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Instability of the continuous spectrum: The N -band Stark ladder*

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It is shown that the energy spectrum of the Bloch electron in an external field is *continuous*. Furthermore, it is shown that all approximations which take into account interband coupling within groups of finite number of bands (the N -band approximation) lead to a *pure-point* spectrum of intertwining Wannier–Stark ladders. This instability of the continuous spectrum under the N -band approximation is related to a theorem due to Weyl and von Neumann. Approximation methods for dealing with interband coupling within a group of finite number of bands are given.

1. INTRODUCTION

Weyl and von Neumann pointed out that the continuous spectrum is very unstable in that arbitrarily small perturbations can turn it into a pure point spectrum. On the contrary, the common belief is that physically meaningful perturbations do not cause such pathologies: They leave the continuous spectrum continuous and the discrete spectrum discrete. Instabilities of the continuous spectrum have been considered to be of mathematical interest having little or nothing to do with physics.

We shall show that a natural physical approximation widely used in solid state physics is of this nature: The approximation discards a presumably small part of the Hamiltonian, thereby changing the original continuous spectrum into a pure point spectrum. The example is taken from the theory of the one-dimensional Bloch electron in an external field. In Sec. 2 it is shown that the spectrum is absolutely continuous from $-\infty$ to ∞ and that it has no gaps. The absolute continuity of the spectrum follows from a general theorem in Sec. 2. This theorem generalizes a known result of Dunford and Schwartz to potentials that are not necessarily monotonic at infinity.

It is an experimental fact that, even though the band index is no longer a constant of motion, the electron leaks out of the band very slowly for external fields that are not too strong. A natural approximation is to assume that the band index is a true constant of motion (and then correct perturbatively). This is the “single band approximation,” and it leads to the pathological character described in the Weyl–von Neumann theorem: The exact continuous spectrum is made a pure point spectrum by it.

The point spectrum (eigenvalues) of the single band approximation has been of considerable interest because it is related to the Wannier–Stark ladder,¹ which consists of an infinite set of eigenvalues with spacing Ea . E is the force field and a is the lattice spacing. In some sense, the Stark ladder is the analog of Landau levels

in external magnetic fields. However, whereas the latter has at least a sound experimental basis, this is not the case for the Stark ladder which is more of a problem than a well-established effect.² The point spectrum is an artifact of the single band approximation since the exact spectrum is absolutely continuous. However, this *does not* prove that there is no Stark ladder effect in the sense of a periodic structure in the physical (optical, say) spectrum. In particular, this does not mean that the single band approximation is “large” or unphysical. On the contrary, the lesson of the Weyl–von Neumann theorem is that the spectrum, in its set theoretic sense, is a very sensitive object.

In Sec. 4 we discuss the N -band Hamiltonian. We prove that the spectrum consists of N intertwined Wannier–Stark ladders. Thus a finite interband interaction preserves the discrete spectrum. We also consider methods of approximations for the interband coupling. An analogy between the time-dependent Schrödinger equation and the N -band Hamiltonian is used to apply the adiabatic approximation to obtain the eigenvalues of the N -band Hamiltonian. This analogy also leads to a conservation law of probability in k .

2. THE MODEL

Consider the one-dimensional single particle Hamiltonian:

$$H = p^2/2m + V(x) + Ex, \quad x \in \mathbf{R}^1. \quad (1)$$

$V(x)$ is periodic and twice differentiable.

This Hamiltonian describes the motion of a charged particle in a periodic crystalline field and in an external constant electric (or gravitational) field. The crystal is assumed to be infinitely big. H is self-adjoint by standard arguments.³

The spectrum of H is the real energy axis; i. e., it is continuous stretching from $-\infty$ to ∞ . Before proving this, let us consider the simpler Hamiltonian:

$$H_0 = p^2/2m + Ex. \quad (2)$$

The unitary transformation

$$U = \exp[ip^3/6m] \quad (3)$$

transforms H_0 into the multiplication operator Ex . H_0 and Ex are thus unitarily equivalent so that in particular they have the same spectrum. The spectrum of an operator which is a multiplication by a function is the range of values this function assumes. In our case the spectrum of Ex , and hence of H_0 , stretches continuously from $-\infty$ to ∞ . Note that H_0 has no eigenvalues embedded in the continuous spectrum.⁴

It is perhaps physically obvious that the addition of a bounded periodic function to H_0 does not change the nature of the spectrum and in particular that the Hamiltonian (1) has no bound states.⁵ Mathematically, a problem arises because the periodic potential remains finite at infinity. It may then happen that interference due to the wiggling of the potential produces bound states. Examples of such bound states were given by von Neumann and Wigner.⁶

The following theorem guarantees the absolute continuity of the spectrum for potentials that go to $-\infty$ in one direction (at least) with no assumption of monotonicity.⁷

Theorem: Let there be given the second order differential operator

$$-\frac{d^2}{dx^2} - q(x) \quad (4)$$

on the interval $[\alpha, \infty)$. Assume that:

- (a) $q(x)$ is positive for x large enough,
- (b) $\int^\infty [(q'/q^{3/2})' + \frac{1}{4}(q')^2 q^{-5/2}] dx < \infty$,
- (c) $\int^\infty q^{-1/2} dx = \infty$,
- (d) $|q(x+a)| > |q(x)|$ for $a > a_0$.

Then the spectrum of any self-adjoint extension of the operator is entirely continuous and covers the whole real axis. In particular, this is the case for the Hamiltonian in Eq. (1).

The above theorem is a standard result in analysis, except for condition (d), which is customarily replaced by a much stronger condition of monotonicity of $q(x)$ (monotonicity is equivalent to $a_0 = 0$). The proof of this theorem is identical to the proof of Corollary XIII. 6. 21 in Dunford and Schwartz.⁸ In other words, Dunford and Schwartz prove a stronger result than the one they state. We shall only point out that (d), or equivalently the assumption of monotonicity, is used once in the proof, to show the absence of L^2 solutions.

To summarize:

- (a) H has absolutely continuous spectrum from $-\infty$ to $+\infty$ for $E \neq 0$. In particular it has no gaps of forbidden energies characteristic to the free ($E = 0$) Bloch Hamiltonian.
- (b) H has no eigenvalues (bound states), not even eigenvalues embedded in the continuous spectrum. In particular there is no ladder structure for the eigenvalues.

3. THE SINGLE BAND APPROXIMATION

Here we shall briefly review the "single band approximation," which reflects the idea that bands are meaningful objects even in the presence of external fields of force.⁹ The approximation involves adding a term to the Hamiltonian which makes the band index a true constant of motion. The matrix elements of the position operator x in the nk representation are^{5,10}

$$(nk|x|mk') = i\delta_{m,n} \frac{d}{dk} \delta(k-k') + x_{mn}(k) \delta(k-k'); \quad (5)$$

$x_{mn}(k)$ are continuous functions in the absence of bands crossing.¹¹ (This is the generic situation in one dimension.¹⁴ Moreover,

$$x_{mn} = \frac{i\hbar}{m} \frac{p_{mn}(k)}{\epsilon_n(k) - \epsilon_m(k)}, \quad (6)$$

$$\frac{1}{2m} \sum_m |p_{mn}(k)|^2 \leq \epsilon_n(k) + \sup_x |V(x)|.$$

Consider the Hermitian operator A with matrix elements

$$\begin{aligned} A_{mn}(k) &= x_{mn}(k), \quad m \neq n, \\ A_{nn}(k) &= 0. \end{aligned} \quad (7)$$

In the single band approximation, the Hamiltonian H in (1) is replaced by

$$H_{SB} = H - EA. \quad (8)$$

One expects that H_{SB} is an approximation to H if A is in some sense small. Phenomenologically, A is associated with tunneling which is a very slow process on atomic scale for large band gaps¹² [see Eq. (6)]. H_{SB} assumes the simple form of an infinite number of decoupled, first-order differential operators, with the operator corresponding to the n th band being

$$iE \frac{d}{dk} + \epsilon_n(k) + Ex_{nn}(k). \quad (9)$$

H_{SB} is diagonal in the band index n and has pure point spectrum. The eigenvalues have two quantum numbers—the band index n and a ladder index ν . The eigenfunctions and eigenvalues are, respectively,

$$\psi_{\nu n}(mk) = \frac{\delta_{\nu, m}}{\sqrt{2\pi/a}} \exp\left(-\frac{i}{E} \int_{-\tau/a}^k dk' [\lambda_{\nu} - \epsilon_n(k') - Ex_{nn}(k')]\right), \quad (10)$$

$$\lambda_{\nu} = \nu Ea + \frac{a}{2\pi} \int_{-\tau/a}^{\tau/a} dk [\epsilon_n(k) + Ex_{nn}(k)],$$

where $\nu = \{0, \pm 1, \pm 2, \dots\}$, $n = \{1, 2, \dots\}$. $\psi_{na}(k, m)$ is just a phase in k . This is a consequence of a conservation law which will be discussed in Sec. 4.

For fixed n , the eigenvalues are equally spaced, hence the name "Stark ladder." The infinite number of ladders, corresponding to the infinite number of bands, are intertwined. There is thus an infinite number of eigenvalues within each energy interval Ea .

4. N-BAND HAMILTONIAN

A. A spectral theorem

Consider the N -band Hamiltonian H_{NB} in $E_N \otimes L^2(B)$,

E_N an N -dimensional vector space and B the Brillouin zone. H_{NB} is given by

$$H_{NB}\psi(n, k) = iE \frac{d}{dk} \psi(n, k) + \epsilon_n(k)\psi(n, k) + E \sum_{m=1}^N x_{nm}(k)\psi(m, k), \quad n=1, \dots, N. \quad (11)$$

H_{NB} describes N bands coupled by the interband interaction $x_{mn}(k)$.¹³ Our purpose is to show that, for any finite N (and in the absence of band crossing), H_{NB} has a purely discrete spectrum in the form of N Stark ladders. Only for $N=\infty$ is the continuous spectrum recovered.

H_{NB} has discrete spectrum by the following argument: The N -band Hamiltonian with $x_{mn}(k)$ set equal to zero has a compact resolvent [this follows from Eq. (10)]. If there is no band crossing, it follows from (6) that the interband interaction $x_{mn}(k)$ is a bounded operator. By a basic theorem of Rellich¹⁴ H_{NB} has a compact resolvent, and so H_{NB} has a purely discrete spectrum with isolated eigenvalues accumulating only at infinity.

The pathological behavior of the spectrum under the perturbation of interband coupling is peculiar to the full infinite bands Hamiltonian. That is, only in this case does the interband coupling make a continuous spectrum discrete or vice versa. In particular, no N -band model recovers the absolute continuity of the true spectrum.

Let $h(k)$ be the operator

$$h\psi(n, k) = \epsilon_n(k)\psi(n, k) + E \sum_{m=1}^N x_{nm}(k)\psi(m, k) \quad (12)$$

and $h_{mn}(k)$ its matrix elements.

Hermiticity and periodicity give two global characteristics of the solutions of N -band Hamiltonians.

(a) The spectrum of eigenvalues has the form of N intertwined Stark ladders.

This follows from periodicity in k -space: If $\psi_\lambda(n, k)$, $\{k \in B, n=1, \dots, N\}$ is an eigenvector with eigenenergy λ , then $\exp(i\nu ka)\psi_\lambda(k, n)$ is an eigenvector with eigenenergy $\lambda + \nu Ea$. A simple continuity argument shows that there are N such ladders: Let the interbands coupling shrink to zero. This shifts the eigenvalues up or down but it does not annihilate or create eigenvalues. Since there are N ladders for zero coupling, there are N ladders also for any non-zero interband coupling.

(b) Probability conservation in k -space: If $\psi_\lambda(k, n)$ is an eigenvector of the N -band Hamiltonian then $\sum_{n=1}^N |\psi_\lambda(k, n)|^2$ is constant, independent of k .

To show this let $(\psi(k), \phi(k))$ denote scalar product in the N -dimensional vector space, i. e.,

$$(\psi(k), \phi(k)) \equiv \sum_{n=1}^N \psi^*(n, k)\phi(n, k). \quad (13)$$

The eigenvector ψ_λ of the N -band Hamiltonian satisfies

$$iE \frac{d}{dk} \psi_\lambda(k, n) = [\lambda - h(k)]\psi_\lambda(k, n). \quad (14)$$

Since λ is real and $h(k)$ self-adjoint, the result follows by Stone's theorem.¹⁵ This conservation relation is the

analog of the conservation of probability for the time-dependent Schrödinger Hamiltonian.

B. Methods of approximation

The N -band Hamiltonian cannot be solved exactly in general and one must resort to approximations.¹³ Although perturbation expansion in the interband interaction is in principle possible, this is not the most convenient method.¹⁶ In particular, the perturbation expansion does not preserve property (b)—conservation of probability in k . [It does preserve property (a).] A more natural approximation is the adiabatic method.¹⁷ This approximation is exact either when $h(k)$ is independent of k or when $h(k)$ is diagonal. The approximation proceeds from the aforementioned k - t analogy.

Let $\lambda_n(k)$ and $\psi_n(m, k)$, $\{n, m=1, \dots, N\}$ be the eigenvalues and eigenvectors of the matrix $h(k)$ in E_N . Furthermore, let

$$\bar{\lambda}_n = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk \lambda_n(k).$$

Then, in the adiabatic approximation, the eigenvalues and eigenfunctions of the N -band Hamiltonian are respectively

$$\lambda_{\nu n} = \bar{\lambda}_n + \nu Ea,$$

$$\psi_{\nu n}^{NB}(m, k) = \psi_n(m, k) \exp(i\nu ka) \exp \frac{i}{E} \int_{-\pi/a}^k dk [\lambda_n(k) - \bar{\lambda}_n],$$

where $n=1, \dots, N$ and $\nu=0, \pm 1, \dots, \pm \infty$. The adiabatic approximation satisfies both properties (a) and (b), i. e., it has the spectrum of N ladders and it conserves probability in k .

SUMMARY

We have shown that the spectrum of the Bloch electron in an external field is continuous. Under a perturbation corresponding to the accounting for interband coupling within groups consisting of a finite number of bands, the spectrum has been shown to become discrete, consisting of intertwined Stark ladders. This phenomenon is related to a theorem of Weyl and von Neumann.¹⁸ Finally we have shown that probability in k is conserved by eigenfunctions of the N -band Hamiltonian, and introduced a method of approximation for the interband interaction which preserves this property.

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