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The transfer matrices and electronic spectrum of the multilayered system in a homogeneous magnetic field

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Abstract. The model of the multilayered media of the Kronig–Penney type with the applied magnetic field oriented parallel to the layer surfaces is investigated. The operator of translation is expressed in terms of the parabolic cylinder functions. The difference equations for the transfer matrix and the electron wavefunction, as well as the rigorous equations on the electron energy spectrum, are obtained. For the array of the flat δ -barriers all the limiting cases are analysed: weak or strong magnetic field, weak or tight binding, multilayered film, infinite lattice. For the latter it is shown that the destruction of the quasi-momentum space homogeneity at the magnetic field switching on begins from the Brillouin zone edges and is quantitatively described by the cotangent singularity.

1. Introduction

By now there exists a number of works devoted to the investigation of electron behaviour in the periodic medium or quantum film with the applied homogeneous magnetic field. The physical importance of diffraction processes is evident because they determine crossover from the Bloch solution in lattice or from the standing waves in slab to the Landau solution [1] is obvious, but the rigorous qualitative and quantitative quantum-mechanical description of the wavefunction and the spectrum evolution is not trivial. The motion of the Bloch electron in the magnetic field has been studied using different approaches and approximations which select one or another important feature of the system (Peierls's substitution [2], magnetic translation groups [3], topological concepts [4], weak and tight binding [5,6], Pippard networks [7], effective mass [8], semiclassical approximation [9], zone subdivision [10], Hofstadter's butterfly [11] etc). Some of the simplified models (such as Harper's equation [6]) are of great interest and have been developed in a wide variety of physical and mathematical contexts (incommensurate structures and so forth) which have caused the corresponding flow of literature [12]. On the other hand, in connection with the adjacent question about spectra in the magnetic field of the volume and lateral superlattices it is interesting to observe the evolution of the skipping orbits [13, 14] and spectra of the magnetic surface levels in the films [15–17] when the multilayered structures are formed.

In this paper a rather simple quasi-one-dimensional model of the multilayered media of the Kronig–Penney type with the piecewise constant potential and with an applied magnetic field oriented parallel to the surfaces of layers is studied. The one-dimensionality permits us to find the explicit expression of the transfer matrix (the operator of translation) in terms

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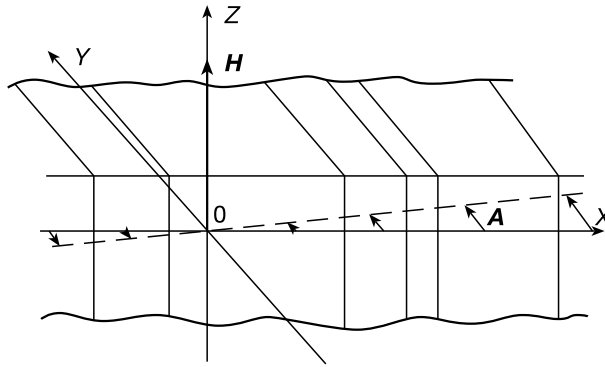


Figure 1. The geometry of the problem.

of the parabolic cylinder functions. We obtain the universal rigorous difference equations (a type of Harper equation, but with a different structure) for the transfer matrix and the wavefunction, as well as the rigorous equation on the electron energy spectrum. Extensive results are presented for the array of flat δ -barriers at different boundary conditions. All the reasonable limiting cases are analysed: weak or strong magnetic field, weak or tight binding (barrier transparency), multilayered film, infinite lattice. For the latter of special interest is the quantitative description of the quasi-momentum space homogeneity destruction at the cost of the breakdown of the translational invariance of the one-electron Hamiltonian at the weak magnetic field. The destruction of homogeneity begins from the Brillouin zone edges and is described by the cotangent singularity.

Our approach generalizes the rigorous one-dimensional solution of Floke–Liapunov [18] which served earlier as the conceptual basis for the three-dimensional Fourier constructions of Bloch and Brillouin [19]. Unfortunately, we cannot directly use this approach for the two- and three-dimensional lattices, because it fails to separate variables, match explicitly the analytical solutions in different cells and obtain the translation operator. To support the usefulness of the detailed analysis of the ideal quasi-one-dimensional model for the diamagnetic lattice we mention the analogy with the role and meaning of the one- and two-dimensional Ising model in the theory of ferromagnetism and phase transitions because of its ‘solubility’ [20].

Apart from the formal interest our model has a practical value, because it is directly applicable to the plane-parallel multilayered synthetic semiconductor or metal nanostructures as well as to the lateral superlattices on the surfaces of the semiconductors or dielectrics, which are now intensively investigated and widely used in microelectronics [21].

2. Description of the model and transfer matrix

Let us consider a multilayered system with plane-parallel boundaries and the magnetic field \mathbf{H} which is oriented parallel to the layers (figure 1).

We direct the z -axis along the magnetic field \mathbf{H} , and the x -axis is transverse to the layers so that the lattice potential is $\tilde{U} = \tilde{U}(X)$. We direct the vector potential along the y -axis and choose Landau gauge $\mathbf{A} = (0, HX, 0)$, so we will solve the steady-state Schrödinger equation

in the standard form for this problem:

$$\left[\frac{\hat{p}_x^2}{2m} + \frac{1}{2m} \left(\hat{p}_y - \frac{eH}{c} X \right)^2 + \frac{\hat{p}_z^2}{2m} + \tilde{U}(X) \right] \Psi = E \Psi \quad (1)$$

$$\Psi = \exp \frac{i}{\hbar} (p_y Y + p_z Z) \psi \quad \hat{p}_{x_j} = -i\hbar \frac{\partial}{\partial X_j} \quad (X_j = X, Y, Z).$$

If the film is bounded in the Z -direction, then the Z -projection of the momentum is elementary quantized $p_z = n_z \hbar / L_z$ where L_z is the size of film and n_z is an integer number. It is not simple to take the boundary conditions along the y -axis into account analytically, so we will assume the system to be unbounded along the y -axis and the parameter p_y to be continuous.

By making all parameters dimensionless, as usual, we arrive at the one-dimensional differential equation

$$\frac{d^2 \psi}{dx^2} - \left[\frac{x^2}{4} + \tilde{a}(x) \right] \psi = 0. \quad (2)$$

x is the X coordinate referenced from the 'orbit centre' X_c and all of them are also expressed in units of 'magnetic length' l , that is

$$x = \bar{x} - \bar{x}_c \quad \bar{x} = \frac{X}{l} \quad \bar{x}_c = \frac{X_c}{l} \quad (3)$$

$$l^2 = \frac{c\hbar}{2|e|H} = \frac{\hbar}{2m\omega_0} \quad X_c = \frac{cp_y}{eH} = \frac{e}{|e|} \frac{p_y}{m\omega_0} \quad \omega_0 = \frac{|e|H}{mc}$$

where ω_0 is the Larmor frequency, and $\tilde{a}(x)$ is the dimensionless energetic parameter

$$\tilde{a}(x) = -\frac{E_t - \tilde{U}(x)}{\hbar\omega_0} \quad E_t = E - \frac{p_z^2}{2m}. \quad (4)$$

In every layer, while the potential energy is constant $\tilde{U} = \text{const}$, the equation (2) is the standard Weber equation [22], with the parameter

$$a \equiv -\left(\nu + \frac{1}{2} \right) = -\frac{E_t - \tilde{U}}{\hbar\omega_0}. \quad (5)$$

Its solutions are the parabolic cylinder functions (the Weber functions) $U(a, x) \equiv D_\nu(x)$ and $V(a, x)$ [23–25]. It is most convenient for us to use $D_\nu(x)$ and $D_\nu(-x)$ as the linear independent solutions. Really, if $\nu \neq n$, where n is an integer, then their Wronskian is different from zero and is equal to [23]

$$W\{D_\nu(x), D_\nu(-x)\} = \det \begin{pmatrix} D_\nu(x) & D_\nu(-x) \\ D'_\nu(x) & D'_\nu(-x) \end{pmatrix} = \frac{\sqrt{2\pi}}{\Gamma(-\nu)} \quad (6)$$

where a derivative with respect to x is denoted by a prime and $\Gamma(-\nu)$ is the Euler gamma function.

At present the asymptotics of these functions are well investigated [22–26] (appendix A). We note here that at $x \rightarrow \pm\infty$, ($|x| \gg |a|$, out of parabolic well) $D_\nu(x)$ decreases to the right and increases to the left (qualitatively resembling e^{-x} but considerably steeper), and $D_\nu(-x)$ —vice versa (like e^x).

Inside the parabolic well at $\nu \approx -a \gg x^2$ both solutions oscillate. At $\nu \rightarrow n$ degeneration appears and both solutions are proportional to the Hermite polynomial $H_n(x/\sqrt{2})$ of the n th order and of definite parity

$$D_n(x) = 2^{-\frac{n}{2}} e^{-\frac{x^2}{4}} H_n \left(\frac{x}{\sqrt{2}} \right) \quad (7)$$

$$D_n(-x) = (-1)^n D_n(x).$$

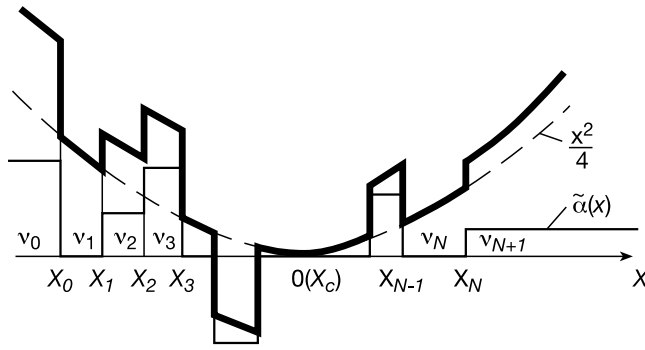


Figure 2. The effective one-dimensional magnetic ‘potential’ $\tilde{a}(x) + x^2/4$ (heavy curve), the layered potential $\tilde{a}(x)$ (light curve) and the magnetic parabolic ‘potential’ $x^2/4$ (dashed curve).

Thus, in the layer on the interval of constancy of the parameter $a = -(\nu + \frac{1}{2})$ and not integer ν , the general solution of the equation (2) has the form

$$\psi(x) = A_+ D_\nu(x) + A_- D_\nu(-x). \quad (8)$$

The matrix of transfer from x_1 to x_2 relates the columns of function ψ and its derivative ψ' in these points [27]

$$\begin{pmatrix} \psi(x_2) \\ \psi'(x_2) \end{pmatrix} = M(x_2, x_1) \begin{pmatrix} \psi(x_1) \\ \psi'(x_1) \end{pmatrix} \quad M(x_2, x_1) = \begin{pmatrix} M(x_2, x_1)_{11} & M(x_2, x_1)_{12} \\ M(x_2, x_1)_{21} & M(x_2, x_1)_{22} \end{pmatrix}. \quad (9)$$

If the points x_1 and x_2 belong to one layer, then with the help of (8) and (6) by the elimination of the integration constants A_+ and A_- we obtain for equation (2) the following form of the transfer matrix:

$$M^{(\nu)}(x_2, x_1) = \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \begin{pmatrix} D_\nu(x_2) & D_\nu(-x_2) \\ D'_\nu(x_2) & D'_\nu(-x_2) \end{pmatrix} \begin{pmatrix} D'_\nu(-x_1) & -D_\nu(-x_1) \\ -D'_\nu(x_1) & D_\nu(x_1) \end{pmatrix} \quad (10)$$

which is evidently unimodular, $\det M^{(\nu)}(x_2, x_1) = 1$.

We also note that if the potential $\tilde{U}(X)$ contains in some point X_n the δ -barrier (plane) of power \bar{U}_n , i.e. that in square brackets in equation (1), there is a term

$$\begin{aligned} \tilde{U}(X) &= \frac{\hbar^2}{2m} \bar{U}_n \delta(X - X_n) = \frac{\hbar^2}{2ml^2} U_n \delta(x - x_n) \\ x_n &= \bar{x}_n - \bar{x}_c \quad \bar{x}_n = \frac{X_n}{l} \quad U_n = l \bar{U}_n \end{aligned} \quad (11)$$

therefore, for the solutions of the equation (2) the matrix of transfer across such a barrier at the point x_n is [28]

$$\hat{U}_n = \begin{pmatrix} 1 & 0 \\ U_n & 1 \end{pmatrix}. \quad (12)$$

3. Layers with rectangular barriers

First, we examine the model with the finite number $N + 2$ of layers, so that the potential energy $\tilde{U}(X)$ is the piecewise constant, not necessarily periodical (figure 2). The parameter ν exhibits the discontinuities in $N + 1$ points x_0, x_1, \dots, x_N so that in the region of the layer $x_{i-1} < x < x_i$ we have $\tilde{U}(X) = \tilde{U}_i$, $\nu = \nu_i$ and the integration constants in (8) are A_{i-} and

A_{i+} . If the step potential \tilde{U}_i nowhere tends to $(-\infty)$ anomalously rapidly, then the presence of the parabolic barrier in (2) provides the finite motion along the x -axis and the fulfillments of the null boundary conditions at the infinity

$$\psi(\pm\infty) = 0. \tag{13}$$

It means that in (8) we have

$$\psi(x) = \begin{cases} A_{0-} D_{v0}(-x) & \text{i.e. } A_{0+} = 0 \quad \text{at } x < x_0 \\ A_{(N+1)+} D_{vN+1}(x) & \text{i.e. } A_{(N+1)-} = 0 \quad \text{at } x > x_N. \end{cases} \tag{14}$$

The lack of translational symmetry of equations (1) and (2) means the nonconservation of quasi-momentum. Nonetheless, it is not so difficult, with the help of the transfer matrix (9), (10) to write out a universal recurrent difference equation [27] which is equivalent to the differential equation (2). It connects the values of the wavefunction in three points at $n > m > p$

$$\psi_n = \alpha_{nmp} \psi_m - \beta_{nmp} \psi_p \tag{15}$$

where $\psi_n = \psi(x_n)$ is the value of the wavefunction in the node x_n and recurrent coefficients α and β are expressible in terms of the elements of the one-step transfer matrix (9) between these points

$$\alpha_{nmp} = M(x_n, x_m)_{11} + \beta_{nmp} M(x_m, x_p)_{22} \quad \beta_{nmp} = \frac{M(x_n, x_m)_{12}}{M(x_m, x_p)_{12}}. \tag{16}$$

There is [27] the equation, analogous to (15), for the ψ'_n derived from the latter by the change of indices ($1 \leftrightarrow 2$) of all elements of the transfer matrix in (16). At the beginning of the recursion ψ_0 and ψ'_0 are given by the boundary condition at $x = x_0$ and ψ_1, ψ'_1 are expressed through them from (9).

If the points x_n are chosen to coincide with the surfaces of the layers (figure 2) and the transfer matrix elements in (16) are taken from (10), then equations (15) may be considered as some analogue of the Harper equation [6] which describes the electron behaviour in the two-dimensional lattice with the perpendicular magnetic field. Equation (15) by definition corresponds to the quasi-one-dimensional model and does not reduce to the Harper equation because $\beta \neq 1$ and α are not periodic in space. On the other hand, equation (15) is rigorous and permits us to investigate the transition from weak to tight binding in the multilayered lattice and, in addition, to describe quantitatively the destruction of the quasi-momentum space homogeneity at the perturbations of the periodic potential.

The renormalization of the wavefunction ψ_n and recurrent coefficients α and β at the roughening may be expressed in terms of the determinants of the tridiagonal matrices composed from the coefficients of equation (15) on the sequence of all nodes [27]. Furthermore, we may investigate these expressions numerically or by using the known asymptotics of $D_v(x)$. In addition, it is evident from (9) and (14) that the spectral equation of the system is

$$(D'_{vN+1}(x_N), -D_{vN+1}(x_N)) M^{(vN)}(x_N, x_{N-1}) \dots M^{(v2)}(x_2, x_1) M^{(v1)}(x_1, x_0) \times \begin{pmatrix} D_{v0}(-x_0) \\ D'_{v0}(-x_0) \end{pmatrix} = 0. \tag{17}$$

By substituting the transfer matrix (10) we obtain

$$\sum_P (-1)^P \prod_{i=0}^N \det \begin{pmatrix} D_{vi}(-x_i) & D_{vi+1}(x_i) \\ D'_{vi}(-x_i) & D'_{vi+1}(x_i) \end{pmatrix} = 0 \tag{18}$$

where P is the operation of sign changing $(x_i, -x_{i+1}) \rightarrow (-x_i, x_{i+1})$ in the arguments of the parabolic cylinder functions from two adjacent determinants for one i in every subsequent

summand (not touching the signs of arguments of the extreme $D_{\nu_0}(-x_0)$ and $D_{\nu_{N+1}}(x_N)$), and the summation is taken over all these transpositions. We also omit the factors $\Gamma(-\nu_i)/\sqrt{2\pi} \neq 0$.

When $N \rightarrow \infty$ and at the finite potentials \tilde{U}_i all sums, products and tridiagonal determinants converge exponentially on the Larmour radius length due to the $D_\nu(\pm x)$ asymptotics at infinity.

If the infinitely high barrier exists in some region $x_{i-1} < x < x_i$, i.e. $\nu_i \rightarrow -\infty$, then on his left boundary the identity $D_{\nu_i}(x_{i-1}) \equiv 0$ and on his right boundary the identity $D_{\nu_i}(-x_i) \equiv 0$ are fulfilled, but the derivatives D'_{ν_i} are not equal to zero as they are constants of the boundary conditions and enter in (18) as factors not affecting the spectra of the regions mutually isolated by the barrier.

In particular at $N = 0$ we have two half-spaces with the plane surface at x_0 in the magnetic field parallel to it and with the spectral equation

$$\det \begin{pmatrix} D_{\nu_0}(-x_0) & D_{\nu_1}(x_0) \\ D'_{\nu_0}(-x_0) & D'_{\nu_1}(x_0) \end{pmatrix} = 0 \quad (19)$$

whence if the left region is impenetrable ($D_{\nu_0}(-x_0) \equiv 0$, $\nu_0 = -\infty$), then the spectral equation is $D_{\nu_1}(x_0) = 0$ and if the right region is impenetrable ($D_{\nu_1}(x_0) \equiv 0$, $\nu_1 = -\infty$), then the spectral equation is $D_{\nu_0}(-x_0) = 0$.

When $N = 1$ we have a plate (layer $x_0 < x < x_1$, adjacent with two half-infinite media) and the spectral equation

$$\det \left[\begin{pmatrix} D_{\nu_0}(-x_0) & D_{\nu_1}(x_0) \\ D'_{\nu_0}(-x_0) & D'_{\nu_1}(x_0) \end{pmatrix} \begin{pmatrix} D_{\nu_1}(-x_1) & D_{\nu_2}(x_1) \\ D'_{\nu_1}(-x_1) & D'_{\nu_2}(x_1) \end{pmatrix} \right] - \det \left[\begin{pmatrix} D_{\nu_0}(-x_0) & D_{\nu_1}(-x_0) \\ D'_{\nu_0}(-x_0) & D'_{\nu_1}(-x_0) \end{pmatrix} \begin{pmatrix} D_{\nu_1}(x_1) & D_{\nu_2}(x_1) \\ D'_{\nu_1}(x_1) & D'_{\nu_2}(x_1) \end{pmatrix} \right] = 0. \quad (20)$$

From here if both media on each side are impenetrable, then $D_{\nu_0}(-x_0) \equiv D_{\nu_2}(x_1) \equiv 0$, $\nu_0, \nu_2 \rightarrow -\infty$ and the equation for the spectrum of a plate with $\nu_1 = \nu$ is

$$\det \begin{pmatrix} D_\nu(x_0) & D_\nu(x_1) \\ D_\nu(-x_0) & D_\nu(-x_1) \end{pmatrix} = 0. \quad (21)$$

Its asymptotics are analysed in appendix B.

4. The δ -barriers array

As usual, in the Kronig–Penney model it is the limit of the Dirac potential comb which is the most readily analysed both qualitatively and quantitatively.

Consider an array of $N - 1$ plane-parallel potential barriers U_n of the form (11) at $x = x_n \equiv x_0 + nd$ ($n = 1, 2, \dots, N - 1$) with the matrices of transfer across them (12). The boundary conditions to the left from $x = x_0$ and to the right from $x = x_0 + Nd$ may correspond to the mixed boundary problem, i.e. to the presence there of the barriers of different height. In every cell (layer) the solution has the form (8) and the constants A_{n+}, A_{n-} with the help of (9), (10) can easily be expressed in terms of the values ψ and ψ' in the nodes x_n . In this paper our prime interest is the energetic spectrum which is determined by the values of the parabolic cylinder functions in the nodes.

The matrices of transfer across the cells $x_{n-1} < x < x_n$ are

$$\begin{aligned} M(x_1, x_0) &= M^{(\nu)}(x_1, x_0) \\ M(x_n, x_{n-1}) &= M^{(\nu)}(x_n, x_{n-1}) \hat{U}_{n-1} \quad n = 2, \dots, N - 1 \end{aligned} \quad (22)$$

hence with the help of (16) and (6) we find the recurrent coefficients $\alpha_n = \alpha_{nmp}, \beta_n = \beta_{nmp}, (m = n - 1, p = n - 2)$ in the difference equation (15) for the neighbouring nodes ($n \geq 2$)

$$\alpha_n = \frac{M_{n-2,n}}{M_{n-2,n-1}} + U_{n-1}M_{n-1,n} \quad \beta_n = \frac{M_{n-1,n}}{M_{n-2,n-1}} \tag{23}$$

i.e. are expressible in terms of the upper-right element of the matrix (10) of transfer along the nodes

$$M_{ij} \equiv M^{(\nu)}(x_j, x_i)_{12} = \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \det \begin{pmatrix} D_i & D_j \\ D_{-i} & D_{-j} \end{pmatrix} \tag{24}$$

possessing the evident properties

$$M_{ij} = -M_{ji} \quad M_{ij}M_{kl} = M_{ik}M_{jl} + M_{il}M_{kj}. \tag{25}$$

Here and later on the parabolic cylinder functions in the nodes x_i are conveniently denoted by $D_i \equiv D_\nu(x_i), D_{-i} \equiv D_\nu(-x_i)$ omitting the index ν which is the same in all layers.

As indicated earlier, the solutions of equations (15) may be written and analysed with the help of the determinants B_l^m of tridiagonal matrices with the $(\beta_n, \alpha_n, 1)$ on the diagonals for the sequence of nodes $m \leq n \leq l$ [27].

The spectrum depends on the concrete boundary conditions at $x = x_0$ and $x = x_0 + Nd$. This dependence decreases with an increase of magnetic field H , of the system width Nd and with a decrease of the boundary barriers. We shall restrict our consideration to two limiting cases: the lattice without the boundary barriers and the lattice in the rectangular infinite potential well.

First, since motion in the magnetic field is finite, one can do without the potential well on the boundary using instead the boundary conditions (14) with $\nu_0 = \nu_{N+1} = \nu_n = \nu$:

$$\begin{aligned} \psi(x_1) &= A_{1-}D_{-1} & \text{i.e. } & A_{1+} = 0 \\ \psi(x_{N-1}) &= A_{N+}D_N & \text{i.e. } & A_{N-} = 0. \end{aligned} \tag{26}$$

In this case the recurrent system (15), with the analogous system for the derivatives ψ'_n [27], may be transformed to the system for the coefficients $A_{n\pm}$ (at the normalization $A_{1-} = 1$)

$$\begin{aligned} A_{n\pm} &= \tilde{\alpha}_{n\pm}A_{(n-1)\pm} - \tilde{\beta}_{n\pm}A_{(n-2)\pm} & n &\geq 3 \\ A_{1+} &= 0 & A_{1-} &= 1 & A_{2\pm} &= \tilde{\alpha}_{2\pm} \end{aligned} \tag{27}$$

with the recurrent coefficients

$$\tilde{\alpha}_{n\pm} = 1 + \tilde{\beta}_{n\pm} - U_{n-1} \frac{D_{\mp(n-1)}}{D_{\mp(n-2)}} M_{n-2,n-1} \quad \tilde{\beta}_{n\pm} = \frac{U_{n-1} D_{\mp(n-1)}^2}{U_{n-2} D_{\mp(n-2)}^2}. \tag{28}$$

Then the equation for the energy spectrum is obtained by equating to zero the tridiagonal determinant

$$A_{N-} = B_N^2 \equiv \begin{vmatrix} \tilde{\alpha}_{2-} & 1 & & & \\ \tilde{\beta}_{3-} & \tilde{\alpha}_{3-} & 1 & & \\ & \tilde{\beta}_{4-} & \tilde{\alpha}_{4-} & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & \tilde{\beta}_{N-} & \tilde{\alpha}_{N-} \end{vmatrix} = 0. \tag{29}$$

We will not analyse the asymptotics of these expressions and will concentrate our attention on the other problem with the infinite well.

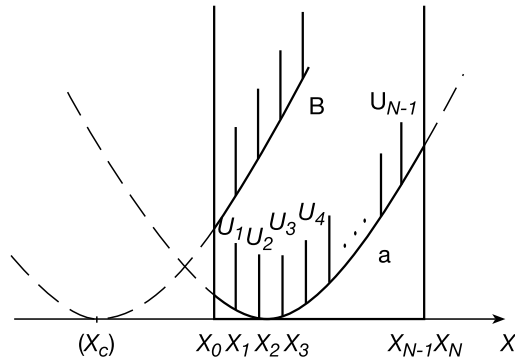


Figure 3. The effective one-dimensional magnetic potential in the infinite rectangular well with the lattice of δ -barriers. The orbit centre (X_c) lies: (a) in the plate volume; (b) outside of the plate.

5. The system of δ -barriers in the infinite rectangular well

Assume that at $x = x_0$ and $x = x_N = x_0 + Nd$ there are infinite potential walls (figure 3) with the null boundary conditions

$$\psi(x_0) = \psi(x_N) = 0. \quad (30)$$

In reality such a model corresponds to the multilayered quantum plate of width $L = Nd$ or to roughly taking into account of the quantum coherence length L related to the electron mean-free path.

From (9) and (30) it follows that the wavefunction in the node n is

$$\psi_n = M(x_n, x_0)_{12} \psi'(x_0) \quad (31)$$

and the spectral equation is

$$M(x_N, x_0)_{12} = 0 \quad (32)$$

i.e. they are determined by the upper-right element of the transfer matrix. We may write out for it the recurrent equation (15) with the coefficients equal to (23) and the expressions through its tridiagonal determinants. However, it is simpler to obtain the results by the direct multiplication of the one-step matrices (22), in fact

$$M(x_n, x_0) = M^{(v)}(x_n, x_{n-1}) \hat{U}_{n-1} M^{(v)}(x_{n-1}, x_{n-2}) \hat{U}_{n-2} \dots M^{(v)}(x_2, x_1) \hat{U}_1 M^{(v)}(x_1, x_0) \hat{U}_0 \hat{U}_0^{-1}. \quad (33)$$

For the subsequent computations it is convenient to include at the end of this expression a unit matrix $\hat{I} = \hat{U}_0 \hat{U}_0^{-1}$ by defining for the first cell some effective transfer matrix \hat{U}_0 for a 'null' δ -barrier. Hence, by elementary induction with the help of (24), (25) we obtain for the matrix element the rigorous finite sum

$$M(x_n, x_0)_{12} = M_{0n} + \sum_{1 \leq i \leq n-1} M_{0i} U_i M_{in} + \sum_{1 \leq j < i \leq n-1} M_{0j} U_j M_{ji} U_i M_{in} + \sum_{1 \leq k < j < i \leq n-1} M_{0k} U_k M_{kj} U_j M_{ji} U_i M_{in} + \dots + M_{01} \prod_{1 \leq i \leq n-1} U_i M_{i+1}. \quad (34)$$

In the right part there are exactly n subsums and in every s th subsum there are exactly C_{n-1}^{s-1} terms. By substitution of (24) for the right-most elements M_{in} in subsums at all i one can see that the integration constants for the wavefunction (8) in the n th cell are given by (34)

with a simple change ($M_{in} \rightarrow -D_{-i}$) at all i for A_n and ($M_{in} \rightarrow D_i$) for A_{-n} and with the common coefficient $\Gamma(-\nu)\psi'(x_0)/\sqrt{2\pi}$ in front.

Hereafter, we assume all δ -barriers to be identical $U_n = U$ and examine the limiting cases of the equation (32) for the spectrum.

5.1. Weak binding and strong magnetic field

In the case $U = l\bar{U}_n \ll 1$ (i.e. $c\hbar\bar{U}_n^2 \ll 2|e|H$) we retain in (34) two leading subsums. In the zero approximation at $U = 0$ we have equation (21) for the spectrum of the uniform plate which is analysed in appendix B (substitution $x_1 \rightarrow x_N$). In the linear approximation over U we get

$$M(x_N, x_0)_{12} = \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \left[(D_0 D_{-N} - D_{-0} D_N) \left(1 + U \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \sum_{i=1}^{N-1} D_i D_{-i} \right) - U \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \left(D_0 D_N \sum_{i=1}^{N-1} D_{-i}^2 + D_{-0} D_{-N} \sum_{i=1}^{N-1} D_i^2 \right) \right] = 0. \tag{35}$$

- (a) If the ‘orbit centre’ lies deeply in the plate volume $X_0 \ll X_c \ll X_N$ (figure 3(a)), then in accordance with (78) $D_{-0} \sim D_N \sim L^\nu \exp(-L^2)$ are small, but $D_0 \sim D_{-N} \sim \Gamma(-\nu)^{-1} L^{-(\nu+1)} \exp(L^2)$ are large. For a not-too-wide multilayered plate we replace the second parentheses by a unit and obtain the equation taking into account corrections to (92) from the lattice

$$D_0 D_{-N} = D_{-0} D_N + U \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \left(D_0 D_N \sum_{i=1}^{N-1} D_{-i}^2 + D_{-0} D_{-N} \sum_{i=1}^{N-1} D_i^2 \right). \tag{36}$$

For a very wide plate $|x_0|, |x_N| \rightarrow \infty$, the coefficient in front of $D_0 D_{-N}$ is the main one, therefore the spectrum equation is

$$\frac{\sqrt{2\pi}}{\Gamma(-\nu)} = -U \sum_{i=1}^{N-1} D_i D_{-i}. \tag{37}$$

Here the dependence on the boundaries disappears. This expression can be readily obtained in the absence of the rectangular well by calculating the determinant (29) in the linear approximation over U .

By the expansion of the left side of (37) near the integer zeros $\nu = n$ of the inverse Γ -function (cf (94)) and by substitution in the right side $\nu = n$, that is $D_i = D_n(x_i)$, we obtain a shift of the Landau levels (93) in the lattice to higher energy.

$$\nu = n + \frac{U}{\sqrt{2\pi} 2^n n!} \sum_{i=1}^{N-1} e^{-\frac{x_i^2}{2}} H_n^2 \left(\frac{x_i}{\sqrt{2}} \right). \tag{38}$$

This result is known from the perturbation theory.

- (b) If the ‘orbit centre’ lies outside of the plate (the ‘skipping orbits’), for example, behind the left boundary (figure 3(b)), then $D_N \sim L^\nu \exp(-L^2)$ is small, $D_{-N} \sim \Gamma(-\nu)^{-1} L^{-(\nu+1)} \exp(L^2)$ is large and $D_0 \sim D_{-0} \sim 1$ are oscillating in accordance with (82), (83) asymptotics or as Airy functions (85). Instead of (96) the following equation is obtained:

$$D_0 = D_{-0} \frac{\frac{D_N}{D_{-N}} + U \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \sum_{i=1}^{N-1} D_i \left(D_i + D_{-i} \frac{D_N}{D_{-N}} \right)}{1 + U \frac{\Gamma(-\nu)}{\sqrt{2\pi}} \sum_{i=1}^{N-1} D_{-i} \left(D_i - D_{-i} \frac{D_N}{D_{-N}} \right)} \equiv f(\nu). \tag{39}$$

For the wide plate and the weak lattice the right part is small. We can find the corrections due to it from perturbation theory by expanding D_0 at the left over $\nu - \nu_0$, where ν_0 is the root of equation $D_0 \equiv D_{\nu_0}(x_0) = 0$ and by substituting $\nu = \nu_0$ in the right part $f(\nu)$

$$\nu = \nu_0 + \left(\frac{\partial D_0}{\partial \nu} \right)_{\nu_0}^{-1} f(\nu_0). \quad (40)$$

In particular, we will obtain the corrections to the theory of Ni and Prange [14] if we take the asymptotics $D_\nu(x)$ in the form of the Airy functions (85).

5.2. The very tight binding

In the case $U = l\bar{U}_n \gg 1$ (i.e. $c\hbar\bar{U}_n^2 \gg 2|e|H$) at the cost of normalization we divide (34) by U^{N-1} and retain the two last subsums. In the limit of $U \rightarrow \infty$ the last term in (34) describes the complete localization in the layers

$$\prod_{0 \leq i \leq N-1} M_{ii+1} = 0. \quad (41)$$

In each i th layer in the zero approximation over U^{-1} the discrete spectrum is given by the equation (21), i.e.

$$M_{ii+1} = D_i D_{-(i+1)} - D_{-i} D_{i+1} = 0 \quad (42)$$

which is analysed in appendix B.

For the wide layers and strong magnetic field ($d \gg 1$) the Landau magnetic localization (93), (95) or (96) becomes apparent. For the narrow layers and weak magnetic field ($d \ll 1$) every discrete level in the layer generates the band of the energy states connected with the magnetic parabolic space variation of the potential energies for the effective well bottom in the layers and is also connected with the smearing caused by the arbitrariness of the 'orbit centre' X_c position in the layer of its localization. Thus, from expression (104) for the i th layer by the replacement $X_0 \rightarrow X_0 + ild$, $X_1 \rightarrow X_0 + (i+1)ld$ we get for $i \gg 1$

$$E_t = E_n + \frac{m\omega_0^2}{2} [ild - (X_c - X_0)]^2 \quad E_n = \frac{\hbar^2}{2m} \left(\frac{\pi n}{L} \right)^2. \quad (43)$$

It is seen from (41) that with the increase of system width $N \rightarrow \infty$ the dependence on X_c becomes periodical with the period ld . At large i the energy density of states in the band with the number n has a singularity of the inverse square root type near the threshold E_n which is typical for the one-dimensional systems

$$\frac{di}{dE_t} = \frac{1}{\sqrt{2m\omega_0}ld} \frac{1}{\sqrt{E_t - E_n}}. \quad (44)$$

The penultimate subsum in (34) describes the penetration of the wavefunction of steady states (42) into the adjacent layers and the shift of their energy levels.

Thus, if layer i is not on the well border ($i \neq 0, N$), then near the root of (42) the perturbed equation is

$$M_{ii+1} = -\frac{1}{U} \left(\frac{D_i}{D_{i+1}} + \frac{D_{i+1}}{D_i} \right) \quad (45)$$

and if the layers are on the well border, then the perturbed equations are

$$M_{01} = -\frac{1}{U} \frac{D_0}{D_1} \quad M_{N-1N} = -\frac{1}{U} \frac{D_N}{D_{N-1}} \quad (46)$$

with ν equal to the root of (42) at the right.

5.3. Very weak magnetic field

Now consider the limiting case corresponding to switching off the magnetic field, when $H \sim \omega_0 \rightarrow 0$, i.e. we have a strong increase of the magnetic length $l \sim 1/\sqrt{H} \rightarrow \infty$ and the parameter $a = -E_t/\hbar\omega_0 \rightarrow -\infty$ in the Weber equation. It means that for electrons moving mainly transverse to the layers (p_y is not anomalously large) we may use the semiclassical asymptotics of the parabolic cylinder functions (82). Then we get for the transfer matrix (10) the following expression:

$$M^{(v)}(x_m, x_n) = \begin{pmatrix} \sqrt{\frac{Y_n}{Y_m}} \cos(\theta_m - \theta_n) & \frac{2}{\sqrt{Y_n Y_m}} \sin(\theta_m - \theta_n) \\ -\frac{\sqrt{Y_n Y_m}}{2} \sin(\theta_m - \theta_n) & \sqrt{\frac{Y_m}{Y_n}} \cos(\theta_m - \theta_n) \end{pmatrix} \quad (47)$$

where

$$Y_n = \sqrt{4|a| - x_n^2} \gg 1 \quad (48)$$

$$\theta_n = \frac{x_n}{4} Y_n + |a| \arcsin \frac{x_n}{2\sqrt{|a|}}.$$

We introduce the dimensionless wavenumber for the motion transverse to the layers

$$k \equiv \tilde{k}l = \sqrt{|a_0|}. \quad (49)$$

The ‘real’ transverse wavenumber \tilde{k} , the energy of transverse motion E_\perp and the effective parameter $|a_0|$ are

$$\tilde{k} = \frac{1}{\hbar} \sqrt{2mE_\perp} \quad E_\perp = E_t - \frac{p_y^2}{2m} \quad |a_0| = \frac{E_\perp}{\hbar\omega_0} = |a| - \frac{\bar{x}_c^2}{4}. \quad (50)$$

Under the assumption that $k \gg 1$ we will expand in k^{-1} the semiclassical phase and pre-exponent

$$\theta_n = k\bar{x}_n - \bar{x}_n - \theta_c \quad \theta_c = k\bar{x}_c + \frac{1}{12}\bar{x}_c^3 \quad Y_n = 2k(1 - \varepsilon_n) \quad (51)$$

where the small expansion parameters are

$$\bar{x}_n = \frac{\bar{x}_n^2(\bar{x}_n - 3\bar{x}_c)}{24k} = \frac{eHX_n^2}{2c\hbar^2\tilde{k}} \left(\frac{eHX_n}{3c} - p_y \right) \ll 1 \quad (52)$$

$$\varepsilon_n = \frac{\bar{x}_n(\bar{x}_n - 2\bar{x}_c)}{8k^2} = \frac{eHX_n}{c(\hbar\tilde{k})^2} \left(\frac{eHX_n}{2c} - p_y \right) \ll 1.$$

We hold terms of the lowest order, so for the magnetic field H we get the linear corrections from the effect of the ‘orbit centre’ $X_c \sim p_y$ and the square corrections from the effect of the ‘node coordinate’ X_n (it is important for the electrons with $X_c \ll X_n$, i.e. $cp_y \ll eHX_n$). In principle, it is not so difficult to hold all quadratic in the magnetic field corrections (of the $p_y^2 H^2$ type and so on [16, 17]), but we do not pursue these objectives. Note, that in semiclassics usually $kd = \tilde{k}ld \gg 1$ and the pre-exponent role is relatively small:

$$1 \gg \bar{x}_n \sim \tilde{k}X_n\varepsilon_n \gg \varepsilon_n. \quad (53)$$

In addition, the condition of the semiclassical approximation (84) itself gives a weak restriction

$$|X_n - X_c| \ll 8\tilde{k}^3 l^4. \quad (54)$$

Since $d = x_n - x_{n-1}$ is the period of the lattice composed from the identical δ -barriers $\hat{U}_n = \hat{U}$, then the matrix (22) of transfer across the cell $n = 1, 2, \dots, N$ taking into account the linear corrections (52) is

$$M(x_n, x_{n-1}) \equiv M^{(v)}(x_n, x_{n-1})\hat{U} = \hat{M} + \hat{\delta}_{n-1} \quad (55)$$

where the transfer matrix across the cell without the magnetic field is

$$\hat{M} = \hat{M}\hat{U} \quad \hat{M} = \begin{pmatrix} \cos kd & \frac{1}{k} \sin kd \\ -k \sin kd & \cos kd \end{pmatrix} \quad \hat{U} = \begin{pmatrix} 1 & 0 \\ U & 1 \end{pmatrix} \quad (56)$$

and a correction to it in the magnetic field is

$$\hat{\delta}_n = \hat{\delta}_n \hat{U} \quad \hat{\delta}_n = (\mathbf{x}_{n+1} - \mathbf{x}_n) \hat{\alpha} + \frac{1}{2} (\varepsilon_{n+1} \hat{\beta}_+ + \varepsilon_n \hat{\beta}_-) \\ \hat{\alpha} = \begin{pmatrix} \sin kd & -\frac{1}{k} \cos kd \\ k \cos kd & \sin kd \end{pmatrix} \quad \hat{\beta}_\pm = \begin{pmatrix} \pm \cos kd & \frac{1}{k} \sin kd \\ k \sin kd & \mp \cos kd \end{pmatrix}. \quad (57)$$

From (33) in the linear in $\hat{\delta}_n$ approximation we get the matrix of transfer across the whole well

$$M(x_N, x_0) = \left(\hat{M}^N + \sum_{n=0}^{N-1} \hat{M}^{N-n-1} \hat{\delta}_n \hat{M}^n \right) \hat{U}^{-1}. \quad (58)$$

For it to be valid the lattice potential should not be too strong $U\mathfrak{x}$, $U\varepsilon \ll k$.

The integer powers of the matrix \hat{M} are expressed by the known Abelés expression [29]

$$\hat{M}^n = U_{n-1}(h) \hat{M} - U_{n-2}(h) \hat{I}. \quad (59)$$

With the help of the second-kind Chebyshev polynomials [24]

$$U_{n-1}(h) = \frac{1}{\sqrt{1-h^2}} \sin n \arccos h \quad (60)$$

one can see from (56) that for our model their argument is the Kronig–Penney function

$$h = \frac{1}{2} Sp \hat{M} = \cos kd + \frac{U}{2k} \sin kd. \quad (61)$$

(a) In the absence of the magnetic field $\hat{\delta}_n = 0$ and in accordance with (32) we obtain the equation for the spectrum of the quasi-one-dimensional lattice in the rectangular infinite well

$$\left(\hat{M}^N \right)_{12} = \frac{1}{k} \sin \tilde{k} l d U_{N-1}(h) = 0. \quad (62)$$

Zeros of sine give zone thresholds $\tilde{k} = \tilde{n}\pi/l d$, $\tilde{n} = 0, \pm 1, \pm 2, \dots$ and the zeros of Chebyshev polynomials are

$$h_{N-1,n} = \cos \frac{n}{N} \pi \quad n = 1, 2, \dots, N-1. \quad (63)$$

They are connected with the characteristic exponents of the multipliers λ (eigenvalues of the matrix of transfer by a period) [18]

$$\det(\hat{M} - \lambda \hat{I}) = 0 \quad \lambda = e^{\pm i K l d} \quad (64)$$

whence follows the dispersion law for the quasi-momentum K

$$\cos K l d = h. \quad (65)$$

Thus the allowed quasi-momentum values

$$K_n = \frac{1}{l d} \arccos h_{N-1,n} = \pm \frac{n}{N} \frac{\pi}{l d} \quad (66)$$

are the discrete points uniformly filling the one-dimensional Brillouin zone of the size $[-\pi/l d, \pi/l d]$.

(b) In the weak magnetic field with the help of (56), (57) and (59) we perform in (58) long but standard calculations of the upper-right element $M(x_N, x_0)_{12}$ and the spectral equation (32) takes the following form

$$\left(\hat{M}^N\right)_{12} = \frac{1}{k} \sin kd U_{N-1}(h) = f(h, H) \tag{67}$$

where a small ($\sim \alpha$ and $\sim \varepsilon$) perturbing function $f(h, H)$ in the right part describes the shift of the roots of equation (62) and destruction of the K -space homogeneity. Aside from H , the function depends on the ‘orbit centre’ location X_c , the energy k and the lattice parameters X_n, U, N, d :

$$f(h, H) = \frac{\alpha_N - \alpha_0}{k} (U_{N-1}(h) \cos kd - U_{N-2}(h)) - \frac{\varepsilon_N + \varepsilon_0}{2k} U_{N-1}(h) \sin kd + \frac{U}{k^2} \sin kd \sum_{n=1}^{N-1} [\alpha_n U_{N-2n-1}(h) - \varepsilon_n U_{N-n-1}(h) U_{n-1}(h) \sin kd]. \tag{68}$$

The shift $\Delta h = h - h_0$ of the roots h_0 of the equation (62) will be obtained by the expansion of the left side (67) in a small shift Δh and by the substituting in the right part $f(h_0, H)$.

The form of the corrections in the magnetic field depends on the location of the left and right sides of the plate because the origin of the coordinates determines a zero of the vector-potential and the form of the Hamiltonian of the input problem (1). The formulae look simpler if we choose the origin on the left surface of the plate, assuming $\bar{x}_0 = 0, \bar{x}_n = nd$ (i.e. $\alpha_0 = \varepsilon_0 = 0$). So, for the roots on the thresholds of zones $\tilde{k}_0 = \tilde{n}\pi/ld$, where $\sin k_0 d = 0$ we have $h_0 = \cos k_0 d = (-1)^{\tilde{n}}, U_{N-1}(1) = N, U_{N-1}(-1) = (-1)^{N-1}N$, from where we get the perturbed values of threshold wavenumbers

$$\tilde{k} = \frac{\tilde{n}\pi}{ld} + \frac{\alpha_N}{Nld} = \frac{\tilde{n}\pi}{ld} + \frac{1}{\tilde{n}} \frac{ld}{2\pi\hbar^2} \frac{eHL}{c} \left(\frac{eHL}{3c} - p_y \right). \tag{69}$$

Out of thresholds, assuming $\sin kd \neq 0$ and denoting $t = \arccos h$ it is convenient to rewrite the equation (67) in the trigonometrical form

$$\sin Nt = \tilde{f}(t, H) \tag{70}$$

where

$$\tilde{f}(t, H) = \frac{\alpha_N - \alpha_0}{\sin kd} (\sin Nt \cos kd - \sin(N-1)t) - \frac{\varepsilon_N + \varepsilon_0}{2} \sin Nt + \frac{U}{k} \sum_{s=1}^{N-1} \left[\alpha_s \sin(N-2s)t - \frac{\varepsilon_s \sin kd}{2 |\sin t|} (\cos(N-2s)t - \cos Nt) \right]. \tag{71}$$

The trigonometrical sums in $\tilde{f}(t, H)$ can be computed, they give the singularity of $\cot t$ type as shown in appendix C. We will perform the computations only near the root $h_0 = h_{N-1,n}$ (example (63)) where $t_n = \pm n\pi/N$, and the left side of (70) in the linear in $\Delta h \ll 1$ order is equal to

$$(-1)^{n+1} \frac{N}{\sin \frac{n}{N}\pi} (h - h_{N-1,n}) \tag{72}$$

and in the right part we may substitute $t = t_n$ and $k = k_n$ where k_n is the solution of the equation (61), i.e. $h(k_n) = h_{N-1,n}$.

If one defines ‘quasi-momentum’ K in accordance with (64), (65) and assumes the right part of (71) to be small $\sim \Delta Kld \ll 1, \Delta K = K - K_n$, then

$$\cos Kld = \cos \frac{n}{N}\pi - \Delta Kld \sin \frac{n}{N}\pi \tag{73}$$

and the allowed values of the ‘quasi-momentum’ are

$$K_n = \pm \left(\frac{n}{N} \frac{\pi}{ld} + \Delta K \right) \quad (74)$$

where $\Delta K = \Delta K(n)$ describes quantitatively the degree of the breakdown of the equality (66), that is the degree of non-homogeneity of the K -space:

$$\begin{aligned} \Delta K(n) = & \frac{\alpha_0 - \alpha_N}{Nld} \frac{\sin \frac{n}{N}\pi}{\sin k_n d} + \frac{U}{Nldk_n} \sum_{s=1}^{N-1} \alpha_s \sin 2\pi \frac{n}{N}s \\ & + \frac{U}{Nldk_n} \frac{\sin k_n d}{\sin \frac{n}{N}\pi} \sum_{s=1}^{N-1} \frac{\varepsilon_s}{2} \left(1 - \cos 2\pi \frac{n}{N}s \right). \end{aligned} \quad (75)$$

We sum up the trigonometrical sums in (75) by using the formulae from the appendix C, because α_s includes the second and the third powers of s and ε_s includes the first and the second powers. If we take the origin of the coordinates on the left boundary of the plate, then in (52) $X_0 = 0$, $X_n = nld$ and, as a final result, we get the sum of contributions from the boundary ΔK_b , from the semiclassical phase ΔK_{α} and pre-exponent ΔK_{ε}

$$\Delta K(n) = \Delta K_b + \Delta K_{\alpha} + \Delta K_{\varepsilon} \quad (76)$$

$$\begin{aligned} \Delta K_b = & \frac{eHL}{2c\hbar^2\tilde{k}_n} \left(p_y - \frac{eHL}{3c} \right) \frac{\sin \frac{n}{N}\pi}{\sin \tilde{k}_n ld} \\ \Delta K_{\alpha} = & \bar{U} \frac{eHL}{4c\hbar^2\tilde{k}_n^2} \left(p_y - \frac{eH}{3c} \left(L - \frac{3l^2d^2}{L \sin^2 \frac{n}{N}\pi} \right) \right) \cot \frac{n}{N}\pi \\ \Delta K_{\varepsilon} = & -\bar{U} \frac{eHL}{4cld\hbar^2\tilde{k}_n^3} \left(p_y - \frac{eH}{3c} \left(L - \frac{l^2d^2}{L} \left(1 + \frac{3}{2} \cot^2 \frac{n}{N}\pi \right) \right) \right) \frac{\sin \tilde{k}_n ld}{\sin \frac{n}{N}\pi}. \end{aligned} \quad (77)$$

The last sum in (75) and the last term in (76) can be neglected if $\alpha_n \gg \varepsilon_n$ (i.e. $kd \gg 1$). We emphasize that the ratio \bar{U}/\tilde{k}_n and hence $\Delta K_{\alpha}/\Delta K_b$ may be not small.

The main result is seen from (77): the value of $\Delta K(n)$ sharply increases at large N when $n \ll N$ or $N - n \ll N$, that is near the Brillouin zone boundaries. This increase is mainly described by the powers of the function $\cot \frac{n}{N}\pi$. With the increase of energy (number of zone) the value ΔK decreases as some powers of $1/k_n$. The dependence of ΔK from the plate width $L = Nld$ is essential while L is small relative to the electron mean-free path. In the opposite case L can be replaced by the order of value by this mean-free path.

The singular addition $\Delta K(n)$, as told, characterizes quantitatively the degree of the quasi-momentum space nonhomogeneity, i.e. the metric tensor of the K_n -space dependence on the coordinates. Also, $\Delta K(n)$ characterizes the width ΔK_{nonh} of the region near the Bragg plane where this nonhomogeneity is most essential, i.e. such K_n where $\Delta K(n) \geq \pi/Nld \equiv \pi/L$. It is an important question in magnetic breakdown and related problems. For example, in the simplest situation, when in (76) the first term in ΔK_{α} is the largest one we get for ΔK_{nonh} the expression

$$\Delta K_{nonh} = \frac{1}{ld} \operatorname{arccot} \frac{4\pi c\hbar^2\tilde{k}_n^2}{\bar{U}eHL^2p_y}.$$

The new analytical type of the revealed singularity, obviously changes the character of the Van Hove singularities [31] in the energy density of states dn/dE_t on the thresholds E_0 of zones. For example, from (65), in the approximation (77) at $1 \gg n/N \gg ld\Delta K(n)$ and $\Delta E \sim n^2$, where $\Delta E = E_t - E_0$, one can see that on the background of usual threshold singularity $(\Delta E)^{-1/2}$ the additions arise of type $\bar{U}H(\Delta E)^{-3/2}$, $\bar{U}H^2(\Delta E)^{-5/2}$ and so on.

6. Conclusions

In conclusion, we discuss the obtained results and mention the obscure questions and the lines of their solutions. The majority of them are as follows.

- (1) We have examined the analytical solutions of the steady-state Schrödinger equation for the model of the multilayered structure with the geometry of (figure 1) in the magnetic field parallel to layers. On the base of the parabolic cylinder functions we gave a transfer matrix formulation of the problem and reduced it to the equivalent difference scheme. The rigorous solutions for the transfer matrix elements, the wavefunctions and the spectral equations were represented in form of the sums, series and tridiagonal determinants of the original structure. Their asymptotics were analysed for a few nontrivial cases.
- (2) Our transfer matrices and wavefunctions provide a means for calculating the electric current and energy flux, the spectrums of reflectance and transmissivity of the multilayered systems in magnetic field.
- (3) It should be noted that the inclusion of electrical field $E_{field} \parallel X$ leads to simple modifications of our rigorous expressions. The additional potential energy $\Delta U = -eE_{field}X$ in (1) induces the following replacements in all results:

$$X_c \rightarrow X_c + \frac{mc^2 E_{field}}{eH^2}$$

$$E_t \rightarrow E_t + \frac{cE_{field}p_y}{H} + \frac{mc^2 E_{field}^2}{2H^2}$$

which take into account the drifting along the y -axis and give the rigorous solutions for the steady states of the ballistic quantum Hall effect situation in the (figure 1) geometrical configuration [32].

- (4) We obtained the rigorous equation (18) for the electronic energy spectrum in the system with arbitrary number of the rectangular potential barriers. For the system of flat δ -barriers the general results were represented in the form of the tridiagonal determinants (a type of (29)) i.e. in the form of the special sums and series (a type of (32), (34)) at the different boundary conditions. The limit of the one-dimensional periodic lattice is easily passed in all formulae. We distinguished the cases of the volume and the surface ('skipping orbits') states.
- (5) The following qualitative conclusions sum up our analytical results.

If one begins the analysis from the behaviour of the free electron in a magnetic field at switching on the disturbing lattice, then it should be noted that the Landau wavefunction has a few typical parameters with the dimension of length with respect to the orbit centre X_c . First, it is the 'magnetic length' $l = (c\hbar/2eH)^{1/2}$ of the exponential increase of the wavefunction amplitude in the parabolic well and of the exponential decrease outside the well. There are no other length-dimensional parameters for the low-energy Landau levels. However, for the high $n \gg 1$ levels $E_n \simeq n\hbar\omega_0$, in the semiclassical situation, there are two other parameters with a strongly different scale: the wavelength $\lambda_M = 2\pi l/\sqrt{n}$ of space oscillations in the middle of the well which, of course, smoothly increases to the well periphery and the classical turning point coordinate $x_t = 2l\sqrt{n}$, so that $\lambda_M \ll l \ll x_t$, and also $n \simeq x_t/\lambda_M$ are in accordance with the oscillation theorem. Alternatively, in the rectangular potential well (layer) of width ld in the N th state with the energy $E_N = \hbar^2 N^2/2ml^2 d^2$ the wavelength is $\lambda_W = ld/N$. It is evident that with the increase of the δ -barrier power \bar{U} the lattice suppresses long wave oscillations on the periphery of the magnetic field parabola where $\lambda_M \gg ld$; as a result the locking effect for the levels with resonance space oscillations rises. In this case that Landau level 'survives',

which satisfies the condition $ld = N\lambda_M$ (i.e. $n = (N/d)^2$). The effect of the ‘orbit centre’ X_c location smears these levels into the bands.

If one begins the analysis from the behaviour of the Bloch electron in the lattice at switching on the disturbing magnetic field than the cotangent singularity of a metric arises near the Bragg planes in the quasi-momentum space, as we have shown in the framework of the considered model, i.e. the destruction of the K -space homogeneity begins from the Brillouin zone boundary. Moreover, because of the noted singularity one should carefully make use of the ordinary semiclassical arrangements of zone analysis of the galvanomagnetic and related phenomena in crystals—the Landau cylinders, the cyclotron mass and so on [8, 9, 30]. The revealed new singularity has to become apparent in such physical phenomena as the magnetic breakdown, the diamagnetic susceptibility and others.

- (6) We have to emphasize that the singularity of the considered type is obviously not specific to the Bloch electrons only in the magnetic field. We can show that this singularity is universal for the arbitrarily extensive semiclassical perturbation, in particular, for the homogeneous electric field it has been done with the help of the Airy functions [32].

That is apparently some general singular natural phenomenon of the phase K -space collapse when the weak extensive disturbance operates in a lattice. We remind ourselves of the other well known diffraction peculiarities in an ideal lattice for the quasi-wave vectors are closed to the Bragg planes: the orthogonality of the isoenergetic surfaces to these planes, the Van Hove singularities and so on.

- (7) In the two-dimensional lattices the effect of zone subdivision at switching on the weak magnetic field is usually described as a fractal process of the formation of a Cantor discontinuum for the energy values [10–12]. The principal dependence on the quantum of the magnetic flux across the unit cell is essential. The account of diffraction on the x - and y -surfaces of the cells lead to a justification [33] of the phenomenological Peierls rule [2] and as a consequence to the one-dimensional along x -axes difference Harper’s equation [6] with the periodic potential which is incommensurate to the lattice potential. In our model the cell (layer) has an infinite area, the diffraction on y -boundaries is absent and the quantum of the magnetic flux across the cell of the infinite size does not reveal itself in the coefficients of the rigorous difference equation (15) as well in the other results. Nevertheless, it is interesting that there is the original analytical singularity of cotangent type in the metric of K -space and connected with the weak magnetic field. The manifestation of this singularity in the two-dimensional lattices and its relation to the fractal density of states for them is still an open question.

It would be interesting to apply a similar analysis to the model with the finite-size rectangular cells which have partially penetrable boundaries parallel to the x - and y -axes. This problem requires numerical calculations since we can not separate variables in the Schrödinger equation even for the simplest Landau gauge and obtain the one-dimensional wave equation of the second order along the y -axes (similar to the x -axes) and thereupon the transfer matrix. Proceeding from the system consisting of a few coupled periodical strips to the limit of the system with the periodic two-dimensional potential $\tilde{U}(X, Y)$ one hopes to observe not only the origin of the Peierls rule in a weak magnetic field [33], but the evolution of the two-dimensional Bloch electron spectrum in the strong magnetic field.

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Appendix A. Asymptotics of the parabolic cylinder functions

The asymptotic expansions for the Weber functions have been well studied and may be found in [22–26]. We present below the most important formulae, retaining only the main terms of the appropriate expansions and considering that ν is not an integer ($a = -\nu - \frac{1}{2}$).

(I) Far out of the parabolic well under the barrier at $|x| \gg |a|$ the decreasing and the increasing solutions are

$$\begin{aligned}
 D_\nu(x) &= |x|^\nu e^{-\frac{x^2}{4}} & x \rightarrow \infty \\
 D_\nu(x) &= \frac{\sqrt{2\pi}}{\Gamma(-\nu)} \frac{1}{|x|^{1+\nu}} e^{\frac{x^2}{4}} & x \rightarrow -\infty
 \end{aligned}
 \tag{78}$$

moreover near the integer values of $\nu \approx n$ at the expense of $1/\Gamma(-\nu) \rightarrow 0$ the increasing at $x \rightarrow -\infty$ part of the solution $D_\nu(x)$ vanishes and asymptotically decreases as the $|x|^n \exp(-x^2/4)$ part. Then

$$D_\nu(-x) = D_\nu(z) \quad z = -x. \tag{79}$$

In differentiation over x , it is obviously sufficient to only take into account the exponent.

(II) Far from the classical turning point $x^2 = 4|a|$ the main terms of the Darwin expansions [26] in the Liouville–Green (or semiclassical WKB) approximation are:

(1) out of the parabolic well under the barrier.

(a) At $a > 0$, i.e. $\tilde{U} > E_t$ and $\tilde{X} = \sqrt{x^2 + 4a} \gg 1$:

$$\begin{aligned}
 D_\nu(\pm x) &= \frac{(2\pi)^{\frac{1}{4}}}{\sqrt{\Gamma(-\nu)}} \frac{1}{\sqrt{\tilde{X}}} e^{\mp\tilde{\Theta}} \\
 D'_\nu(\pm x) &= \mp \frac{(2\pi)^{\frac{1}{4}}}{\sqrt{\Gamma(-\nu)}} \frac{\sqrt{\tilde{X}}}{2} e^{\mp\tilde{\Theta}} \\
 \tilde{\Theta} &= \frac{1}{2} \int_0^x \tilde{X} dx = \frac{x}{4} \tilde{X} + a \operatorname{arsh} \frac{x}{2\sqrt{a}}
 \end{aligned}
 \tag{80}$$

(b) at $a < 0$, i.e. $\tilde{U} < E_t$ and $X = \sqrt{x^2 - 4|a|} \gg 1$

$$\begin{aligned}
 D_\nu(\pm x) &= \frac{\sqrt{\Gamma(1+\nu)}}{(2\pi)^{\frac{1}{4}}} \frac{1}{\sqrt{X}} e^{\mp\tilde{\Theta}} \\
 D'_\nu(\pm x) &= \mp \frac{\sqrt{\Gamma(1+\nu)}}{(2\pi)^{\frac{1}{4}}} \frac{\sqrt{X}}{2} e^{\mp\tilde{\Theta}} \\
 \tilde{\Theta} &= \frac{1}{2} \int_{2\sqrt{|a|}}^x X dx = \frac{x}{4} X + a \operatorname{arch} \frac{x}{2\sqrt{|a|}}
 \end{aligned}
 \tag{81}$$

(2) inside the parabolic well above the barrier at $a < 0$, i.e. $\tilde{U} < E_t$ and $Y = \sqrt{4|a| - x^2} \gg 1$

$$\begin{aligned}
 D_\nu(\pm x) &= \frac{\sqrt{\Gamma(1+\nu)}}{(2\pi)^{\frac{1}{4}}} \frac{2}{\sqrt{Y}} \cos\left(\pm\Theta - \frac{\pi\nu}{2}\right) \\
 D'_\nu(\pm x) &= \mp \frac{\sqrt{\Gamma(1+\nu)}}{(2\pi)^{\frac{1}{4}}} \sqrt{Y} \sin\left(\pm\Theta - \frac{\pi\nu}{2}\right) \\
 \Theta &= \frac{1}{2} \int_0^x Y dx = \frac{x}{4} Y + |a| \arcsin \frac{x}{2\sqrt{|a|}}
 \end{aligned}
 \tag{82}$$

from which at $\nu \approx -a \gg 1$ by using known Γ -function properties it is not so difficult to get a pure oscillatory limit

$$D_\nu(\pm x) = \frac{1}{\sqrt{\pi}} 2^{\frac{\nu}{2}} \Gamma\left(\frac{1+\nu}{2}\right) \cos\left(\pm\sqrt{\nu}x - \frac{\pi\nu}{2}\right). \tag{83}$$

We note that the semiclassical condition [1] requires the relative smallness of the derivative

$$\left| \frac{d\lambda}{dx} \right| \sim \left| \frac{x}{Y^3} \right| \ll 1 \quad (84)$$

where $\lambda \sim Y^{-1}$ is the typical wavelength, whence

$$x^{2/3} \ll 4|a| - x^2.$$

(III) In the region near the classical turning point $x^2 = 4|a|$ where the potential is almost linear, in the Langer approximation at $(-a) = \nu + \frac{1}{2} \gg 1$ the solutions may be expressed in terms of Airy functions $Ai(\tau)$ and $Bi(\tau)$ [24, 25]

$$\begin{aligned} D_\nu(x) &= A(\nu, \tau) Ai(\tau) \\ D_\nu(-x) &= A(\nu, \tau) (\cos \pi a Ai(\tau) + \sin \pi a Bi(\tau)) \end{aligned} \quad (85)$$

where

$$\begin{aligned} A(\nu, \tau) &= 2^{\frac{\nu}{2}} \Gamma\left(\frac{1+\nu}{2}\right) \left(\frac{\tau}{\xi^2 - 1}\right)^{1/4} & \xi &= \frac{x}{2\sqrt{|a|}} \\ \tau &= \begin{cases} -\left[\frac{3}{2}|a| \left(\arccos \xi - \xi\sqrt{1-\xi^2}\right)\right]^{2/3} & \xi \leq 1 \\ \left[\frac{3}{2}|a| \left(\xi\sqrt{\xi^2-1} - \operatorname{arch} \xi\right)\right]^{2/3} & \xi \geq 1 \end{cases} \end{aligned} \quad (86)$$

whence in the immediate vicinity $\Delta x = x - 2\sqrt{|a|}$ of the turning point we have at $|\Delta x| \ll 2\sqrt{|a|}$, that $\tau = |a|^{1/6} \Delta x$ and

$$A(\nu, \tau) = 2^{\frac{\nu}{2}} \Gamma\left(\frac{1+\nu}{2}\right) |a|^{1/6} \quad (87)$$

i.e. the last coefficient is independent of τ .

Appendix B. The spectrum of plate in the parallel magnetic field

Equation (21) gives the spectrum of a plate in the magnetic field

$$M(x_1, x_0)_{12} \equiv M_{01} = \frac{\Gamma(-\nu)}{\sqrt{2\pi}} (D_0 D_{-1} - D_{-0} D_1) = 0. \quad (88)$$

The knowledge of asymptotics of the parabolic cylinder functions $D_i \equiv D_\nu(x_i)$ and $D_{-i} \equiv D_\nu(-x_i)$ permits us to select the limiting cases for the plate of the width $L = (x_1 - x_0)l$.

B.1. The wide plate and the strong magnetic field ($L \gg l$)

(a) If the 'orbit centre' lies deeply in the plate volume $X_0 \ll X_c \ll X_1$ (figure 3(a)), then with the help of (78) and (79) we see that

$$D_{-0} D_1 = |x_0 x_1|^\nu e^{-\frac{x_0^2 + x_1^2}{4}} \quad (89)$$

is exponentially small and

$$D_0 D_{-1} = \left(\frac{\sqrt{2\pi}}{\Gamma(-\nu)}\right)^2 \frac{1}{|x_0 x_1|^{1+\nu}} e^{\frac{x_0^2 + x_1^2}{4}} \quad (90)$$

is exponentially large except for such ν when

$$\frac{\sqrt{2\pi}}{\Gamma(-\nu)} = 0. \quad (91)$$

The spectral equation (88) takes the form

$$\left| \frac{\sqrt{2\pi}}{\Gamma(-\nu)} \right| = |x_0 x_1|^{\nu+\frac{1}{2}} e^{-\frac{x_0^2+x_1^2}{4}}. \tag{92}$$

At $|x_0|, |x_1| \rightarrow \infty$ we have (91), its roots are the integer numbers $\nu = n$ that gives the Landau spectrum $E_t = E_n$

$$E_n = \hbar\omega_0(n + \frac{1}{2}) \quad n = 0, 1, 2, \dots \tag{93}$$

By the expansion of the inverse Γ -function near its n th zero

$$\frac{1}{\Gamma(-\nu)} = (-1)^{n+1} n!(\nu - n) \tag{94}$$

we get from (92) the solutions

$$\nu = n + \frac{1}{\sqrt{2\pi}n!} |x_0 x_1|^{n+\frac{1}{2}} e^{-\frac{x_0^2+x_1^2}{4}} \tag{95}$$

that describe the upward shift of the n th Landau level if one replaces n by ν in (93).

- (b) If the ‘orbit centre’ lies outside the plate (the classical ‘skipping orbits’, figure 3(b)), for example, behind the left boundary x_0 , then taking into account the right boundary influence the spectral equation is

$$D_0 = D_{-0} \frac{D_1}{D_{-1}}. \tag{96}$$

From (78) one can see the exponential smallness of the ratio in the right part

$$g(x_1, \nu) \equiv \frac{D_1}{D_{-1}} = \frac{\Gamma(-\nu)}{\sqrt{2\pi}} |x_1|^{1+2\nu} e^{-\frac{x_1^2}{2}} \ll 1 \tag{97}$$

at $x_1 \rightarrow \infty$ we get the spectral equation for the half-space $D_\nu(x_0) = 0$. By substituting the asymptotics of $D_\nu(x_0)$ and $D_\nu(-x_0)$ across the Airy functions (85) it is not so difficult to reproduce the results of Nee and Prange [14] for the spectrum of the ‘skipping orbits’ near the left boundary

$$Ai(\tau_0) = 0 \tag{98}$$

where $\tau_0 < 0$ and is expressed across x_0 with the help of (86) or (87). From (96) in this case we get the equation which describes the shift of the levels from reflections on the right boundary

$$Ai(\tau_0) = \frac{g(x_1, \nu) \sin \pi a Bi(\tau_0)}{1 + g(x_1, \nu) \cos \pi a} \tag{99}$$

the right part is usually small and may be treated as perturbation.

B.2. The narrow plate and the weak magnetic field ($L \ll l$)

By using the semiclassical asymptotics (82) and the known properties of the Γ -function we reduce (88) to the form

$$M_{01} = \frac{1}{\sqrt{Y_0 Y_1}} \sin(\Theta_1 - \Theta_0) = 0 \tag{100}$$

where $\Theta_{0,1} = \Theta(x_{0,1})$ and $Y_{0,1} = Y(x_{0,1})$, i.e. just to the equation for the spectrum of the standing waves in the plate

$$\begin{aligned} \Theta_1 - \Theta_0 &= n\pi \quad n = 0, 1, 2, \dots \\ \Theta_{0,1} &= |a| \left(\xi_{0,1} \sqrt{1 - \xi_{0,1}^2} + \arcsin \xi_{0,1} \right) \quad \xi_{0,1} = \frac{x_{0,1}}{2\sqrt{|a|}}. \end{aligned} \tag{101}$$

In fact, this spectrum was explicitly examined by Papapetrou [15] and Friedman [16, 17], who considered the magnetic field as weak perturbation.

We only note the dependence of the energy levels on the position of the 'orbit centre' X_c and the plate boundaries $X_{0,1}$. So, at $|a| \gg 1 \gg |x_{0,1}|$ with the expansion in $\xi_{0,1} \ll 1$ we get

$$2|a|(\xi_1 - \xi_0)[1 - \frac{1}{6}(\xi_0^2 + \xi_0\xi_1 + \xi_1^2)] = n\pi \quad (102)$$

whence the law of the quantization for the dimensionless spectral parameter $|a|$ with the corrections of the second order in $|x_{0,1}| \ll 1$ is

$$|a| = \left(\frac{n\pi l}{L}\right)^2 + \frac{1}{12}(x_0^2 + x_0x_1 + x_1^2) \quad (103)$$

or in the real variables

$$E_t = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2 + \frac{m\omega_0^2}{6}(\Delta X_0^2 + \Delta X_0\Delta X_1 + \Delta X_1^2) \quad (104)$$

where $\Delta X_{0,1} = X_{0,1} - X_c$.

Appendix C

For the computation of the trigonometrical sums in (71) and (75) we consider the geometric progression

$$\sum_{k=0}^{m-1} e^{ik\gamma} = \frac{e^{i\gamma m} - 1}{e^{i\gamma} - 1} \quad (105)$$

its singularities are determined by the zeros of the function $\sin \gamma/2$. Let us differentiate (105) over γ successively three times, separate the real and the imaginary parts and substitute $m = N$, $\gamma = 2\pi n/N$, where $n = 1, 2, \dots, N-1$. We obtain the following sums

$$\begin{aligned} \sum_{s=1}^{N-1} \begin{Bmatrix} \sin 2\pi \frac{n}{N}s \\ \cos 2\pi \frac{n}{N}s \end{Bmatrix} &= \begin{Bmatrix} 0 \\ -1 \end{Bmatrix} & \sum_{s=1}^{N-1} s \begin{Bmatrix} \sin 2\pi \frac{n}{N}s \\ \cos 2\pi \frac{n}{N}s \end{Bmatrix} &= -\frac{N}{2} \begin{Bmatrix} \cot \pi \frac{n}{N} \\ 1 \end{Bmatrix} \\ \sum_{s=1}^{N-1} s^2 \begin{Bmatrix} \sin 2\pi \frac{n}{N}s \\ \cos 2\pi \frac{n}{N}s \end{Bmatrix} &= -\frac{N}{2} \begin{Bmatrix} N \cot \pi \frac{n}{N} \\ N-1 - \cot^2 \pi \frac{n}{N} \end{Bmatrix} \\ \sum_{s=1}^{N-1} s^3 \begin{Bmatrix} \sin 2\pi \frac{n}{N}s \\ \cos 2\pi \frac{n}{N}s \end{Bmatrix} &= -\frac{N}{4} \begin{Bmatrix} (2N^2 - 3(1 - \cot^2 \pi \frac{n}{N})) \cot \pi \frac{n}{N} \\ N(2N - 3(1 - \cot^2 \pi \frac{n}{N})) \end{Bmatrix}. \end{aligned} \quad (106)$$

In the right part one can see the singularity of the $\cot \pi n/N$ power type at large N if $n \ll N$ or $n - N \ll N$. We also note the known sums

$$\sum_{s=1}^{N-1} s = \frac{1}{2}N(N-1) \quad \sum_{s=1}^{N-1} s^2 = \frac{1}{2}(N-1)N(2N-1). \quad (107)$$

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