm{i}qx)V(x)\,\mathrm{d}^3x$$

where Λ is a basic cell of L. Then (Avron *et al* 1974) H_0 is unitarily equivalent to the direct integral

$$\int_{\mathrm{B}}^{\oplus} H_0(k)\,\mathrm{d}^3k$$

on

$$\mathscr{H} = \int_{\mathrm{B}}^{\oplus} l^2(\tilde{L}_k)\,\mathrm{d}^3k,$$

where $\mathrm{B} = \mathbb{R}^3/\tilde{L}$ is the Brillouin zone. We assume $V \in L^2_{\mathrm{loc}}(\mathbb{R}^3, \mathrm{d}^3x)$ or, equivalently, in view of (1),

$$v^2 \equiv \int_\Lambda |V(x)|^2\,\mathrm{d}^3x < \infty. \tag{3}$$

The properties of H_0 are summarised in the following proposition.

Proposition 1 (Avron *et al* 1974, Thomas 1973). H_0 is self-adjoint on $D(H_0) = D(-\Delta)$† and bounded below. Σ_{H_0} is absolutely continuous. Σ_{H_0} consists thus of the union of a countable number of connected disjoint closed sets, which we shall call 'bands'. Let now

$$H = H_0 + U \tag{4}$$

where U is a multiplication operator on $\mathscr{H}$, satisfying the condition

$$U \in L^2(\mathbb{R}^3) + L^\infty_\epsilon(\mathbb{R}^3) \tag{5}$$

in the notation of Hunziker (1966). This condition allows for potentials of type

$$U(x) = \sum_{i=1}^{N} \frac{\lambda_i}{|x - x_i|} \qquad N < \infty$$

where the λ_i, $i = 1, \ldots, N$, are real constants (related to 'dielectric constants' in Bassani *et al*) and $x_i = 1, \ldots, N$, arbitrary points in L.

Proposition 2. H is self-adjoint on $D(H) = D(-\Delta)$ and bounded below.

Proof. V is a Kato-small perturbation of $(-\Delta)$, that is $D(V) \supseteq D(-\Delta)$ and for all $\psi \in D(-\Delta)$ and all $\epsilon > 0$ there exists $b(\epsilon) < \infty$ such that

$$\|V\psi\| \leq \epsilon\|-\Delta\psi\| + b(\epsilon)\|\psi\|. \tag{6}$$

† For any operator A on $\mathscr{H}$, $D(A)$ denotes its domain and Σ_A its spectrum, and if $z \notin \Sigma_A$, $R_A(z) \equiv (z - A)^{-1}$.

Since V is assumed to be only *locally* L^2, the standard Kato proof of (Reed and Simon 1975, theorem X-16) does not apply immediately. However, the result follows easily from Avron *et al* (1974). Let E be negative real. We have for all $\psi \in D(H_0)$, $V\psi = V(E+\Delta)^{-1}(E+\Delta)\psi$ because $(V(E+\Delta)^{-1})$ is bounded:

$$\|V(E+\Delta)^{-1}\|^2 = \int_B \mathrm{d}^3k \, \|\tilde{v}(k)(E-T(k))^{-1}\|^2_{l^2(\tilde{L}_k)} \leq |B| v^2 \sum_{j \in \tilde{L}_k} (E-j^2)^{-2} \equiv \epsilon^2. \tag{7}$$

This also shows that (6) holds, with ϵ as defined by (7), and $b(\epsilon) = \epsilon |E|$, and ϵ may be made arbitrarily small by choosing E sufficiently large negative. By (5), U is a Kato-small perturbation of $(-\Delta)$ (Reed and Simon 1975, theorem X-16), hence so is $(U+V)$, and the final assertion follows from the Kato–Rellich theorem (Reed and Simon, theorem X-12).

Proposition 3. If $z \notin \Sigma_H$, the operator

$$A(z) = UR_{H_0}(z)$$

is a compact operator.

Proof. By Hunziker (1966) it is sufficient to prove that

$$A_1(z) \equiv U_1 R_{H_0}(z)$$

is Hilbert–Schmidt for $z \notin \Sigma_{H_0}$ and $U_1 \in L^2(\mathbb{R}^3)$, and by standard arguments it is sufficient to prove this for any negative real $E \notin \Sigma_{H_0}$. As in Thomas (1973), this follows by writing

$$A_1(E) = A_2 A_3(E)$$

where $A_2 \equiv U_1(1-\Delta)^{-1}$ is Hilbert–Schmidt (Hunziker 1966) and

$$A_3(E) \equiv (1-\Delta)(E-H)^{-1} = \int_B^{\oplus} (1+T(k))(E-T(k))^{-1}[1-\tilde{v}(k)(E-T(k))^{-1}]^{-1} \, \mathrm{d}^3k$$

is bounded for E sufficiently large negative (Avron *et al* 1974).

Proposition 4. (*a*) $\Sigma_{H_0} \subseteq \Sigma_H$. (*b*) The part of Σ_H in the complement of Σ_{H_0} (in particular, in a 'forbidden energy band') consists of isolated point eigenvalues of finite multiplicities, which may accumulate at most at the extremities of a band.

Proof. (*a*) Define, for each $x \in L$, the operators T_x by

$$(T_x f)(y) = f(x+y) \qquad f \in \mathscr{H} \quad x \in L \quad y \in \mathbb{R}^3.$$

It follows by the same argument of Hunziker (1966, lemma 3), that

$$\lim_{|x| \to \infty} \|UT_x f\| = 0 \qquad \forall f \in D(H_0).$$

Now, for $x \in L$, T_x and H_0 commute on $D(H_0)$ by (1). The rest of the argument is as in Hunziker (1966).

(*b*) We use the Lippman–Schwinger equation

$$R_H(z) = R_{H_0}(z) + R_{H_0}(z) U R_H(z) \qquad z \notin \Sigma_H.$$

$(R_{H_0}(z)U)$ has a unique bounded extension $(R_{H_0}(\bar{z})U)^* = UR_{H_0}(z)$, which is a compact operator by proposition 3. The rest follows as in Hunziker (1966). Avron (1977) considered perturbations of trace-class in the crystal-momentum representation, neglecting interband transitions ('small' coupling constant). As he remarked, there are qualitative differences between the spectrum with and without these approximations, in the case of a potential growing at infinity, and we should like to comment on the qualitative differences in the impurity case. Under a reasonable set of assumptions, the number of eigenvalues of H in a 'forbidden energy band' is finite, in contrast to what is expected in the Coulomb case†. This is not surprising, of course, because the trace-class condition is a 'short-range' condition, but the point is that the finiteness of the number of eigenvalues is here, under this condition, an almost universal phenomenon, due to the fact, emphasised by Avron (1977), that classically or semi-classically the orbits in k-space do not extend to infinity.

To analyse the situation, firstly we write $\mathscr{H}$ as a direct sum over a 'band index' (Odeh and Keller 1964)

$$\mathscr{H} = \bigoplus_{n=1}^{\infty} \mathscr{H}_n. \tag{8}$$

More precisely, each $\phi \in \mathscr{H}$ may be represented by a sequence $\{\phi_n\}_{n=1}^{\infty}$ such that

$$\|\phi\|^2 = \int_B \mathrm{d}^3k \sum_{n=1}^{\infty} |\phi_n(k)|^2 \qquad \phi_n(k) \equiv \langle \psi_n^k, \phi \rangle$$

where ψ_n^k are the 'Bloch waves' (Odeh and Keller 1964, corollary 2 in their notation). We define the Hamiltonian in correspondence with (8), by

$$H = H_0 + U$$

$$H_0 = \bigoplus_{n=1}^{\infty} H_{0n}$$

$$U = \bigoplus_{n=1}^{\infty} U_n$$

$$(H_{0n}\phi_n)(k) = \epsilon_n(k)\phi_n(k) \qquad k \in B$$

$$(U_n\phi_n)(k) = \frac{1}{|B|}\int_B \mathrm{d}^3k'\, U_n(k, k')\phi_n(k') \qquad k \in B$$

$$U_n(k, k') = \overline{U_n(k', k)} \equiv \sum_{t \in L} \lambda_n(t) \exp[\mathrm{i}(k-k')t]$$

under the condition

$$C_n \equiv \sum_{t \in L} |\lambda_n(t)| \qquad C \equiv \sup_n C_n < \infty. \tag{9}$$

The above definition is equivalent to the one given by Avron (1977). If the $\lambda_n(t)$ are interpreted as matrix elements of U between Wannier functions $a_n(\cdot - t)$ (in the notation and definition of Odeh and Keller, appendix). The model is a generalisation of a model of Koster and Slater (1954). We assume that $\Sigma_{H_{0n}}$, the range of $\epsilon_n(\cdot)$ (the

† The Coulomb case has been studied by Bentosela (1977), who provided a rigorous justification of the 'effective mass approximation'.

'band' Σ_n), is absolutely continuous, and that $\Sigma_n \cap \Sigma_m = \emptyset$ for $n \neq m$, i.e. the bands do not overlap. Hence the spectrum $\Sigma_{H_0} = \cup \Sigma_{H_{0n}}$ is absolutely continuous. The operator U is easily seen to be trace-class, whence (a) and (b) of proposition 3 hold (Avron 1977). By methods of Ghirardi and Rimini (1965, see also Simon 1971) one may prove the following proposition.

Proposition 5. Suppose there exist non-degenerate critical points of maximum and minimum of $\epsilon_n(\cdot)$ in B, for each n. Let $E_n \equiv \max_{k\in B}\epsilon_n(k)$, and $e_n \equiv \min_{k\in B}\epsilon_n(k)$, and

$$A_n(E) \equiv \frac{1}{|B|^2}\int_{B\times B} \mathrm{d}^3k\, \mathrm{d}^3k' \frac{|U_n(k,k')|^2}{(E-\epsilon_n(k))(E-\epsilon_n(k'))} \qquad \text{for } E > E_n \text{ or } E < e_n.$$

Then the number N_n^+ of eigenvalues of H in the interval $(E_n, E_n + C_n]$, where C_n is defined by (9), satisfies

$$N_n^+ \leqslant \lim_{E \downarrow E_n} A_n(E) < \infty.$$

Similarly, the number N_n^- of eigenvalues of H in the interval $[e_n - C_n, e_n)$ satisfies

$$N_n^- \leqslant \lim_{E \uparrow E_n} A_n(E) < \infty.$$

Let $G_n \geqslant 0$ denote the magnitude of the gap between the bands Σ_n and Σ_{n+1}. We assume finally: there exists $\gamma > 0$ independent of n such that

$$\max\{C_n, C_{n+1}\} \leqslant G_n - \gamma \qquad \forall n = 1,2,\ldots. \tag{10}$$

This assumption is quite natural, since we neglected interband transitions in our definition, and C_n is a measure of the magnitude of the perturbation.

Corollary. Under assumption (10), the number of eigenvalues of H in any forbidden energy band is finite.

Proof. By proposition 4 applied to our case, the eigenvalues of H may accumulate at most at the extremity of a band. Now, it is easy to prove that

$$\sum_H = \overline{\bigcup_{n=1}^{\infty} \sum_{H_n}} \qquad H_n \equiv H_{0n} + U_n.$$

Further, by (10), there exists no point at the extremity of any particular band which is a limit point of a sequence of eigenvalues, each one coming from one of the bands (in principle *infinite* in number) which are situated above it. Hence, it is sufficient to prove that the number of eigenvalues of H_n in any two half-open intervals having, respectively, E_n and e_n as end points, is finite. This follows from proposition 5.

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