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1994 J. Phys.: Condens. Matter 6 6245

(http://iopscience.iop.org/0953-8984/6/31/024)

J. Phys.: Condens. Matter 6 (1994) 6245–6255. Printed in the UK

Energy spectrum of a Bloch electron on a two-dimensional lattice with long-range hopping in a magnetic field

V M Gvozdikov
Department of Physics, Kharkov State University, Kharkov, 310077, Ukraine

Received 4 December 1993

Abstract. The density of states (DOS) of the Bloch electron on a two-dimensional (2D) lattice in an external perpendicular magnetic field is exactly calculated in the case of a rational flux through an elementary cell in the model with exponentially decreasing, as a function of inter-site spacing, overlap integrals. A generalization of this model to the case of an array of parallel chains with tight-binding correlations between them is considered, and the appropriate DOS is calculated. A quasiclassical quantization rule is obtained for arbitrary electron dispersion along the chains in the low-flux limit, which yields, for energies near the band bottom, Landau levels that broaden into bands of width proportional to a magnetic breakdown-like probability factor. The analogy between the Wannier–Stark ladder and the Landau spectrum for a Bloch electron on a 2D lattice is considered. Possible applications to organic conductors and superconducting superlattices are discussed.

1. Introduction

The problem of the electron energy spectrum on a two-dimensional (2D) lattice has been in the spotlight during the past decades since it has many applications in solid-state physics: in superconductor networks [1], in the quantum Hall effect [2], in anyon superconductivity [3], in flux phases of the Hubbard model [4], and so on. Beginning with the works of Azbel [5] and Hofstadter [6] it is well known that the energy spectrum of electrons in a 2D lattice depends strongly on the ratio Φ/Φ_0, where Φ is the flux per unit cell and $\Phi_0 = hc/e$ is the flux quantum. For the irrational flux case, the energy spectrum is of fractal nature, whereas the integrated density of states (DOS), as was first pointed out in [7], approaches some regular curve when the irrational number Φ/Φ_0 is successively approximated by rational fractions. The DOS for rational flux per unit cell, $\Phi/\Phi_0 = p/q$, of a square lattice with nearest-neighbour electron hopping has also been calculated analytically for the first time in [7]. The results of this work were used recently in the study of electronic diamagnetism in 2D lattices [8, 9].

The present paper is devoted to the energy spectrum calculations within the frame of a certain 2D model lattice that assumes an exponential form of inter-site overlap integrals. The plan of the paper is as follows. In section 2, a brief description of the transfer-matrix method is given in the context of its application to the DOS calculation in the frame of the model of [7]. Section 3 contains the exact transfer-matrix derivation of the DOS for a Bloch electron on a 2D lattice with exponentially decreasing, as a function of inter-site distance, overlap integrals, provided that magnetic flux through a unit cell is a rational fraction of the flux quantum Φ_0. Section 4 deals with a generalization of the model to the case of a 2D periodic set of parallel atomic chains. The DOS of such a system is also examined in this section. Section 5 is devoted to the quasiclassical analysis of the energy spectrum of

0953-8984/94/316245+11$19.50

the model adopted in the previous section. An appropriate quantization rule is obtained and the Landau band energy spectrum is found in the low-flux limit for an arbitrary electron dispersion relation along the chains. In conclusion a discussion on possible applications of the obtained results is presented.

2. The DOS for a 2D lattice with nearest-site electron hopping

In the present section the method of calculation of the DOS, utilized in [7], is slightly reformulated on the basis of the transfer-matrix approach, which makes it possible to generalize calculations to the case of a 2D lattice with long-range electron hopping. Such calculations are done below in a model with exponentially decreasing, as a function of inter-site distance, overlap integrals.

The Hamiltonian of a single electron in a 2D square lattice with nearest-neighbour hopping is given by

$$H = 2t[2 - \cos(p_x a/\hbar) - \cos(p_y a/\hbar)]. \tag{1}$$

Here t is the overlap integral between the nearest sites, a is the lattice constant and $p_{x,y}$ are momentum projections on the axes X and Y respectively.

The corresponding Schrödinger equation $H\Psi(x, y) = E\Psi(x, y)$ in an external perpendicular magnetic field B in the Landau gauge $A = B(0, X, 0)$ can be written, after Peierls substitution $P \to P - eA/c$, in the well known form of Harper's equation

$$t[f(n+1) + f(n-1)] = [E - E(n, \nu)]f(n) \tag{2}$$

$$E(n, \nu) = 4t - 2t\cos(\nu - 2\pi n\Phi/\Phi_0). \tag{3}$$

Here the wavefunction $f(x)$ and discrete variables n and n' have been introduced by the relationships: $\Psi(x, y) = \exp(ip_y y/\hbar)f(x)$, $x = an$, $y = an'$, $\nu = p_y a/\hbar$ and $\Phi = Ba^2$. In the case of a rational flux per unit cell, $\Phi/\Phi_0 = p/q$, one can easily solve equation (2) in different ways. For the sake of the following calculations it is useful to introduce a transfer matrix

$$T_n(E) = \begin{vmatrix} 0 & \vdots & -1 \\ \cdots & \vdots & \cdots \\ -1 & \vdots & [E(n, \nu) - E]/t \end{vmatrix}. \tag{4}$$

Equation (2) can now be written in the matrix form

$$\begin{vmatrix} f(n) \\ f(n+1) \end{vmatrix} = T_n(E) \begin{vmatrix} f(n+1) \\ f(n) \end{vmatrix}. \tag{5}$$

Since $E(n\nu)$ as a function of n has period q, we arrive at the following dispersion equation after a small amount of standard manipulations

$$\cos(k_x a) = \tfrac{1}{2}\,\mathrm{Sp}\,T(E) \tag{6}$$

where $T(E) = T_1(E)T_2(E)\ldots T_q(E)$. The quantity $T(E)$ is also a function of $\nu = k_y a$. Owing to the obvious symmetry relation $k_x \leftrightarrows k_y$, the dependence of $T(E)$ on $k_y a$ should

be identical to that given by equation (6), since, after substitution $X \leftrightarrows Y$, we alternatively arrive at equation (6), but this time with $\cos(k_y a)$ on the left-hand side. Thus, the summation of both equations yields

$$2\cos(k_x a) + 2\cos(k_y a) = P_q(E) \tag{7}$$

where

$$P_q(E) = \mathrm{Sp}[T_1(E)T_2(E)\ldots T_q(E)]_{v=0} \tag{8}$$

is a polynomial of degree q in E. The proof of the above statement is also given in [7]. The DOS $g(E)$ then can be calculated with the help of the standard definition

$$g(E) = \frac{1}{2\pi^2 q}\int_0^{\pi}\left|\frac{\mathrm{d}k_x}{\mathrm{d}E}\right|\mathrm{d}(k_y a). \tag{9}$$

Substituting (7) into (9) and performing integration, we have

$$g(E) = (1/2\pi^2 q)|\mathrm{d}P_q(E)/\mathrm{d}E|K'[\tfrac{1}{4}|P_q(E)|] \tag{10}$$

where $K'(k) = K[(1-k^2)^{1/2}]$, and $K(k)$ is a complete elliptic integral of the first kind. In essence, this is exactly the result of [7], except that the polynomial $P_q(E)$ in equation (10) is determined, according to (8), as a trace of the product of q matrices $T_n(E)$, whereas in [7] this polynomial is presented as a determinant of some $q \times q$ matrix. For lattices with nearest-site electron hopping, both the above ways of $P_q(E)$ calculation require approximately equal effort. If, however, one takes into consideration electron hopping to more remote sites, the amount of calculation necessary to obtain polynomial $P_q(E)$ from the determinant will grow enormously and employment of the formula (8) becomes much more preferable.

3. The DOS for 2D long-range hopping model lattice

Consider a 2D lattice with a rectangular unit cell of sides a_x and a_y, and described by the Hamiltonian

$$H = H(P_x) + H(P_y) \tag{11}$$

where

$$H(P_j) = \sum_{m_j} t(m_j)\exp[\mathrm{i}P_j a_j m_j)/\hbar]. \tag{12}$$

The overlap integrals $t(m_j)$ are taken here in the exponentially decreasing form with respect to the distance $|m_j|a_j$ between the lattice sites

$$t(m_j) = t_0\exp(-q|m_j|a_j). \tag{13}$$

When an external perpendicular magnetic field B is applied, one can, proceeding in the same fashion as before, obtain a more general equation than equation (2) for the wavefunction

$$\sum_{n'\neq n} t_0\exp(-q|n'-n|a)f(n') = [E - E(n,\nu)]f(n). \tag{14}$$

The on-site energy $E(n, \nu)$ here is determined by the sum

$$E(n, \nu) = \sum_{m_y} t_0 \exp[-qa|m_y| + \mathrm{i}(\nu - 2\pi n\Phi/\Phi_0)m_y]. \tag{15}$$

Performing summation, we have

$$E(n, \nu) = t_0 \sinh(qa)[\cosh(qa) - \cos(\nu - 2\pi n\Phi/\Phi_0)]^{-1}. \tag{16}$$

Indices at a_j are omitted in equations (14)–(16) and in what follows.

In the case $qa \gg 1$, one can neglect electron hopping beyond the nearest-neighbour sites, and arrive at Harper's equation (2) with $t = t_0 \exp(-qa)$ and $E(n, \nu) = 2t_0 \exp(-qa)\cos(\nu - 2\pi n\Phi/\Phi_0)$. In the general case of an arbitrary qa, the model under study permits electron inter-site hopping to neighbours of all orders. As shown in the author's papers [10, 11], equation (14) can be solved easily with the help of a transfer-matrix approach. Proceeding along the lines of [10, 11], one can represent the solution of equation (14) in the form

$$f(n) = A(n) + B(n) \tag{17}$$

where the quantities $A(n)$ and $B(n)$ are determined by the right-hand sides of equations

$$A(n) = t(n, \nu) \sum_{n' \geqslant n} \exp[-qa(n' - n)] f(n') \tag{18}$$

$$B(n, \nu) = t(n, \nu) \sum_{n' < n} \exp[-qa(n - n')] f(n'). \tag{19}$$

Symbol $t(n, \nu)$ stands for

$$t(n, \nu) = t_0[E - E(n, \nu) - t_0]^{-1}. \tag{20}$$

Now, one can readily obtain the recurrence equations for $A(n)$ and $B(n)$, which may be written in the following matrix form

$$\begin{vmatrix} A'(n+1) \\ B'(n+1) \end{vmatrix} = T_n(E) \begin{vmatrix} A'(n) \\ B'(n) \end{vmatrix}. \tag{21}$$

The transfer matrix $T_n(E)$ has the form

$$T_n(E) = \begin{vmatrix} [1 - t(n, \nu)]\mathrm{e}^{qa} & -t(n, \nu)\mathrm{e}^{qa} \\ t(n, \nu)\mathrm{e}^{-qa} & [1 + t(n, \nu)]\mathrm{e}^{-qa} \end{vmatrix}. \tag{22}$$

and $A'(n) = A(n)/t(n, \nu)$ and $B'(n) = B(n)/t(n, \nu)$.

Since for rational flux through the unit cell, $\Phi/\Phi_0 = p/\tilde{q}$, the energy $E(n, \nu)$ of equation (15) is a periodic function of n with period $\tilde{q}$, one can, by trivial repetition of the arguments that hold for the above derivation of the DOS, check that $g(E)$ for the present model is given again by equation (10). The only difference is that in the model under consideration the transfer matrix $T_n(E)$ is defined by equation (22). The energy bands location is determined by the condition $|P_{\tilde{q}}(E)| \leqslant 4$. The number of bands depends on the

degree of the polynomial $P_{\tilde{q}}(E)$, which, in turn, is fixed by the value of the rational fraction $p/\tilde{q}$. Within each of the permitted energy bands the DOS $g(E)$ has a well known 'pagoda' shape with a logarithmic singularity in the middle of the band.

As for possible applications of the considered model, it should be noted that to a greater or lesser degree long-range correlations are present in every physical system. Nonetheless, it is customary to explore problems related to 2D Bloch electrons in a uniform magnetic field within the frame of a tight-binding Hamiltonian. Moreover, this approach is often justified on the grounds that overlap integrals are exponentially decreasing functions of inter-site distance, so that one can neglect electron hopping beyond the nearest neighbours [12]. The result obtained above shows that a model with exponentially decreasing overlap integrals in essence is not much more complicated than a tight-binding one, and can be readily solved exactly with the help of a transfer-matrix technique, at least in the rational flux case. Meanwhile, some problems, such as, for example, plasma oscillations in superlattices in a magnetic field, should be treated beyond the nearest-neighbour correlation approach. The exponential form of interlayer correlations in this system stems from the long-range Coulomb interactions across the layers [11]. Another typical example is with superconducting superlattices and superstructures in which long-range correlations between layers arise due to the sharp growth of the coherence length when temperature approaches the critical one, T_c. Such enhancement of the interlayer correlation range near T_c manifests itself in a well known dimensional 3D to 2D crossover, which takes place with increase of external magnetic field [13]. An analogous phenomenon holds for 2D superconducting superstructures in a magnetic field. Inasmuch, as in general, inter-site correlations do not need to be exactly of the exponential form, the most adequate approach to the discussed problem should be based on the concept of an arbitrary dispersion relation as is usual in the standard electron theory of metals [14]. As a first step towards this, in the next section we will consider a 2D lattice model in which an arbitrary dispersion relation of electrons in one of the two dimensions is assumed.

4. Generalization of the method to a 2D anisotropic lattice

The transfer-matrix approach developed in the previous sections can be readily modified for the case of a 2D regular anisotropic structure. To see this, consider a 2D Hamiltonian of the form

$$H = 2t[1 - \cos(p_x a/\hbar)] + \epsilon(p_y b/\hbar)]. \tag{23}$$

The first term on the right-hand side of this equation is the usual tight-binding Hamiltonian describing electron hopping between chains, whereas the periodic function $\epsilon(p_y b/\hbar) = \epsilon(p_y b/\hbar + 2\pi)$ refers to an arbitrary electron dispersion in chains assumed to be parallel to the Y axis. After separation of variables in a way described in section 2, we have

$$tf(n+1) + tf(n-1) + [E - 2t - \epsilon(\nu - 2\pi n\Phi/\Phi_0)]f(n) = 0. \tag{24}$$

Here $\nu = p_y b/\hbar$. This equation generalizes Harper's equation since it depends on an arbitrary function $\epsilon(\nu)$, which in the original Harper's equation (2) equals $2t[1 - \cos(\nu - 2\pi n\Phi/\Phi_0)]$. Equation (24), after the fashion of section 2, can be written in the matrix form (5) with the transfer matrix (4) in which the on-site energy should be taken in the form

$$E(n, \nu) = 2t + \epsilon(\nu - 2\pi n\Phi/\Phi_0). \tag{25}$$

The principal difference between the case under consideration and that of section 2 emanates from the X–Y anisotropy and results in the loss of symmetry relation $p_x \leftrightarrows p_y$. The latter means that equation (7) does not hold true in this case and that direct integration in equation (9) is impossible. Nevertheless, with the help of equation (6) the DOS (9) can be represented in the form

$$g(E) = \frac{1}{2\pi^2 q} \int_0^{\pi} [4 - P_q^2(E, \nu)]^{-1/2} \left| \frac{\mathrm{d}P_q(E, \nu)}{\mathrm{d}E} \right| \mathrm{d}\nu. \tag{26}$$

The polynomial $P_q(E, \nu)$ entering equation (26) is

$$P_q(E, \nu) = \mathrm{Sp}[T_1(E, \nu)T_2(E, \nu) \ldots T_q(E, \nu)] \tag{27}$$

and the transfer matrix $T_q(E, \nu)$ is given by equations (4) and (25). Since for rational flux, $\Phi/\Phi_0 = p/s$, the function $P_s(E, \nu)$ is a polynomial of degree s in E, the DOS (26) consists of s bands with boundaries determined by the condition $4 \geqslant P_s(E, \nu)$.

Unfortunately, one cannot complete integration on ν in equation (26) without specific choice of the dispersion relation $\epsilon(\nu)$. As a concrete example of how equation (26) operates, consider again a model with exponential correlations between electrons on lattice sites (13), but this time assume that such correlatins hold only within the chains, which means that $\epsilon(\nu)$ should be taken in the form given by equation (16). For the simplest case of rational flux, $\Phi/\Phi_0 = 1$, equations (26) and (16), after substitution $x = \cos\nu$, yield

$$g(E) = \frac{1}{2\pi t} \int_{-1}^{1} [(1 - x^2)Q(E, x)]^{1/2} [\cosh(qb) - x] \mathrm{d}x \tag{28}$$

where

$$Q(E, x) = \epsilon(4 - \epsilon)(x - x_+)(x - x_-) \qquad \epsilon = E/t \tag{29}$$

$$x_+ = \cosh(qb) + \sinh(qb)/(4 - \epsilon) \tag{30}$$

$$x_- = \cosh(qb) - \sinh(qb)/\epsilon. \tag{31}$$

The actual limits of integration in equation (28) are determined by the two conditions: $(1 - x)^2 Q(E, x) > 0$ and $|x| \leqslant 1$. A simple analysis shows that the top and the bottom edges of the energy band are $\epsilon_{\max} = 4 + \coth\gamma$ and $\epsilon_{\min} = \tanh\gamma$ respectively, whereas the analytic form of the DOS within the band is different for different values of qb and ϵ. (Here and in what follows $\gamma = qb/2$.) Three cases should be distinguished: (i) $\tanh\gamma > 1/4$, (ii) $\sqrt{5} - 2 < \tanh\gamma < 1/4$, and (iii) $0 < \tanh\gamma < \sqrt{5} - 2$. For each of these cases the energy band is divided into four sections by three points $\epsilon_1 = \coth\gamma$, $\epsilon_2 = 4 + \coth\gamma$ and $\epsilon_3 = 4$, of which the first two are roots of the equations $x_-(\epsilon_1) = 1$ and $x_+(\epsilon_2) = -1$. The hierarchy of energies for each of the above cases is different and correspondingly equal to: $\epsilon_{\min} \leqslant \epsilon_1 < 4 < \epsilon_2 \leqslant \epsilon_{\max}$ for case (i), $\epsilon_{\min} < 4 < \epsilon_1 < \epsilon_2 \leqslant \epsilon_{\max}$ for case (ii), and $\epsilon_{\min} < 4 < \epsilon_2 < \epsilon_1 \leqslant \epsilon_{\max}$ for case (iii). As long as ϵ belongs to one of these energy intervals, the corresponding hierarchy between the four roots 1, -1, $x_+(\epsilon)$ and $x_-(\epsilon)$ of the equation $(1 - x^2)Q(E, x) = 0$ remains fixed. On the other hand, the relative positions of these roots define the actual limits of integration in equation (28), and change each time ϵ transfers from one interval into another. Therefore, the DOS is given by 12 different analytic

expressions for every energy interval of the above three cases (i)–(iii). Considering here for brevity only case (i), and performing the integration in equation (28), we have

$$g(E) = 2\pi I(E, \gamma)[|E(4t - E)|]^{-1/2}. \tag{32}$$

The function $I(E, \gamma)$ can be expressed in terms of elliptic integrals of the first and third kinds, and has a form varying from one energy interval to another. When $\epsilon_{\min} \leqslant \epsilon < 4$

$$I(E, \gamma) = \alpha[(\cosh\gamma - a)F(\pi/2, k) + (a - d)\Pi(\pi/2, \beta, k)] \tag{33}$$

where $\alpha = 2/[(a - c)(b - d)]^{1/2}$ and $\beta = (d - c)/(a - c)$. It is also assumed that $a > b > c > d$ whereas specific choice of these constants and parameter k depends on ϵ. If $\epsilon_{\min} \leqslant \epsilon \leqslant \epsilon_1$, then $a = x_+$, $b = 1$, $c = x_-$, $d = -1$, and $k = \{[(x_+ - 1)(x_- - 1)]/2(x_+ - x_-)\}^{1/2}$. If $\epsilon_1 \leqslant \epsilon \leqslant 4$, then symbols in (33) should be redenoted in the following way: $b \Rightarrow c$, $c \Rightarrow b$, $k \Rightarrow 1/k$.

For the energy interval $4 < \epsilon \leqslant \epsilon_{\max}$ the function $I(E, \gamma)$ is given by

$$I(E, \gamma) = \alpha[(\cosh\gamma - d)F(\pi/2, k) + (d - c)\Pi(\pi/2, \delta, k)] \tag{34}$$

where $\delta = (b - c)/(b - d)$. The other constants entering equation (34) are: $a = x$, $b = 1$, $c = -1$, $d = x_+$ and $k = \{2(x_- - x_+)/[(x_- + 1)(1 - x_+)]\}^{1/2}$, if $4 < \epsilon \leqslant \epsilon_{\max}$; and when $\epsilon_2 < \epsilon \leqslant \epsilon_{\max}$, the following substitutions should be done: $c \Rightarrow d$, $d \Rightarrow c$, $k \Rightarrow 1/k$. If $\epsilon = 4$, then the DOS is

$$g(E) = (\tau/2\pi t)[(\cosh\gamma - a)F(\pi/2, k) - (a + 1)^{1/2}E(\pi/2, k)] \tag{35}$$

with $a = \cosh\gamma - \frac{1}{4}\sinh\gamma$, $\tau = [\sinh\gamma(a + 1)]^{-1/2}$ and $k = [2/(a + 1)]^{1/2}$.

The logarithmic Van Hove singularities in the DOS are typical features of any 2D system. Their locations in the considered system are determined by the quadratic equation $k(\epsilon) = 1$, which has different coefficients when ϵ belongs to different energy intervals. The corresponding solutions are trivial though rather cumbersome, and therefore there is no need to present them here in an explicit form.

The above analysis shows that, although in the model under consideration $g(E)$ can be obtained in an explicit analytic form, the corresponding calculations are rather tedious even in the simplest case, so that for practical purposes a numerical computation of the DOS on the basis of equation (28) appears more preferable. Nevertheless, analytic consideration of the Landau energy spectrum can be done within the quasiclassical approach even for a more general 2D model in which an arbitrary dispersion relation along one of the two directions is assumed.

5. Landau bands in a 2D strongly anisotropic lattice

Now turn back to equation (24) and consider the low-flux limit, which means that $\Phi/\Phi_0 \ll 1$. Of course, one can readily make flux Φ small compared with flux quantum Φ_0 just by application of a small field B, but the point is that even in the highest available fields of the order 10–100 T the ratio Φ/Φ_0 in conventional crystals is extremely small, $\Phi/\Phi_0 \sim 10^{-3}$–10^{-4}. The latter is due to the fact that an enormous field of the order 10^5 T should be applied to the crystal lattice to obtain total flux through a unit cell equal

to Φ_0. The smallness of the parameter Φ/Φ_0 gives ground for the following power series expansion

$$\epsilon(\nu - 2\pi n\Phi/\Phi_0) \simeq \epsilon(\nu) - \epsilon'(\nu)2\pi n\Phi/\Phi_0 + \tfrac{1}{2}\epsilon''(\nu)(2\pi n\Phi/\Phi_0)^2 + \cdots. \tag{36}$$

Keeping in equation (24) terms only up to the first order in $2\pi n\Phi/\Phi_0$, we have

$$tf(n+1) + tf(n-1) + [E - 2t\epsilon(\nu) - \hbar\Omega(\nu)n]f(n) = 0. \tag{37}$$

Here $\Omega = eB/mc$ is the cyclotron frequency, and $m = m(\nu)$ stands for the effective mass, which depends through the parameter $\nu = p_y b/\hbar$ on position at the Fermi surface. For m^{-1} we have: $m^{-1}(\nu) = m_*^{-1}u(\nu)$, where $m_* = \hbar^2/abt$ and $u(\nu) = \epsilon(\nu)/t$. In conventional metals the width of the conduction band is of the order of $t = P_f^2/2m$, with $P_f \simeq \hbar/a_B$ and m the electron mass (a_B is the Bohr radius). The estimation of the mass m_* in this case yields $m_* \simeq m$, while $u(\nu)$ is of the order of unity or less.

The energy spectrum given by equation (37) is well known in the literature as the Wannier–Stark ladder since equation (37) corresponds exactly to that of a tight-binding chain in a uniform electric field [15]. In analogy with the Wannier–Stark ladder the energy spectrum of the Schrödinger equation (37) consists of a periodic set of discrete levels with separation $\hbar\Omega$, which is nothing but the Landau spectrum

$$E_n(\nu) = 2t + \epsilon(\nu) + \hbar\Omega(\nu)n. \tag{38}$$

The analogy between the Wannier–Stark ladder and the Landau spectrum is, however, not complete because the Wannier–Stark ladder is infinite in both directions whereas the Landau spectrum is limited from the bottom. To see this in more detail, consider the spectrum just above the bottom of the energy band. In this case $\epsilon'(\nu) = 0$ and a term proportional to Φ^2 should be taken into consideration in equation (36). So, after substitution of equation (36) into equation (24), we arrive at the following equation:

$$tf(n+1) + tf(n-1) + [E - 2t + \epsilon(\nu) - (\sigma n)^2]f(n) = 0 \tag{39}$$

where

$$\sigma = \epsilon''(\nu_0)^{1/2}\sqrt{2\pi}\,\Phi/\Phi_0. \tag{40}$$

The derivative in equation (40) is taken in the minimum ν_0 of the dispersion relation $\epsilon(\nu)$.

To solve the difference equation (39), it is convenient to introduce a function $\phi(x)$ depending on some dimensionless variable x:

$$\phi(x) = \sum_n f(n)e^{inx}. \tag{41}$$

In terms of $\phi(x)$ the difference equation (39) can be written as a differential one

$$-\sigma^2\frac{d^2\phi}{dx^2} + 2t(1 - \cos x)\phi = [E - \epsilon(\nu)]\phi. \tag{42}$$

This equation has the form of a Schrödinger one for a 'particle' moving in the potential $U(x) = 2t(1 - \cos x)$. Its energy spectrum may be readily found with the help of

the quasiclassical approach. Thus, after some standard manipulations we obtain from equation (42) a quasiclassical quantization rule

$$\oint k(x, y)\,\mathrm{d}x = J(n, y) \tag{43}$$

with $k(x) = [(y-1+\cos x)]^{1/2}$ and $y = [E+\epsilon(\nu)]/2t$. The right-hand side of equation (43) is given by

$$J(n, y) = (2\pi\sigma/t^{1/2})\{(n+\tfrac{1}{2}) + [(-1)^n/\pi]\sin^{-1}[W\cos(pa)]\}. \tag{44}$$

Here p is a wavevector in direction across the chains, and W stands for the quasiclassical tunnelling probability under the crest of the periodic potential $U(x)$

$$W = \exp(-H_*/H). \tag{45}$$

The characteristic magnetic field H_* determines the scale of fields such that for $H > H_*$ the discrete Landau levels are broadened into bands. The field H_* is given by

$$H_* = \frac{\Phi_0}{\pi ab}\theta\int_{-x_0}^{x_0}|k(x)|\,\mathrm{d}x. \tag{46}$$

Here $\theta = [t/\epsilon''(\nu_0)]^{1/2}$ and $\pm x_0$ are the turning points of the 'particle' in the potential $U(x)$. The integral (43) can be expressed in terms of complete elliptic integrals of the first and second kinds.

$$\oint k(x, y)\,\mathrm{d}x = 16[(y^2-1)F(\pi/2, y) + E(\pi/2, y)]. \tag{47}$$

Taking into account that for low-lying levels, in which we are interested, the parameter $y \ll 1$, and that in this limit the right-hand side of equation (47) is equal to $\simeq 2\pi y$, we have

$$E_n(p) = \epsilon(\nu_0) + \hbar\Omega\{(n+\tfrac{1}{2}) + [(-1)^n/\pi]\sin^{-1}[W\cos(pa)]\}. \tag{48}$$

The effective mass entering the cyclotron frequency in (48) is now given by $m(\nu_0) = m_*/\theta$.

Thus, one can see from equation (47) that the energy spectrum of the system under consideration consists of a set of equidistant Landau levels with separation $\hbar\Omega$, which are broadened into Landau bands due to the lifting of their degeneracy on orbit centre position in a periodic 2D lattice. The width of these bands is proportional to the field-dependent tunnelling probability $W(H)$, which is of the same form as in coherent magnetic breakdown [16].

6. Conclusion

The energy spectrum of a 2D Bloch electron in a strong quantizing magnetic field is an old classical problem intimately connected with a number of applications in solid-state physics partially enumerated in the introduction. Although this problem has been extensively explored for the past decades, only a few exact results in this field are known. One of them is the simple analytic expression for the DOS given by Wannier *et al* [7] for a square lattice

with a tight-binding electron Hamiltonian in the rational flux case. Only nearest-neighbour site correlations have been assumed in [7]. On the other hand, long-range correlations are inevitably present in every physical system and in some cases (see above for details) should be taken into consideration. In this connection the result of [7] is generalized in the third section of the present paper to the case of a 2D lattice model with exponentially decreasing, as a function of inter-site distance, overlap integrals. It was done on the basis of a transfer-matrix approach developed earlier in the problem of plasma oscillations in superlattices [11]. The transfer-matrix approach proved to be useful also in the energy spectrum study of yet another 2D lattice model. In this model, considered in the fourth section, a 2D lattice consists of a periodic set of parallel chains with arbitrary electron dispersion, which are correlated in the transverse directions by dint of nearest-neighbour electron hopping. Such a model to all appearances is applicable to organic conductors of the (TMTSF) $_2$X family [17] (TMTSF = tetramethyltetraselenafulvalene), which are layered crystals with layers consisting of a weakly correlated periodic set of organic conducting chains. In the rational flux case the DOS of this model depends on polynomials (27) and has an integral form (26) that permits one to obtain an explicit expression for any specific form of dispersion relation $\epsilon(\nu)$ and readily lends itself to numerical computations. For intra-chain overlap integrals that are exponentially decreasing with inter-site distance, the exact DOS in the rational flux case is expressed in terms of elliptic integrals (32). In the low-flux limit, i.e. when $\Phi/\Phi_0 \ll 1$, the energy spectrum can be derived for arbitrary electron dispersion $\epsilon(\nu)$. In this case the Schrödinger equation (37) takes the form of a difference equation, which is well known in the Wannier–Stark problem of an electron in a uniform electric field on a one-dimensional lattice. Such similarity makes it possible to consider equidistant Landau spectrum (38), by analogy with the Wannier–Stark ladder, as some sort of 'magnetic Wannier–Stark ladder'. A more detailed analysis of this analogy based on the Green functions technique will be published elsewhere.

A simple quantization rule (43) is also derived for low-lying levels, with respect to the band bottom. This quantization rule yields an energy spectrum (48) composed of equidistant Landau levels broadened into bands whose width is proportional to the probability factor (45) similar to that of magnetic breakdown systems.

In conclusion, two remarks on possible applications of the above results are in order. The first one is that the difference equation (39) also arises in the problem of the upper critical magnetic field, H_{c2}, calculated in a 1D superconducting superlattice [18]. The physical reason for this lies in the fact that H_{c2} is determined by the lowest edge of the Landau spectrum of a 'particle' in an external magnetic field, as is well known in the theory of superconductivity. The unconventional, from the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity point of view, non-linear temperature behaviour of $H_{c2}(T)$, observed in 1D superlattices [13], is, in the long run, due to non-linearities in H of the lowermost Landau band edge. Since the above results pertain to the 2D geometry, a favourable opportunity appears to explain non-linearities in $H_{c2}(T)$ of a 2D superstructure in the same fashion as in a 1D superconducing superlattice. In particular, the so-called positive curvature of the $H_{c2}(T)$ in a 2D superconducting superlattice made of mismatched dislocation network in a PbTe/PbS multilayer [19] can be explained in this way. The corresponding results will be published elsewhere.

The second remark addresses the problem of a magnetic-field-induced series of structural Peierls-like phase transitions periodic in inverse field, which has been observed in 2D organic conductors of the (TMTSF)$_2$X family [17]. A very similar phenomenon was predicted recently in periodic 2D magnetic breakdown structures [20], and in a 2D conductor subjected to a perpendicular quantizing magnetic field and simultaneously modulated by a 1D periodic

potential lying in the plane of this 2D conductor [21]. Since, as was pointed out above, the energy spectrum (48) is applicable to 2D organic conductors, and, on the other hand, it is of the same type as that exploited in [20, 21], an intriguing opportunity appears to explain a cascade of Peierls-like structural phase transitions in organic conductors on the basis of the Landau band energy spectrum found in this paper.

Of course, the presented list of possible applications is far from being complete and can be readily extended because many problems in condensed matter physics are intimately related to the problem of a Bloch electron on a 2D lattice.

Acknowledgment

The research described in this publication was made possible, in part, by Grant No U2K000 from the International Science Foundation.

References

[1] Alexander S 1983 *Phys. Rev.* B **27** 1541–57
[2] Prange R E and Girvin S M (ed) 1987 *The Quantum Hall Effect* (New York: Springer)
[3] Wilczek F 1990 *Fractional Statistics and Anyon Superconductivity* (Singapore: World Scientific)
[4] Affleck I and Marson B 1988 *Phys. Rev.* B **37** 3774–84
[5] Azbel M Ya 1964 *Zh. Eksp. Teor. Fiz.* **46** 929–41 (1964 *Sov. Phys.–JETP* **19** 634–44)
[6] Hofstadter D 1976 *Phys. Rev.* B **14** 2239–49
[7] Wannier G H, Obermair G M and Ray R 1979 *Phys. Status Solidi* b **93** 337–42
[8] Hasegawa Y, Lederer P, Rice T M and Wiegmann P M 1989 *Phys. Rev. Lett.* **63** 907–10
[9] Montambaux G 1989 *Phys. Rev. Lett.* **63** 1657
[10] Gvozdikov V M 1992 *Fiz. Nizk. Temp.* **18** 1128–34 (1992 *Sov. J. Low Temp. Phys.* **18** 790–5)
[11] Gvozdikov V M 1990 *Fiz. Nizk. Temp.* **16** 1156–63 (1990 *Sov. J. Low Temp. Phys.* **16** 668–72)
[12] Barelli A and Kreft C 1991 *Preprint* CPT-91/PE.2515, Centre de Physique Theorique, Marseille
[13] Jin B Y and Ketterson J B 1989 *Adv. Phys.* **38** 189–366
[14] Lifshits I M, Azbel M Ya and Kaganov M I 1973 *Electron Theory of Metals* (New York: Consultants Bureau)
[15] Callaway J 1964 *Energy Band Theory* (New York: Academic)
[16] Kaganov M I and Slutskin A A 1983 *Phys. Rep.* **98** 189–307
[17] Gor'kov L P 1984 *Usp. Fiz. Nauk* **144** 381–413 (1984 *Sov. Phys.–Usp.* **27** 809–901)
[18] Gvozdikov V M 1990 *Fiz. Nizk. Temp.* **16** 5–15 (1990 *Sov. J. Low. Temp. Phys.* **16** 1–6)
[19] Mironov O A, Savitskii B A, Sipatov A Yu *et al* 1988 *Pis. Zh. Eksp Teor. Fiz.* **48** 100–2 (1988 *JETP Lett.* **48**)
[20] Gvozdikov V M and Kaner E A 1986 *Pis. Zh. Eksp. Teor. Fiz.* **43** 393–5 (1986 *JETP Lett.* **43** 507–9)
[21] Gvozdikov V M 1992 *Fiz. Nizk. Temp.* **18** 997–1004 (1992 *Sov. J. Low Temp. Phys.* **18** 700–5)