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A note on the extension of the Kane function

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Abstract. We give an exact expression for the extension of the Kane function for periodic potentials with an inversion centre. The variance of the Kane function is the sum of the semi-classical expression and the variance of the Wannier function of Kohn type.

1. Introduction

The motion of a Bloch electron in external fields has challenged theoreticians for about half a century [1, 2]. Even if the external—electric or magnetic—fields are constant, which means that the physics is invariant under lattice translation, the mathematics involved in the quantum-mechanical description can be quite complicated.

In 1960, Wannier remarked that in the case of a homogeneous electric field the energy spectrum should consist of ladders of equally spaced eigenvalues, later referred to as Wannier–Stark ladders [3]. But he also believed that 'energy states in the electric field case have not much intrinsic interest because they are *a priori* known to be not normalizable and hence not truly stationary'. If a restriction is made to a single energy band of the Bloch electron, explicit solutions can be found which give rise to Stark ladders and are square integrable [4, 5]. These functions, known as Kane functions, practically became a standard approximation and it was believed for a long time that the coupling of different bands would not change the spectrum qualitatively.

The rigorous proof of the continuous spectrum by Avron *et al* [6] and preceding controversies [7] did little or no harm to the popularity of the Kane functions. Since in many cases of practical interest, the tunnelling rate is smaller by orders of magnitude than the spacing of the Stark ladder, the picture of stationary states plus dissipation on account of the tunnelling is still a reasonable approximation. Wannier–Stark ladders, and their time-dependent adjuncts, Bloch oscillations, have been observed in optical experiments on superlattices in electric fields [8–10], giving proof of strongly localized eigenfunctions. Therefore, Kane functions or, equivalently, Wannier functions are the basic ingredients for most theoretical studies of superlattices in electric fields [11–14]. Recent results on the optical absorption of superlattices in electric fields show a good quantitative agreement between experimental data and calculations based on Wannier functions [15].

From limiting cases (no periodic potential, tight-binding approximation), it is plausible that the wave functions should narrow as the field strength increases. A semiclassical, 'if the unit is right, the result is right' approach gives an effective extension of the wave packet $\Delta x = \Delta E/|eF|$, where ΔE is some effective miniband width, e is the elementary charge, and F is the field strength. This was pointed out by many authors [8, 9, 11, 13], and is a good

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estimate in the limit of small fields. On the other hand, for $F \to \pm\infty$, the Kane function goes over to a symmetric or antisymmetric Wannier function which has a finite width of the order of the lattice constant [14].

The question arises of whether one can find an expression for the extension of the Wannier function that would cover field strengths from zero to infinity. In this paper we show that the variance of the Kane function is exactly the sum of the semiclassical expression for the variance and the variance of the Kane function in the limit $F = \infty$.

2. Preliminaries

Unless otherwise noted, integrals and sums run from $-\infty$ to $+\infty$ and asymptotic behaviour of functions and series refers to the limit $\pm\infty$. Trivial prefactors of wave functions are excluded if they are not relevant.

We consider the one-dimensional Schrödinger equation of a particle with charge $-e$ in a periodic potential U under a static electric field F:

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + U(x) + eFx\right]\psi(x) = (\hat{H}\psi)(x) = \mathcal{E}\psi(x) \tag{1}$$

where $U(x+a) = U(x)$, and a is called the period of U. We assume that the potential U is symmetric around $x = 0$, i.e.,

$$U(-x) = U(+x)$$

and piecewise continuous.

For $F = 0$, the eigenfunctions of equation (1) can be given in the form of Bloch functions:

$$\varphi_{k\nu}(x) = \sqrt{\frac{1}{2\pi}}\mathrm{e}^{\mathrm{i}kx}u_{k\nu}(x) \qquad u_{k\nu}(x+a) = u_{k\nu}(x) \tag{2}$$

and the spectrum consists of energy bands $E_\nu(k)$. The lattice-periodic functions are normalized according to

$$(u_{k\nu}|u_{k\nu'}) = \frac{1}{a}\int_{-a/2}^{+a/2}\mathrm{d}x\; u^*_{k\nu}(x)u_{k\nu}(x) = \delta_{\nu\nu'}.$$

We assume non-degenerate energy bands, which is the usual case for one-dimensional problems. Then $E_\nu(k)$ possesses continuous derivatives of arbitrary order and the Bloch functions can be chosen such that $\varphi_{k+2\pi/a,\nu}(x) = \varphi_{k\nu}(x)$ [16].

According to Kane, an approximate solution for the eigenfunctions ψ and eigenvalues $\mathcal{E}$ of equation (1) is [4]

$$\begin{aligned}\psi_\nu(x) &= \sqrt{\frac{a}{2\pi}}\int_{-\pi/a}^{+\pi/a}\mathrm{d}k\;\tilde{\psi}_\nu(k)\varphi_{k\nu}(x)\\ \mathcal{E}_\nu &= \frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a}\mathrm{d}k\;[E_\nu(k) + eFX_{\nu\nu}(k)]\end{aligned} \tag{3}$$

where

$$\tilde{\psi}_\nu(k) = \exp\left\{\frac{1}{\mathrm{i}eF}\int_0^k \mathrm{d}k'\;[\mathcal{E}_\nu - E_\nu(k') - eFX_{\nu\nu}(k')]\right\} \tag{4}$$

$$X_{\nu\nu}(k) = \frac{\mathrm{i}}{a}\int_{-a/2}^{+a/2}\mathrm{d}x\; u^*_{k\nu}(x)\frac{\partial u_{k\nu}(x)}{\partial k}. \tag{5}$$

Only one representative of the Kane functions is shown for each band ν, because it is evident that if $\psi_\nu(x)$ is an approximate eigenfunction with eigenvalue $\mathcal{E}_\nu$, then $\psi_\nu(x - am)$ is also an approximate eigenfunction with approximate eigenvalue $\mathcal{E}_\nu + meFa$ (m integer). The Kane functions represent a complete set of eigenfunctions and fulfil

$$\int \mathrm{d}x\ \psi_\nu^*(x - am)\psi_{\nu'}(x - am') = \delta_{\nu\nu'}\delta_{mm'}. \tag{6}$$

Henceforth we shall omit the band index ν on the understanding that the considerations below apply for each band. Then ψ denotes the Kane function for a fixed band ν. We note that, up to a prefactor, the definition of the Kane functions (3)–(5) is independent of the choice of the Bloch functions: a different set of Bloch functions $\exp[\mathrm{i}f(k)]\varphi_k(x)$, f real, $f(-\pi/a) = f(+\pi/a)$, would result in Kane functions $\exp[\mathrm{i}f(0)]\psi(x)$. We will make use of this fact by fixing the phase of the Bloch function as described below.

First, we determine lattice-periodic functions v_k that are subject to the following restrictions: $v_{k=0}$ is real; $(\mathrm{Re}\, v_k|\mathrm{Im}\, v_k) = 0$; and v_k is continuous with respect to k. Because U is symmetric, these lattice-periodic functions have the following properties:

(i) either $\mathrm{Re}\, v_k$ is symmetric for each k and $\mathrm{Im}\, v_k$ is antisymmetric for each k or $\mathrm{Re}\, v_k$ is antisymmetric for each k and $\mathrm{Im}\, v_k$ is symmetric for each k; and

(ii) $v_{+k}(x) = v_{-k}^*(x)$.

The functions $\mathrm{e}^{\mathrm{i}kx}v_k(x)$ also fulfil (i) and (ii) but are not necessarily periodic in k. The Schrödinger equation (1) for $F = 0$ implies that $\mathrm{e}^{\mathrm{i}(k+2\pi/a)x}v_{k+2\pi/a}(x) = c\mathrm{e}^{\mathrm{i}kx}v_k(x)$, $|c| = 1$, for non-degenerate bands. From properties (i) and (ii) it follows that c is either $+1$ or -1. For $c = +1$, we set $\varphi_k(x) = \mathrm{e}^{\mathrm{i}kx}v_k(x)/\sqrt{2\pi}$, which gives $X(k) = 0$. For $c = -1$ we define $\varphi_k(x) = \mathrm{e}^{\mathrm{i}k(x-a/2)}v_k(x)/\sqrt{2\pi}$ which results in $X(k) = a/2$.

The resulting Bloch functions φ_k are periodic in k with a period of $2\pi/a$. The alternatives $c = +1$ and $c = -1$ from the last paragraph correspond to the cases A and B of the paper by Kohn [16] and it is shown therein that $\varphi_k(x)$ has continuous derivatives in k of arbitrary order. The above prescription can also be used for clean numerical calculations of Kane functions.

Now we are able to give an expression for the Kane function (3) in the limit $F \longrightarrow \pm\infty$. Since $X(k) = \text{constant}$,

$$\lim_{F\to\pm\infty} \psi(x) = w(x) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ \varphi_{k\nu}(x). \tag{7}$$

The function w is real, is either symmetric or antisymmetric around $x = 0$ or $x = a/2$, depending on whether $u_{k=0}$ is symmetric or antisymmetric, and obeys the same normalization (6) as the Kane functions. Furthermore, w coincides with the special Wannier function described by Kohn and decays rapidly, i.e., $w(x) = \mathrm{O}(|x|^{-\mu})$ for any $\mu > 0$.

3. The variance of the Kane function

Let χ be a quantum-mechanical wave function which is normalized to unity, i.e.,

$$||\chi||^2 = \int \mathrm{d}x\ |\chi(x)|^2 = 1.$$

Then $|\chi(x)|^2 \geqslant 0$ is interpreted as the probability density. The variance σ^2 is defined as

$$\sigma^2[\chi] = \int \mathrm{d}x\ |\chi(x)|^2 x^2 - \left[\int \mathrm{d}x\ |\chi(x)|^2 x\right]^2$$

and $\sigma = \Delta x$ is interpreted as the extent of the wave function.

We can now formulate the following lemma. The variance of the Kane function is given by

$$\sigma^2[\psi] = \sigma^2[w] + \left(\frac{\Delta E}{eF}\right)^2 \tag{8}$$

with w being the Wannier function of Kohn type, defined in equation (7), and

$$(\Delta E)^2 = \frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ E^2(k) - \left[\frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ E(k)\right]^2. \tag{9}$$

The above equation means, physically, that the variance of the Kane function is the sum of the variance of the Wannier function and the semiclassical approximation for the variance.

Proof. Since the variance is invariant under translation, we assume, without loss of generality, that w is centred at $x = 0$. First, we note from the definition (4) that the function $\tilde{\psi}(k)$ is periodic in k and has continuous derivatives of arbitrary order. Therefore, we may expand $\tilde{\psi}$ as a Fourier series according to

$$\tilde{\psi}(k) = \sum_m c_m \mathrm{e}^{-\mathrm{i}kam} \tag{10}$$

where

$$c_m = \frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ \mathrm{e}^{+\mathrm{i}kam}\tilde{\psi}(k).$$

The Fourier coefficients c_m are rapidly decaying.

Let us now derive an important property of the Fourier coefficients c_m. Let $\tilde{f}$ be any function that is periodic and continuous in $(-\infty, +\infty)$. From $|\tilde{\psi}(k)|^2 \equiv 1$ if follows that

$$\frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ \tilde{\psi}^*(k)\tilde{f}(k)\tilde{\psi}(k) = \frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ \tilde{f}(k).$$

If f_m denotes the mth Fourier coefficient of $\tilde{f}$, then

$$\sum_m \sum_{m'} c_m^* f_{m-m'} c_{m'} = f_0. \tag{11}$$

In turn, since a function can be defined by its Fourier coefficients, equation (11) is valid for any sequence f_m, provided that the sum of the f_m is absolutely convergent.

Inserting the Fourier expansion (10) into the definition of the Kane function (3) and taking into account that $\mathrm{e}^{-\mathrm{i}kam}\varphi_k(x) = \varphi_k(x - ma)$, the Kane function can be expressed in terms of the Wannier function as

$$\psi(x) = \sum_m c_m w(x - ma). \tag{12}$$

The variance of the Kane function now becomes

$$\sigma^2[\psi] = \sum_m \sum_{m'} c_m^* B_{mm'} c_{m'} - \left[\sum_m \sum_{m'} c_m^* A_{mm'} c_{m'}\right]^2 \tag{13}$$

where

$$B_{mm'} = \int \mathrm{d}x\ w^*(x - am)w(x - am')x^2$$

$$A_{mm'} = \int \mathrm{d}x\ w^*(x - am)w(x - am')x.$$

If we shift the argument by $-a(m+m')/2$ in the above integrals, $B_{mm'}$ and $A_{mm'}$ can be decomposed as

$$B_{mm'} = \int \mathrm{d}x\ w^*\left(x - a\frac{m-m'}{2}\right) w\left(x + a\frac{m-m'}{2}\right)\left[x^2 + xa(m+m') + a^2\frac{(m+m')^2}{4}\right]$$
$$= B^{(1)}_{mm'} + B^{(2)}_{mm'} + B^{(3)}_{mm'}$$
$$A_{mm'} = \int \mathrm{d}x\ w^*\left(x - a\frac{m-m'}{2}\right) w\left(x + a\frac{m-m'}{2}\right)\left[x + a\frac{m+m'}{2}\right]$$
$$= A^{(1)}_{mm'} + A^{(2)}_{mm'}.$$

The matrix elements $B^{(1)}_{mm'}$ depend only on the difference $m - m'$ and decay rapidly as $|m - m'| \longrightarrow \infty$. Therefore, we may use the property (11) of the Fourier coefficients which leads us to

$$\sum_m \sum_{m'} c^*_m B^{(1)}_{mm'} c_{m'} = B^{(1)}_{00} = \sigma^2[w].$$

Since w is real and either symmetric or antisymmetric,

$$w^*\left(x - a\frac{m-m'}{2}\right) w\left(x + a\frac{m-m'}{2}\right)$$

is a symmetric function and, therefore, $B^{(2)}_{mm'} = 0$. The orthonormality of the functions $w(x-am)$ results in $B^{(3)}_{mm'} = a^2m^2\delta_{mm'}$. Likewise, by similar arguments we find that $A^{(1)}_{mm'} = 0$ and $A_{mm'} = ma\delta_{mm'}$.

On inserting the results for $B_{mm'}$ and $A_{mm'}$ into expression (13), the variance takes the form

$$\sigma^2[\psi] = \sigma^2[w] + \sum_m |c_m|^2 a^2 m^2 - \left(\sum_m |c_m|^2 am\right)^2.$$

The evaluation of the second and third contribution yields

$$\sum_m |c_m|^2 a^2 m^2 - \left(\sum_m |c_m|^2 am\right)^2$$
$$= \frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k \left|\frac{\mathrm{d}\tilde{\psi}(k)}{\mathrm{d}k}\right|^2 - \left[\frac{a}{2\pi}\int_{-\pi/a}^{+\pi/a} \mathrm{d}k\ \tilde{\psi}^*(k)\,\mathrm{i}\frac{\mathrm{d}\tilde{\psi}(k)}{\mathrm{d}k}\right]^2.$$

By the definition of $\tilde{\psi}$, equation (4), with $X(k) = $ constant, the above expression is equal to $(\Delta E)^2$, equation (9), and this proves the proposition (8). □

It is worthwhile mentioning that a similar relation was found for the energy uncertainty of the Kane function, which is defined as

$$\varepsilon^2[\psi] = \int \mathrm{d}x\ \psi^*(x)(\hat{H}^2\psi)(x) - \left[\int \mathrm{d}x\ \psi^*(x)(\hat{H}\psi)(x)\right]^2.$$

Avron *et al* [17] showed that

$$\varepsilon^2[\psi] = (eF)^2\sigma^2[w].$$

Taking this together with the result of this paper (8), one can now, for example, establish a relation between the variance and the energy uncertainty of the Kane function.

4. Summary

We have seen that for the important case of periodic potentials with an inversion centre, an exact expression can be given for the variance of the Kane function. Up to an additive constant, which is equal to the variance for $F \to \pm\infty$, the semiclassical expression is correct. The extension of the wave function monotonically decreases with $|F|$ and its lower limit is given by the extension of the Wannier function of Kohn type, which is the limit of the Kane function for $F \longrightarrow \pm\infty$.

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