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Stationary states of an electron in periodic structures in a constant uniform electrical field

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Abstract. On the basis of the transfer-matrix technique, an analytical method for investigating the stationary states for an electron in one-dimensional periodic structures in an external electrical field, displaying the symmetry of the problem, is developed. These solutions are shown to be current carrying. It is also shown that the electron spectrum for infinite structures is continuous, and that the corresponding wave functions do not satisfy the symmetry conditions of the problem.

1. Introduction

The question of how an external (constant, uniform) electrical field influences the electron motion in periodic structures has been of great interest for decades [1–4]. Nevertheless, disagreements as regards the nature of the energy spectrum still persist. Some analytical investigations [3, 5, 6] have shown that the energy spectrum should be discrete irrespective of the potential form, and consist of so-called Wannier–Stark ladders with uniformly spaced levels. But other studies (see [4, 7–9] and references therein, including the rigorous mathematical results for the smooth potentials) indicate that, with certain restrictions imposed on the potential, the spectrum is continuous, and that a discrete spectrum may exist only for periodic structures consisting of δ-potentials (under certain conditions) and δ'-potentials (always).

In the simplest model, the problem is reduced to that of solving the one-dimensional Schrödinger equation whose Hamiltonian includes the periodic potential and the potential of an electric field. It is known [5] that the properties of the equation depend strongly on the choice of gauge for the field. When a scalar potential is used, the Hamiltonian is time independent, as in the absence of the field (the problem with zero field will be referred to as a zero-field problem (ZFP)), but its symmetry is different from the translational one. In this case it is important to reveal the changes in the band-gap energy spectrum of the ZFP that are caused by the field, and to find the wave functions satisfying the new symmetry conditions (these functions will play a role which is similar to that of the Bloch functions in the ZFP). A directly opposite situation arises for a vector representation. Now, switching on the field does not break the translational symmetry, and the Hamiltonian becomes time dependent. As a result, the electron energy is no longer a quantum number, and the initial problem can be treated as that of a Bloch electron accelerated by the field.

The mathematical difficulties associated with making use of the scalar potential are well known, since their first exposition in the famous paper [3] by Wannier. To overcome them,

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the author had to treat a finite number of the Bloch bands. This approximation was rightly disputed later [4, 7]. Recent investigations (see, for example, [8, 9]) show that the solution of the problem essentially depends on the alternation order of the Bloch bands and gaps in the high-energy region in the spectrum of the ZFP. It is known that for periodic finite-value potentials the bandwidth increases to infinity with increasing energy, while the gap width vanishes. Taking into account a finite number of Bloch bands is equivalent to treating the whole high-energy region as a gap. Such an approximation is sure to lead to a discrete spectrum.

As far as we are aware, no rigorous analytical solution to the problem with a scalar potential of a general form has been found. Also, the stationary electron states, displaying the symmetry of the problem, remain to be investigated. In this work we propose an exact analytical method for finding such stationary states. The connection between them and the Bloch states is discussed here. The energy spectrum of an electron and the Zener tunnelling are also considered.

2. The symmetry of the wave functions

The basis for our approach is the transfer-matrix method (TMM) [10], which we have used previously [11] for solving the ZFP. We recall that one of the main points of that formalism is the notion of out-of-barrier regions (OBRs), where the total potential is equal to zero. Here we shall use this notion as well, having made the necessary generalizations appropriate to the problem at hand. This can be done in either of two ways. Firstly, one may consider the total potential in the OBR to coincide with the Stark potential which is a linear function of x (in this case the treatment should be based on the Airy-function formalism). Secondly, one may consider the potential in these regions to be a constant which depends linearly on the cell number. The proportionality coefficient depends on the electrical field strength. Both of these variants can be used in our approach. However, in this work we concentrate on the latter, because there is a more evident association with the ZFP in this case.

The stationary Schrödinger equation for a structure of N periods (unit cells) may be written as

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi = 0 \tag{1}$$

where: E is the electron energy; m is its mass; $V(x)$ is defined by the expressions $V(x) = v(x) - n\Delta$ if $x \in (a_n, b_{n+1})$ $(n = 0, \ldots, N-1)$ and $V(x) = -n\Delta$ if $x \in (b_n, a_n)$; $b_n = nD$; $a_n = l + nD$ $(n = 0, \ldots, N)$; $\Delta = e\mathcal{E}D$; e is the (modulus of the) electron charge; l is the OBR width; D is the period of the structure; $\mathcal{E}$ is the electric field strength; $v(x)$ is a bounded function with period D.

It should be noted that boundary conditions at the points $x = 0$ and $x = a_N$ are not needed here, for we do not solve the boundary-value problem. Semi-infinite and infinite structures will be considered below. Notice also that the parameter l may be equal to zero, for the OBR may always be included in the initial potential (as the point with an infinitesimal neighbourhood) without changing the solution of equation (1) (the new and initial potentials are equivalent functions). Thus the present method can be used for any initial potential.

It is known [3] that if the function $\Psi_E(x)$ is a solution of equation (1), then $\Psi_{E+\Delta}(x-D)$ is a solution too. On the basis of this statement, one can assume that there are solutions (to be referred to as $\Psi_{\mathcal{E}}(x; E)$) among those of equation (1) satisfying the condition

$$\Psi_{\mathcal{E}}(x + D; E) = \text{constant} \times \Psi_{\mathcal{E}}(x; E + \Delta) \tag{2}$$

where the constant is a complex value. Our main goal is to find the functions $\Psi_{\mathcal{E}}(x; E)$ and to examine their properties.

The solutions to the Schrödinger equation, both with the scalar and with the vector potentials, are generally found in the form of an expansion in orthogonal functions (for example, in the Bloch functions). In this case the required and basis functions are supposed to belong to the same class of functions. The disadvantage of such an approach is that, in finding wave functions obeying the symmetry conditions, it is not always clear to what class of functions they are to belong. So, for example, in the absence of the field, the same condition of translational symmetry (it coincides with (2) when $\Delta = 0$) leads, for the bands, to the Bloch functions being bounded everywhere, but for the gaps it provides functions that are unbounded at plus and minus infinity. As will be shown below, the functions $\Psi_{\mathcal{E}}(x; E)$ are unbounded when $x \to -\infty$. Thus, if we attempted to find these functions in the Bloch or Wannier expansions, we could obtain an incorrect result, because both sets of functions belong to other classes. The transfer-matrix method is free from this drawback, because the expansion technique is not used there.

3. The functional equation for wave functions in the transfer-matrix method

The general solution of equation (1) in the OBR is

$$\Psi(x; E) = A_n^{(+)}(E)\exp[\mathrm{i}k_n(x - b_n)] + A_n^{(-)}(E)\exp[-\mathrm{i}k_n(x - b_n)] \tag{3}$$

where $k_n = \sqrt{2m(E + n\Delta)/\hbar^2}$; $n = 0, \ldots, N$.

Here the main problem is that of finding the coefficients $A_n^{(+)}(E)$ and $A_n^{(-)}(E)$; $n = 0, \ldots, N$. Once the coefficients have been found, the determination of the $\Psi_{\mathcal{E}}(x; E)$ in the barrier regions should present no serious problems. In the general case, for this purpose one can use, for example, a numerical technique [12].

The connection between the coefficients of the solutions for the first two OBRs is given by

$$\mathcal{A}_0(E) = \alpha(E)\mathbf{Y}(E)\mathbf{\Gamma}(E)\mathcal{A}_1(E). \tag{4}$$

Here $\mathbf{Y}$ is a transfer matrix (see [10]), describing the barrier at the unit cell $n = 0$ (provided that there is no step at the point b_1), and $\alpha\mathbf{\Gamma}$ is a matrix matching the solutions at the step at $x = b_1$:

$$\mathbf{Y} = \begin{pmatrix} \tilde{q} & \tilde{p} \\ \tilde{p}^* & \tilde{q}^* \end{pmatrix} \qquad \mathbf{\Gamma} = \begin{pmatrix} q_s & p_s \\ p_s & q_s \end{pmatrix} \qquad \mathcal{A}_n = \begin{pmatrix} A_n^{(+)} \\ A_n^{(-)} \end{pmatrix} \tag{5}$$

$$\tilde{q} = \frac{1}{\sqrt{T}}\exp[-\mathrm{i}(J + k_0 l)] \qquad \tilde{p} = \sqrt{\frac{R}{T}}\exp\left[\mathrm{i}\left(\frac{\pi}{2} + F - k_0 l\right)\right]$$

$$q_s = (\alpha + \alpha^{-1})/2 \qquad p_s = (\alpha^{-1} - \alpha)/2 \qquad \alpha(E) = \sqrt{k_1(E)/k_0(E)}.$$

The phases $J(E)$, $F(E)$ and the transmission coefficient $T(E)$ (see [10]) describing the barrier in the zero cell are assumed to be known; $R = 1 - T$.

Let

$$\mathbf{Z} = \mathbf{Y}\mathbf{\Gamma} = \begin{pmatrix} q & p \\ p^* & q^* \end{pmatrix}.$$

Then the relationship (4) can be rewritten as

$$\mathcal{A}_0(E) = \alpha(E)\mathbf{Z}(E)\mathcal{A}_1(E) \tag{6}$$

and the connection between any two adjacent OBRs will be determined by

$$\mathcal{A}_n(E) = \alpha(E + n\Delta)\mathbf{Z}(E + n\Delta)\mathcal{A}_{n+1}(E) \qquad n = 0, 1, \ldots, N-1. \tag{7}$$

Given (7), the connection between the zeroth and Nth unit cells can be written in the form

$$\mathcal{A}_0(E) = \alpha_{(1,N)}(E)\mathcal{Z}_{(1,N)}(E)\mathcal{A}_N(E) \tag{8}$$

where

$$\mathcal{Z}_{(1,N)}(E) = \mathbf{Z}(E)\cdots\mathbf{Z}(E + (N-1)\Delta) \tag{9}$$

$$\alpha_{(1,N)}(E) = \prod_{n=0}^{N-1}\alpha(E + n\Delta) = \sqrt{\frac{k_0(E + N\Delta)}{k_0(E)}}.$$

Defining for all n the vector

$$\tilde{\mathcal{A}}_n(E) = \alpha_{(1,n)}(E)\mathcal{A}_n(E)$$

we can rewrite equation (8) as

$$\mathcal{A}_0(E) \equiv \tilde{\mathcal{A}}_0(E) = \mathcal{Z}_{(1,N)}(E)\tilde{\mathcal{A}}_N(E). \tag{10}$$

Now, by analogy with the ZFP [11] we will attempt to find the wave functions whose expressions for the extreme OBRs (i.e. for the zeroth and Nth unit cells) are connected by means of symmetry. For this purpose we will demand that the coefficients of the zeroth and first OBRs must satisfy the condition

$$\tilde{\mathcal{A}}_1(E) = C(E)\mathcal{A}_0(E + \Delta) \tag{11}$$

where $C(E)$ is a complex function. Then, by equation (6), $\mathcal{A}_0(E)$ must obey the functional equation

$$\mathcal{A}_0(E) = C(E)\mathbf{Z}(E)\mathcal{A}_0(E + \Delta). \tag{12}$$

It is easy to check that $\mathcal{A}_0(E)$ is determined by this equation to within a scalar periodical function, $\omega(E)$; $\omega(E + \Delta) = \omega(E)$. That is, if the function $\mathcal{A}_0(E)$ is a solution, then so will be $\omega(E)\mathcal{A}_0(E)$.

Now, taking into account (11) and (12) in the relation (8), we have

$$\tilde{\mathcal{A}}_N(E) = G_N(E)\mathcal{A}_0(E + N\Delta) \tag{13}$$

where

$$G_N(E) = \prod_{n=0}^{N-1} C(E + n\Delta).$$

As in the ZFP [11], equations (10) and (13) provide theoretically a way of deriving, in explicit form, the expressions for the N-barrier transfer matrix (9) in terms of $\mathcal{A}_0(E)$, i.e. in terms of unit-cell characteristics. However, as will be seen from the following, in this approach it gives no benefits for calculating the $\mathcal{Z}_{(1,N)}(E)$.

Considering (13) and the relation $G_{n+1}(E) = C(E)G_n(E + \Delta)$, one can show that

$$\tilde{\mathcal{A}}_{n+1}(E) = C(E)\tilde{\mathcal{A}}_n(E + \Delta).$$

Such a connection between the coefficients of two adjacent OBRs guarantees fulfilment of the symmetry condition (2); that is,

$$\Psi_{\mathcal{E}}(x + D; E) = \alpha^{-1}(E)C(E)\Psi_{\mathcal{E}}(x; E + \Delta). \tag{14}$$

So, in the TMM the symmetry condition leads to the functional equation (12) for the coefficients of the general solution of the Schrödinger equation.

4. Solutions of the functional equation

According to the theory of functional equations [13], in order to solve equation (12) one needs to define the auxiliary functions $\boldsymbol{\eta}_n(E)$, where $n = 0, 1, \ldots$, with the help of the relationships

$$\boldsymbol{\eta}_0(E) = C(E)\mathbf{Z}(E)\boldsymbol{\eta}_0(E) \tag{15}$$

$$\boldsymbol{\eta}_n(E) = C(E)\mathbf{Z}(E)\boldsymbol{\eta}_{n-1}(E + \Delta). \tag{16}$$

Then the solution of equation (12) can be written, as is easily checked, in the form

$$\mathcal{A}_0(E) = \lim_{n\to\infty} \boldsymbol{\eta}_n(E). \tag{17}$$

In fact, this means that we have to solve the auxiliary equation (15) and to prove the existence of the limit (17).

Considering equations (15) and (16), we can write the limit (17) also as

$$\mathcal{A}_0(E) = G_\infty(E)\mathcal{Z}_{(1,\infty)}(E)\tilde{\boldsymbol{\eta}}_0 \tag{18}$$

where

$$\tilde{\boldsymbol{\eta}}_0 = \lim_{n\to\infty} \boldsymbol{\eta}_0(E + n\Delta).$$

The finding of $\mathcal{A}_0(E)$ is seen to be associated with calculating the matrix $\mathcal{Z}_{(1,\infty)}(E)$ for the semi-infinite structure. That is why deriving expressions for $\mathcal{Z}_{(1,N)}(E)$ in terms of $\mathcal{A}_0(E)$ is of no interest in this approach.

Let us begin by solving equation (15). It can be rewritten as

$$\frac{\eta_0^{(-)}}{\eta_0^{(+)}} = \frac{C^{-1} - q}{p} = \frac{p^*}{C^{-1} - q^*} \qquad \boldsymbol{\eta}_0 = \begin{pmatrix} \eta_0^{(+)} \\ \eta_0^{(-)} \end{pmatrix}. \tag{19}$$

This equation coincides as regards form with equation (8) (see reference [11]) in the ZFP. The only difference is that the matrix $\mathbf{Z}(E)$ describes the one-cell potential which involves the electric field effect. Here the graduation of the energy scale into Bloch bands ('allowed' energy regions) and gaps ('forbidden' energy ones) arises as well. But such a division does not yield the energy spectrum for the given problem and is of auxiliary significance.

Since $\det \mathbf{Z}(E) = 1$, the solutions of the characteristic equation (19) (the right-hand equality) are two reciprocal quantities. In choosing the required root, for any energy region, we must proceed from the fact that the function $C(E)$ must have a limit when $E \to \infty$. Otherwise, the limit $\tilde{\boldsymbol{\eta}}_0$ does not exist either, and hence expression (18) loses its meaning.

Let us show that the solutions of the auxiliary equation (19), having the properties needed, are expressed by

$$C_1(E) = \frac{1}{q + y} \qquad \eta_0^{(+)}\big|_1 = 1 \qquad \eta_0^{(-)}\big|_1 = \frac{y}{p}$$

$$C_2(E) = \frac{1}{q^* - y} \qquad \eta_0^{(+)}\big|_2 = -\frac{y}{p^*} \qquad \eta_0^{(-)}\big|_2 = 1$$

$$C_2 = C_1^{-1} \qquad y = -\frac{\mathrm{i}|p|^2 \operatorname{sgn}(u)}{|u| + \sqrt{u^2 - |p|^2}} \qquad u = \operatorname{Im}(q).$$

First of all, it should be noted that the limit $\tilde{\boldsymbol{\eta}}_0$ is calculated on the set of equidistant points E_n, where $E_n = E + n\Delta$; $n = 0, 1, \ldots$. This set will be denoted by $S_{E,\Delta}$; in doing this, we emphasize its dependency on the parameters E and Δ. It is supposed that E varies

on the interval $(0, \Delta]$. The set $S_{E,\Delta}$ consists of the two subsets $S^a_{E,\Delta}$ and $S^f_{E,\Delta}$ whose points belong to the bands ($|u| > |p|$) and gaps ($|u| \leqslant |p|$), respectively. As will be shown below, the behaviours of the vector function $\boldsymbol{\eta}_0(E_n)$ on the subsets $S^a_{E,\Delta}$ and $S^f_{E,\Delta}$ differ qualitatively. Therefore, there exists no limit $\tilde{\boldsymbol{\eta}}_0$ when both of the subsets are infinite.

It follows from general considerations that the numbers of points in $S^a_{E,\Delta}$ and $S^f_{E,\Delta}$ depend on the widths of the bands and gaps as well as on their locations on the energy scale. As will become clear from the following, in order to show the role of both factors, it is sufficient to investigate the rectangular barrier ($v(x) = v_0$). By using the explicit expressions for the tunnelling parameters of the rectangular barrier (see, for example, [10]), one can show that for the matrix element $\tilde{p}$ in the high-energy region, the inequality $|\tilde{p}| \lesssim (v_0/2)E^{-1}$ is valid. The asymptote of the phase $J(E)$ is the function $k_0(E)d$ ($d = b_1 - a_0$ is the barrier width)—for the larger the electron energy is, the more similar its motion is to that of the free electron. Thus, in the high-energy region the centres of the gaps (the points which satisfy the equation $\sin(J(E) + k_0 l) = 0$ are meant) for periodical structures formed with the rectangular barriers asymptotically coincide on the energy scale with the points E_L, where

$$E_L = L^2\epsilon \qquad \epsilon = \frac{\pi^2\hbar^2}{2mD^2} \qquad L = 0, 1, \ldots.$$

The distance between the gap centres in the high-energy region is, consequently, a multiple of the constant ϵ. In this case, the gap width tends to zero with increasing E, while the bandwidth, in contrast, goes to infinity (see [7–9]). These findings are not changed by the presence of the step in the right-hand boundary of the barrier, because the corresponding matrix $\boldsymbol{\Gamma}$ is real, and, also, $|p_s(E)| \sim E^{-1}$ as for the rectangular barrier. That is, for the matrix $\mathbf{Z}(E)$ we have

$$|p(E)| \lesssim \frac{v_0}{2E} \qquad \arg(q) \approx k_0(E)D. \tag{20}$$

Here it is also taken into account that $q = \tilde{q}q_s + \tilde{p}p_s$, $p = \tilde{q}p_s + \tilde{p}q_s$; $|\tilde{q}|^2 - |\tilde{p}|^2 = 1$, $q_s^2 - p_s^2 = 1$. The asymptotics in the high-energy region is not changed either when going to the general-form barrier, because in this case the inequality $|\tilde{p}(E)| \lesssim (v_{max}/2)E^{-1}$ holds, and the asymptotics of $p_s(E)$ remains the same; here v_{max} is the maximum of the moduli of $v(x)$.

It follows from the above that the subset $S^a_{E,\Delta}$ is always infinite, and that $S^f_{E,\Delta}$ is infinite in exceptional ('resonance') cases only: $E = \Delta = r\epsilon$, where r is a rational number. There is no limit $\tilde{\boldsymbol{\eta}}_0$ under these conditions, for the moduli of the functions $\eta_0^{(-)}(E)|_1$ and $\eta_0^{(+)}(E)|_2$ are equal to unity on $S^f_{E,\Delta}$, but on $S^a_{E,\Delta}$ they vary between the limits zero and unity.

At the given Δ, the set of energy values for which 'resonance' takes place is simply a countable set. This is in essence connected with the fact that the gap width goes to zero in the limit $L \to \infty$. Any arbitrary small variation of E removes the points E_n, beginning at some number $\mathcal{N}$, from the gaps. Since all of these points belong to the subset $S^a_{E,\Delta}$, where the inequality $|u| > |p|$ holds, there exists a $\delta > 0$ such that for all $n > \mathcal{N}$ the condition $|u(E_n)| \geqslant |p(E_n)|^{1-\delta}$ is valid (note that $|p|^2 < 1$ in the high-energy region). It follows from this that at these points we have

$$|y| = \frac{|p|^2}{|u| + \sqrt{u^2 - |p|^2}} < \frac{|p|^2}{|u|} \leqslant |p|^{1+\delta}.$$

Hence,

$$|\eta_0^{(-)}(E_n)|_1 = \frac{|y|}{|p|} \leqslant |p(E_n)|^{\delta} \lesssim \gamma E_n^{-\delta}$$

where $\gamma = (v_{max}/2)^{\delta}$. The same asymptotics arises for $\eta_0^{(+)}(E_n)|_2$. This means that almost everywhere on the energy scale

$$\tilde{\eta_0}\big|_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \tilde{\eta_0}\big|_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{21}$$

Now, substituting (21) into (18), we get the final expressions for the two solutions of functional equation (12):

$$\mathcal{A}_0^{(1)} = \begin{pmatrix} Q_{(1,\infty)} G_\infty \\ P^*_{(1,\infty)} G_\infty \end{pmatrix} \qquad \mathcal{A}_0^{(2)} = \begin{pmatrix} P_{(1,\infty)} G_\infty^{-1} \\ Q^*_{(1,\infty)} G_\infty^{-1} \end{pmatrix} \tag{22}$$

where $G_\infty = G_\infty^{(1)} = 1/G_\infty^{(2)}$; $Q_{(1,\infty)}$ and $P_{(1,\infty)}$ are the elements of $\mathcal{Z}_{(1,\infty)}$. Then from (13) it follows that

$$\tilde{\mathcal{A}}_\infty^{(1)}(E) = \begin{pmatrix} G_\infty(E) \\ 0 \end{pmatrix} \qquad \tilde{\mathcal{A}}_\infty^{(2)}(E) = \begin{pmatrix} 0 \\ G_\infty^{-1}(E) \end{pmatrix}. \tag{23}$$

Expressions (3), (8), and (22) provide two independent functions $\Psi_{\mathcal{E}}^{(1)}(x; E)$ and $\Psi_{\mathcal{E}}^{(2)}(x; E)$. Both solutions are current-carrying ones. The corresponding probability flows, $I_{(1)}(E)$ and $I_{(2)}(E)$, are

$$I_{(1)}(E) = \hbar m^{-1} k_0(E) |G_\infty(E)|^2 \qquad I_{(2)}(E) = \hbar m^{-1} k_0(E) |G_\infty(E)|^{-2}. \tag{24}$$

Now we have to prove that the limit in (17) exists. Otherwise expressions (22)–(24) are meaningless.

5. On the existence of the solutions $\Psi_{\mathcal{E}}(x; E)$

For a complex-valued matrix $\mathbf{H}$ and vector $\mathcal{A}$, let us define the norms

$$\|\mathbf{H}\| = \max_j \sqrt{\sum_{i=1}^{2} |h_{ij}|^2} \qquad j = 1, 2$$
$$\|\mathcal{A}\| = |A^{(+)}| + |A^{(-)}|.$$

In particular, this means that $\|\mathbf{Z}\|^2 = 1 + 2|p|^2$. Considering the first solution, we will prove that for any given E and $\varepsilon > 0$ we can find a number N such that

$$\|\boldsymbol{\eta}_n(E) - \boldsymbol{\eta}_{n-1}(E)\| < \varepsilon \tag{25}$$

for $n > N$. Since

$$\boldsymbol{\eta}_n(E) = G_n(E) \mathcal{Z}_{(1,n)}(E) \boldsymbol{\eta}_0(E_n)$$

(here $E_n = E + n\Delta$) we have

$$\|\boldsymbol{\eta}_n(E) - \boldsymbol{\eta}_{n-1}(E)\| \leqslant |G_{n-1}(E)| \, \|\mathcal{Z}_{(1,n-1)}(E)\| \, F(E) \tag{26}$$

where $F(E) = \|C(E_n)\mathbf{Z}(E_n)\boldsymbol{\eta}_0(E_n) - \boldsymbol{\eta}_0(E_{n-1})\|$.

Let us show that the first two norms are bounded as $n \to \infty$. We have

$$|G_\infty(E)|^{-1} = \prod_{n=0}^{\infty} |C(E_n)|^{-1} = \prod_{n=0}^{\infty} |q(E_n) + y(E_n)| \leqslant \prod_{n=0}^{\infty} |q(E_n)| \left(1 + \frac{|y(E_n)|}{|q(E_n)|}\right). \tag{27}$$

The convergence of both norms in (27) is equivalent to that of the series $\sum_{n=0}^{\infty} n^{-2}$, because $|q| = \sqrt{1 + |p|^2}$, $y \sim |p|^2$, $|p| \sim n^{-1}$. Since this series converges, the infinite product $|G_\infty(E)|$ does as well.

For the matrix describing the semi-infinite structures, we have

$$\|\mathcal{Z}_{(1,\infty)}(E)\|^2 \leqslant \prod_{n=0}^{\infty} \|\mathbf{Z}(E_n)\| = \prod_{n=0}^{\infty}(1+2|p(E_n)|^2).$$

Obviously, this product converges for the same reason as (27). In addition, since

$$\|\mathcal{Z}_{(1,\infty)}(E)\|^2 \equiv 1 + 2\frac{R_{(1,\infty)}(E)}{T_{(1,\infty)}(E)}$$

we have that $T_{(1,\infty)}(E) \neq 0$. Hence the semi-infinite structure must be not absolutely opaque to an electron.

Now, it remains to show that F in (26) approaches zero with increasing n. Using (15) we have

$$F = \|\boldsymbol{\eta}_0(E_n) - \boldsymbol{\eta}_0(E_{n-1})\| \lesssim 2\gamma n^{-\delta}. \tag{28}$$

Since the norms $|G_\infty(E)|$ and $\|\mathcal{Z}_{(1,\infty)}(E)\|$ are bounded, we have

$$\max_j(|G_j(E)|\,\|\mathcal{Z}_{(1,j)}(E)\|)$$

where $j = 1, 2, \ldots$. Together with (28), this guarantees fulfilment of the inequality (25), which proves the existence of the limit in (17). For the second solution, the arguments are similar.

6. Conclusions

At first glance it appears that the functions $\Psi_{\mathcal{E}}(x; E)$ can be calculated by this method only for the region located to the right of the zero cell. However, it should be noted that any unit cell of the periodical structure may be taken as the zero cell. Then, by making use of the transfer matrix which connects solutions for the zero cell with those for the regions to the left of it, one can calculate the functions $\Psi_{\mathcal{E}}(x; E)$ for the whole axis Ox.

Since both functions $\Psi_{\mathcal{E}}(x; E)$ are current carrying, their moduli increase infinitely in the classically inaccessible range when $x \to -\infty$, according to the general properties of the one-dimensional Schrödinger equation. Thus, for infinite structures, the $\Psi_{\mathcal{E}}(x; E)$ are not solutions to the problem. However, for any E (excluding a countable set for certain values of Δ), the (non-degenerate) solution for the infinite structure can be obtained as a linear combination of these functions. As a result, we arrive at two important conclusions. First, for the limited periodical potentials the energy spectrum of an electron in the problem for infinite structures is continuous (so the Wannier–Stark states, according to the model, may exist only as quasi-stationary ones). Second, the stationary wave functions of an electron in the infinite structures, being linear combinations of the functions $\Psi_{\mathcal{E}}(x; E)$, do not satisfy the symmetry condition (2). (There is a common misconception that the continuity of the spectrum in this problem is obvious. The following arguments are used in this case, namely that the energy spectrum is continuous since

(a) the range where x is large is classically accessible to an electron; and

(b) the periodical potential is negligible in comparison with the Stark potential when $x \to \infty$, and, consequently, the electron motion in this range is of the free-electron type (see, for example, [3]).

However, it should be noted that the first statement is valid only if $V(x)$ remains finite at plus infinity. But if $V(x) \to -\infty$ as $x \to \infty$, then the electron spectrum may be both continuous and discrete, depending on the monotonicity and rate of decrease of $V(x)$ at $x \to \infty$ (see,

for example, [14]). It also follows from this that the second argument is erroneous, because on the whole axis OX the derivatives of $V(x)$ (and, hence, its monotonicity) are determined by the periodical component of the potential.)

It is interesting also to dwell for a moment on the question of the connection of the given problem to the ZFP. We will start with the fact that the wave functions $\Psi_{\mathcal{E}}(x; E)$ are defined in terms of the solutions of auxiliary equation (19), formally describing the electron motion in the periodic structures in the absence of an electric field. In addition, for finite structures the functions $\Psi_{\mathcal{E}}(x; E)$, in view of their properties, are close to the solutions of the ZFP, if $N\Delta \ll E$ (N is the number of unit cells in the structure). In particular, if the values of E are in the band, then the $\Psi_{\mathcal{E}}(x; E)$, in the given interval, are close to the usual Bloch functions. This is the case when an electrical field has a weak effect on the electron with the energy E. However, the ZFP is not a limiting case for the given problem when the periodical structure is considered for the whole axis Ox. The wave functions $\Psi_{\mathcal{E}}(x; E)$ are then unbounded when $x \to -\infty$, for all values of the electric field strength.

Some comments should also be made about the role of the Zener tunnelling (ZT), which has aroused great interest (see, for example, [6] and references therein) since [2] first appeared. Strictly speaking, this concept refers to electron transitions between bands, and therefore it relates to the non-stationary case. In the models with the vector potential, the Zener tunnelling is caused by the accelerating effect of the field, resulting in a Bloch electron passing (tunnelling) from the lower bands to the upper. In our approach we investigate stationary states. Nevertheless, we can draw some conclusions on this question. This is possible because symmetry condition (14), governing the functions $\Psi_{\mathcal{E}}(x; E)$, links their E- and x-dependencies. In particular, for $\Psi_{\mathcal{E}}(x; E)$, relationship (13) is valid. Note also that $\tilde{\mathcal{A}}_{\infty}$ (see (23)) is a bounded non-zero value. This provides the asymptotics $\mathcal{A}_n \sim n^{-1/4}$ and $\mathcal{A}_0(E) \sim E^{-1/4}$ (as for Airy's functions). Thus the probability that an electron is in the nth unit cell or that it has the energy E decreases with the increasing of these parameters according to a power law instead of the exponential one. This result makes the conclusion presented in reference [8] more precise.

Also, it follows from the above that the well-known Bloch oscillations can exist only as decaying ones. As regards the experimental evidence of long-lived Bloch oscillations and Wannier–Stark ladders in superlattices, it is not a question of the correctness of our approach. This evidence implies only that one needs to find a mathematical model which would be more suitable for describing superlattices. In the future we intend to present such a model.

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