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Quantum mechanics of electrons in periodic potentials and strong magnetic fields

Vladimir M. Gvozdikov

Grenoble High Magnetic Fields Laboratory,
Max-Planck-Institute für Festkörperforschung and CNRS,
25 Avenue des Martyrs, Grenoble 38042, France,
Max-Planck-Institut für Physik komplexer Systeme,
D-01187 Dresden, Germany,
and
Kharkov National University, Kharkov 61077, Ukraine
email: vladimir.m.gvozdikov@univer.kharkov.ua
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Abstract

We present here a review on quantum mechanics of an electron on periodic potential in quantized magnetic field: the so called Landau bands. The problem of the energy spectrum of an electron on a lattice in an external magnetic field, now known as the Azbel-Hofstadter problem, was extensively studied in the 60-th - 70-th. These studies brought forth some mystery because the energy spectrum in the Azbel-Hofstadter problem turned out to be consisting of the Landau bands for rational flux through a unit cell, and becomes fractal for the irrational flux through a unit cell. We descibe here the basic solution and explain how they are used in modern calculations.

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1 Quantum mechanics of an electron in periodic potential and strong magnetic field

Recently a good deal of theoretical activity was devoted to the studies of the role which the periodic potential plays in unusual quantum magnetic oscillations observed in layered organic quasi-two-dimensional (Q2D) conductors [1-4]. These novel materials attract much interest because of the observation in them a whole set of new phenomena as well as due to that their electronic properties to much extend are similar to those of layered high-T_c superconducting cuprates. The de Haas-van Alphen (dHvA) [5-7] and Shubnikov-de Haas (SdH) [8-13] studies of the electron spectrum have shown numerous deviations from the Lifshitz-Kosevich theory[14] which, as is well known, provides a basis for the Fermi surface exploration in conventional 3D metals.

Although the shape of the magnetization pattern and chemical potential behavior considered as a function of the external magnetic field in the layered Q2D organic conductors was a subject of recent theoretical publications [15-20] some points remain unclear since they are in conflict with recent experiments.

While the quantum mechanics of electrons in quantized homogeneous magnetic fields is a subject of many studies [21-27] the periodic potential case is still not fully understood [28-34].

Recent interest in the dynamics of electrons in periodic potentials under strong magnetic fields is triggered by new experimental data in organics. Consider a discrete representation of the Schrödinger equation

$$\sum_m H_{nm}\Psi_m = E\Psi_n. \tag{1}$$

This equation is written in a most general form and relates the quantum amplitudes Ψ_n at different discrete states marked by integer index n. The physical meaning of the state Ψ_n does not fixed in Eq. (1). In particular, we can imagine a chain of sites (atoms) with the Ψ_n being an amplitude of finding an electron on a site n. And off diagonal matrix elements $H_{mn} = \sigma_{nm}$ being the hopping integrals between sites m and n. (See Fig. 1).

The diagonal elements $H_{nn} \equiv \varepsilon_n$ are the energy of an electron at a site n.

Consider the most simple case when all sites are identical ($\varepsilon_n = \varepsilon_0$) and hopping only on the nearest sites are possible (i.e. only hopping integrals $\sigma_{nn+1} = \sigma$ are nonzero). The Schrödinger equation in this case reads

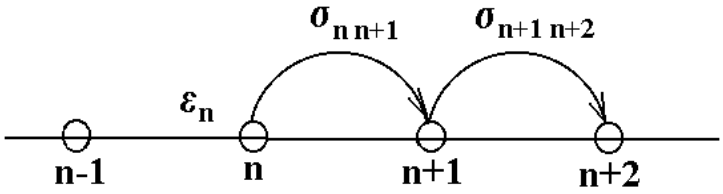

Figure 1: A chain of sites (atoms) with the Ψ_n being an amplitude of finding an electron on a site n. The off diagonal matrix elements $H_{mn} = \sigma_{nm}$ being the hopping integrals between sites m and n.

$$(E - \varepsilon_0)\,\Psi_n - \sigma\,(\Psi_{n+1} + \Psi_{n-1}) = 0. \tag{2}$$

The solution of Eq. (2) can be found in the form

$$\Psi_n = \Psi_0 e^{ikan} \tag{3}$$

where a is the distance between the sites and k is a new quantum number. Substituting Eq. (3) into Eq. (2) we obtain the energy spectrum

$$E\,(k) = E_0 + 2\sigma \cos ka. \tag{4}$$

Since the energy $E\,(k) = E\,(k + 2\pi/a)$ is a periodic function of the wave number k the physically distinguishable states are placed only within the unit cell $-\pi/a \leq k \leq \pi/a$ of the k-space. Because of that k is called the quasi-wave vector.

The DOS for electrons on a chain, therefore, is given by

$$g_1\,(E) = \frac{a}{\pi}\int_{-\pi/a}^{\pi/a} dk\delta\,(E_0 - 2\sigma\cos ka)\,. \tag{5}$$

We put for simplicity $E_0 = 0$ in Eq. (5) and took into account that each site may be occupied by two electrons with the opposite spins. Completing a trivial integration, we finally have

$$g_1\,(E) = \frac{a}{\pi}\frac{1}{\sqrt{(2\sigma)^2 - E^2}}. \tag{6}$$

We see that the energy spectrum of a chain consists of a one band with the $+2\sigma$ and -2σ standing for it's upper and lower bounds. The DOS $g_1(E)$ has a square-root singularities at the bands edges as it is shown in Fig. 2.

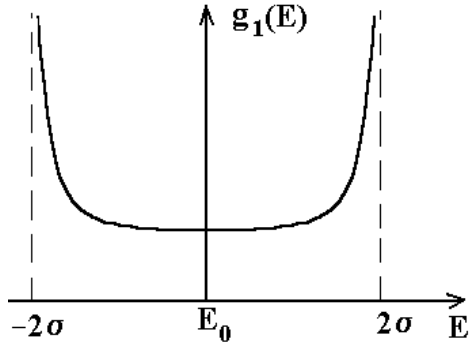

Figure 2: The singularities in the DOS at the energy bands bounds known as a van Hove singularities.

The singularities in the DOS at the energy bands bounds also known as a van Hove singularities. The type of the singularity (i.e. it's dependence on E) as well as the shape of the DOS depend on the dimensionality of the system.

2 Periodic potential

Let the potential $U(z)$ in the Schrödinger equation be a periodic function. In this case the discrete energy levels created by the cylinder potential will be broaden into a dispersive energy bands. The most simple way to see this effect in action is to resort to the simple Kronig-Penny model Writing the Schroedinger equation in the appropriate (for the usage of the transfer matrix formalism) form, we have

$$\frac{d^2\Psi_\varepsilon(z)}{dz^2} + K_{nm}^2(z)\Psi_\varepsilon(z) = 0 \tag{7}$$

with

$$K_{nm}^2(z) = \frac{2\mu}{\hbar^2}\left[\varepsilon - U_{eff}^{nm}(z)\right] \tag{8}$$

where the effective potential is given by the the periodic Kronig-Penny potential. We arrive at the dispersion equation with

$$\frac{1}{2}\mathrm{Sp}\hat{T}(E) = \cos Ka \cos \kappa_{nm} b - \frac{\kappa_{nm}^2 + K^2}{2\kappa_{nm} K} \sin Ka \sin \kappa_{nm} b \tag{9}$$

where the following notations have been introduced

$$K^2 = \frac{2\mu\varepsilon}{\hbar^2}, \tag{10}$$

$$\kappa_{nm}^2 = \frac{2\mu}{\hbar^2}\left[\varepsilon - U_0 G_{nm}\left(\frac{\Phi}{\Phi_0}\right)^{|m|+1}\right], \tag{11}$$

$$G_{nm} = \frac{(n_\rho + |m|)!}{(|m|+1)! n_\rho!}. \tag{12}$$

The interesting point is that a position of the bound state relative to the appropriate Landau level E_n depends on the sign of the potential $U(z)$.

3 The transfer-matrix approach

Consider a chain of atoms with identical hopping integrals $\sigma_{nn+1} = \sigma$ and arbitrary site energies ε_n. The Schrödinger equation in this case reads

$$(E - \varepsilon_n)\,\Psi_n - \sigma\Psi_{n+1} - \sigma\Psi_{n-1} = 0. \tag{13}$$

This equation can be rewritten in the matrix form

$$\begin{pmatrix} \Psi_n \\ \Psi_{n+1} \end{pmatrix} = \hat{T}\,(n) \begin{pmatrix} \Psi_{n-1} \\ \Psi_n \end{pmatrix}, \tag{14}$$

where a transfer-matrix has been introduced

$$\hat{T}\,(n) = \begin{pmatrix} 0 & 1 \\ -1 & \frac{E-\varepsilon_n}{\sigma} \end{pmatrix}. \tag{15}$$

When $\hat{T}$ is applied to a spinor it shifts the site index by unity, i.e. $n \to n+1$. In case when a period contains N sites, the transfer-matrix is simply a product of N matrices

$$\hat{T} = \hat{T}\,(N)\,\hat{T}\,(N-1)\,...\hat{T}\,(1)\,. \tag{16}$$

One can see from Eq. (13) that $\det \hat{T}(n) = 1$. Since the multiplicative property of the determinates: $\det\left(\hat{A}\hat{B}\right) = \det \hat{A} \det \hat{B}$ the $\det\hat{T} = 1$ too.

The transfer-matrix approach is an effective mathematical tool both for periodic and random or quasi-random chains, but we will discuss here only periodic chains. For periodic systems with the spatial period L we can write a solution of the matrix equation

$$\bar{\Psi}_{n+1} = \hat{T}\bar{\Psi}_n \tag{17}$$

in the form

$$\bar{\Psi}_n = \bar{\Psi}_0 e^{ikan}. \tag{18}$$

Since $\bar{\Psi}_0$ is a two component spinor with nonzero elements the Eqs. (17) and (18) require the following condition should be meet

$$\det\left(\hat{T} - \hat{I}e^{ika}\right) = 0, \tag{19}$$

where $\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is a unit matrix.

In explicit form this equation yields

$$\left(T_{11} - e^{ika}\right)\left(T_{22} - e^{ika}\right) - T_{12}T_{21} = 0. \tag{20}$$

Using the fact that $\det T = T_{11}T_{22} - T_{12}T_{21} = 1$, we finally obtain

$$\cos kL = \frac{1}{2}\mathrm{Sp}\hat{T}(E). \tag{21}$$

This equation determines the energy spectrum of the periodic system in the transfer-matrix approach.

In particular case of a chain with one site per unit cell the transfer-matrix is given by Eq. (15) with $\varepsilon_n = E_0$ so that

$$\mathrm{Sp}\hat{T} = \frac{E - E_0}{\sigma} \tag{22}$$

and we arrive at the dispersion relation

$$E(k) = E_0 + 2\sigma \cos kL, \tag{23}$$

which is exactly what we have found before (see Eq. (4)). Consider now a more complex example of a chain with two alternating energies on sites,

$\varepsilon_1 = 0$, $\varepsilon_2 = \varepsilon$, correspondingly. The transfer-matrix then is given by a product of two matrices

$$\hat{T}(E) = \begin{pmatrix} 0 & 1 \\ -1 & \frac{E}{\sigma} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & \frac{E-\varepsilon}{\sigma} \end{pmatrix}. \tag{24}$$

The dispersion equation (21) now reads

$$\cos kL = \frac{E(E-\varepsilon)}{2\sigma^2} - 1. \tag{25}$$

The solution of the quadratic equation (25) yields two energy bands

$$E_{\pm}(k) = \frac{\varepsilon \pm \sqrt{\varepsilon^2 + \left(4\sigma \cos \frac{kL}{2}\right)^2}}{2}. \tag{26}$$

The bands boundaries are given by

$$E_+^{\max} = \frac{1}{2}\left[\varepsilon + \sqrt{\varepsilon^2 + (4\sigma)^2}\right], \quad E_+^{\min} = \varepsilon, \tag{27}$$

$$E_-^{\max} = 0, \qquad E_-^{\min} = \frac{1}{2}\left[\varepsilon - \sqrt{\varepsilon^2 + (4\sigma)^2}\right]. \tag{28}$$

The DOS in the transfer-matrix formalism is very easy to calculate, using the evident relation

$$g(E) = \frac{L}{2\pi}\left|\frac{dk}{dE}\right|. \tag{29}$$

Combining this equation with the dispersion relation of Eq. (21), we have

$$g(E) = \frac{L}{2\pi}\left|\frac{df(E)}{dE}\right| \left(1 - f^2(E)\right)^{-1/2}, \tag{30}$$

where $f(E) = \frac{1}{2}\mathrm{Sp}\hat{T}(E)$.

Elementary algebraic manipulation with respect of Eq. (20) then yield

$$g(E) = \frac{L}{2\pi} \frac{|(E-\varepsilon) + E|}{\sqrt{E(E-\varepsilon)\left[(4\sigma)^2 - E(E-\varepsilon)\right]}}. \tag{31}$$

The dependence of the DOS $g(E)$ is shown on Fig. 3.

The energy spectrum consists of two continuous bands $E_-^{\min} \div E_-^{\max}$ and $E_+^{\min} \div E_+^{\max}$ with the gap ε between them. The DOS $g(E)$ has a square-root van Hove singularities at the bands edges. Putting $\varepsilon = 0$, $L = a$ in Eq. (32)

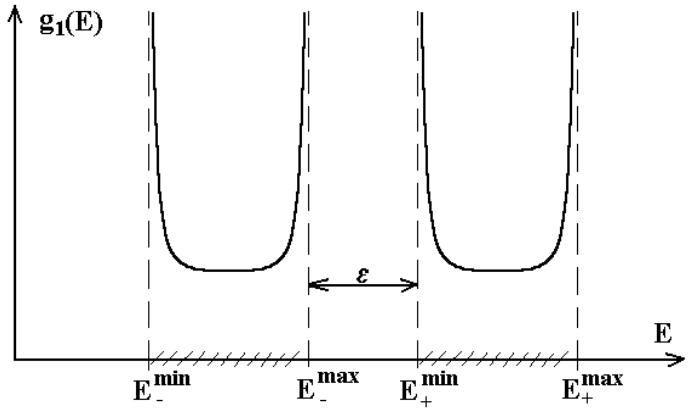

Figure 3: The energy spectrum consists of two continuous bands $E_{-}^{\min} \div E_{-}^{\max}$ and $E_{+}^{\min} \div E_{+}^{\max}$ with the gap ε between them.

we arrive at the DOS of a chain with a one site per unit cell $g_1(E)$ given by Eq. (6).

Note that the transfer-matrix method, in particular, the dispersion equation (20) as well as the DOS of Eq. (30), are general relations valid for any periodic one-dimensional system with an arbitrary transfer-matrix $\hat{T}(E)$. Therefore, the problem of the energy spectrum calculations in any periodic quantum system reduces to finding the transfer-matrix $\hat{T}(E)$.

In a broad sense of the word "site" may be either atom, or chain of atoms, or closed Landau orbit for electron in a magnetic field.

We will illustrate this point in the next section by calculations of the DOS in a two-dimensional lattice.

4 The DOS of electron on a two-dimensional lattice

Consider a two-dimensional lattice shown in Fig. 4. A unit cell is a rightangular four-corner with the sides a and b. The hopping integrals in X and Y directions respectly are σ_1 and σ_2. Since the motion of an electron along the X and Y axes is independent the energy spectrum of electron on a 2D lattice is simply a sum of the two dispersion relations given by Eq. (4)

$$E(k_x k_y) = E_0 + 2\sigma_1 \cos k_x a + 2\sigma_2 \cos k_y a. \tag{32}$$

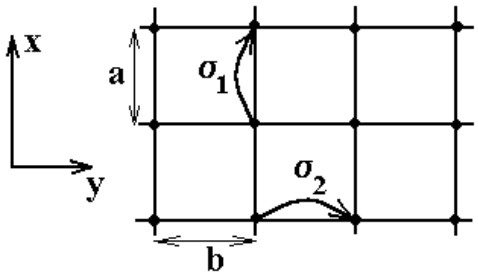

Figure 4: A two-dimensional lattice with a unit cell a rightangular four-corner with the sides a and b. The hopping integrals in X and Y directions respectly are σ_1 and σ_2.

This energy spectrum satisfies the conditions necessary for the convolution rule discussed before. Therefore, the DOS of a 2D lattice is a convolution of two 1D DOS's, given by Eq. (6):

$$g_2(E) = \frac{ab}{\pi^2} \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{(2\sigma_1)^2 - \omega^2}\sqrt{(2\sigma_2)^2 - (E-\omega)^2}}. \tag{33}$$

performing integration, we find:

$$g_2(E) = \frac{2ab}{\pi^2} \begin{cases} \left(\Omega^2 - E^2\right)^{1/2} K\left[W(E)\right], & |E| \le 2\delta \\ \frac{1}{\sqrt{\sigma_1\sigma_2}} K\left[\frac{1}{W(E)}\right], & 2\delta \le |E| \le 2\Omega \\ 0, & |E| > 2\Omega \end{cases}, \tag{34}$$

where $K(W)$ stands for the complete elliptic integral of the first kind and

$$\Omega = 2(\sigma_1 + \sigma_2), \delta = 2|\sigma_1 - \sigma_2|, W(E) = \frac{4\sqrt{\sigma_1\sigma_2}}{\sqrt{\Omega^2 - E^2}}. \tag{35}$$

The DOS $g_2(E)$ is shown schematically in Fig. 5.

The DOS has two logarithmic van Hove singularities at $E = \pm 2\delta$. Nearby these points the $g_2(E) \sim \ln|E \pm 2\delta|$. In the case of a square-lattice $\sigma_1 = \sigma_2 = \sigma$, $\delta = 0$ and these two singularities merge, so that the DOS becomes a more simple analytically

$$g_2(E) = \frac{2a^2}{\pi^2\sigma} K\left[\left\{1 - \left(\frac{E}{4\sigma}\right)^2\right\}^{1/2}\right]. \tag{36}$$

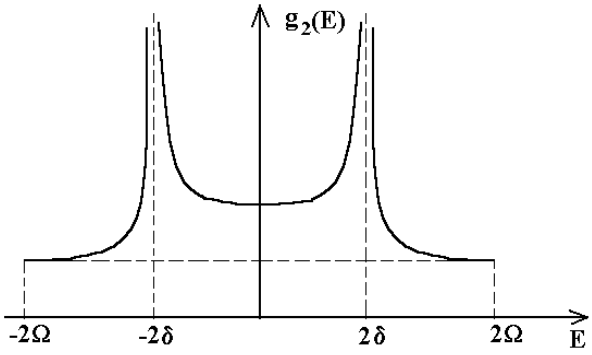

Figure 5: The DOS has two logarithmic van Hove singularities at $E = \pm 2\delta$. Nearby these points the $g_2(E) \sim \ln|E \pm 2\delta|$.

A schematic graph for the $g_2(E)$ in this case is shown in Fig. 6.

The logarithmic singularity now is exactly at the middle of the band whose width is twice as larger than in the 1D case. The asymptotes of the function $g_2(E)$ in the limit $E \to \pm 2\sigma$ and $E \to \pm 2\Omega$ flat and almost energy independent in both cases shown in 6. The origin of this is clear: near the band edges where the dispersion $E(\mathbf{p})$ has an extremum it can be approximated by the quadratic therm $E(\mathbf{p}) \approx E(0) + \mathbf{p}^2/2m$.

On the other hand, as we have already shown the DOS in two-dimensions with the parabolic dispersion is a constant.

We can go further and apply a convolution rule to a tree-dimensional crystal to obtain the DOS $g_3(E)$ in this case

$$g_3(E) = \int_{-\infty}^{\infty} g_2(E-\omega)\, g_1(\omega)\, d\omega. \tag{37}$$

A three-dimensional crystal can be considered as a "chain" each site of which is a plane 2D crystal. Unfortunately, the analytic expression for the $g_3(E)$ can be obtained only near the band edges, where $g_2(E) \approx N(0) = const$.

Counting E from the band edge, we can write the DOS of a 2D lattice near the band edge in the form

$$g_2(E) = N(0)\,\theta(E). \tag{38}$$

Substituting then this equation into the convolution rule (37), we have

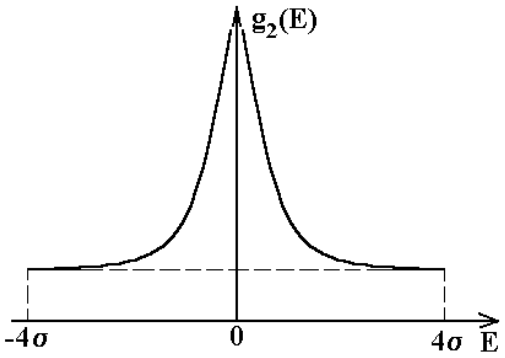

Figure 6: The logarithmic singularity now is exactly at the middle of the band whose width is twice as larger than in the 1D case.

$$g_3(E) = N(0) \int_0^{2\sigma+E} \frac{\theta(\varepsilon)\, d\varepsilon}{\sqrt{(2\sigma)^2 - (\varepsilon - E)^2}}. \tag{39}$$

After the elementary integration, we obtain

$$g_3(E) = \begin{array}{ll} \frac{N(0)}{2\pi}\left(\pi + 2\arcsin\left(\frac{E}{2\sigma}\right)\right), & -2\sigma \le E \le 2\sigma \\ N(0), & E > 2\sigma \end{array}. \tag{40}$$

Therefore, near the band edges the 3D DOS $g_3(E)$ behaves like it is shown schematically in Fig. 7.

5 A transfer-matrix in the quasi-classical approach

In this section we shall consider a charged particle motion in an external magnetic field and in the field of periodic potential. The most adequate method to treat this problem is the transfer-matrix approach. We start with the transfer-matrix method The stationary Schrödinger equation for a particle in an external one-dimensional potential $U(x)$ can be written in a rather simple form

$$\frac{d^2\Psi}{dx^2} + k^2(x)\,\Psi = 0, \tag{41}$$

where $k(x) = p(x)/\hbar$ and

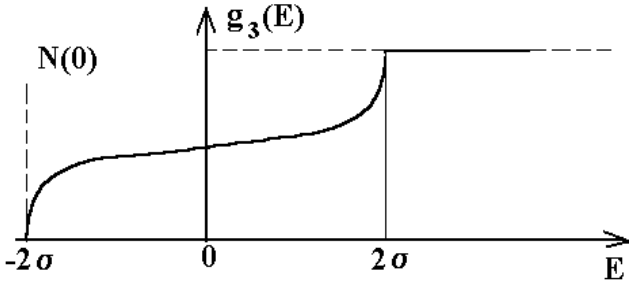

Figure 7: The derivative $dg_3(E)/dE$ diverges at the points $\pm 2\sigma$ which is typical for the van Hove singularities in a three-dimensional crystals.

$$p(x) = \sqrt{2m(E - U(x))} \tag{42}$$

is the classical momentum of a particle. In as much as there are no general solution to the second order differential equation, the exact solutions are known only for a few specific potentials $U(x)$. For example, if $U(x) = U_0 = const$ the solution is a trivial plane wave

$$\Psi(x) = Ae^{\pm ikx} \tag{43}$$

with $k = \frac{1}{\hbar}\sqrt{2m(E - U_0)}$ for $E > U_0$, and an exponent

$$\Psi(x) = Ae^{\pm |k| x} \tag{44}$$

for $E < U_0$.

But if $U(x)$ vary slowly in the space, under the condition that

$$\hbar \left| \frac{dp}{dx} \right| \ll p^2, \tag{45}$$

the solution can be found for an arbitrary shape of the potential energy $U(x)$ in the form of a modulated plane wave

$$\Psi(x) = \frac{C}{\sqrt{p(x)}} e^{\pm \frac{i}{\hbar} \int p(x) dx}, \qquad \text{for } E > U(x) \tag{46}$$

and

$$\Psi(x) = \frac{C}{\sqrt{p(x)}} e^{\pm \frac{1}{\hbar} \int |p(x)| dx}, \qquad \text{for } E < U(x). \tag{47}$$

This is the so called quasi-classical solution which one can find in every textbook on quantum mechanics.

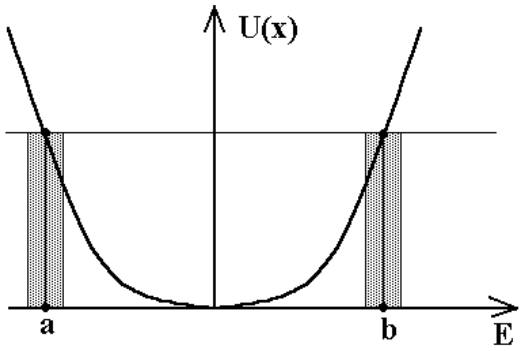

Figure 8: A classical motion of a particle in the potential wel. These quasi-classical solutions are invalid at some stripes near the turning points (dashed lines).

One can see in Fig. 8, which illustrates a classical motion of a particle in the potential well, that quasiclassical solutions are invalid with some stripes near the turning points (dashed in Fig. 8).

In the textbooks it is shown that the quasi-classical wave function of the energy E on both sides of the turning point (let it be a) can be written in the form

$$\Psi(x) = \begin{array}{ll} \frac{C}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int_x^a |p|\,dx\right), & x < a \\ \frac{2C}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_a^x p dx - \frac{\pi}{4}\right), & x > a \end{array} \tag{48}$$

and

$$\Psi(x) = \begin{array}{ll} \frac{B}{\sqrt{|p|}} \exp\left(\frac{1}{\hbar}\int_x^a |p|\,dx\right), & x < a \\ \frac{B}{\sqrt{p}} \cos\left(\frac{1}{\hbar}\int_a^x p dx + \frac{\pi}{4}\right), & x > a \end{array} . \tag{49}$$

Note that coefficients as well as the signs before the phase shift $\pi/4$ in Eqs. (48) and (49) differs.

A trivial consequence of these matching rules is the Bohr-Sommerfeld quantization rule. We can write the wave function within the interval $a < x < b$ by two ways: starting from the exponentially decaying $\Psi(x)$ at $x < a$ and $x > b$ and then applying to them the matching rule equation (48) to transit inside the interval $a < x < b$. Completing this, we have

$$\frac{2C}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_a^x pdx-\frac{\pi}{4}\right)=\frac{2C'}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_x^b pdx-\frac{\pi}{4}\right). \tag{50}$$

The equality (50) is possible only under the two following conditions

$$C'=(-1)^n C \tag{51}$$

and

$$2\int_a^b pdx=2\pi\hbar\left(n+\frac{1}{2}\right). \tag{52}$$

The latter is the famous Bohr-Sommerfeld quantization rule, which yields an energy of a particle in a potential well $U(x)$ as a function of the quantum number n. We can generalize the Bohr-Sommerfeld quantization rule to the case of a particle in a periodic potential. It will be done in the next section.

6 The quasi-classical transfer-matrix in the Landau problem

Consider a particle in the periodic quasi-classical potential shown in Fig.9.

If the potential wells were separated by the impenetrable barriers the energy spectrum was given by the Bohr-Sommerfeld quantization rule of Eq. (52). Each of the energy levels in this case was infinitely degenerated since all the wells in our periodic system are assumed to be of the same shape. But because of the finite transparency of the barriers which separate the wells this degeneracy would be lifted up yielding an energy bands of finite width instead of the sharp levels. Let us see how does it comes within the transfer-matrix approach to the quasi-classical solution of the Schrödinger equation.

A quasi-classical wave function in the region of the n-th potential barrier $b_n<x<a_{n+1}$ can be written in the form

$$\Psi_n=\frac{C_n}{\sqrt{|p|}}\exp\left(-\frac{1}{\hbar}\int_{b_n}^x|p|\,dx\right)+\frac{D_n}{\sqrt{|p|}}\exp\left(\frac{1}{\hbar}\int_{b_n}^x|p|\,dx\right). \tag{53}$$

To transfer from the turning point b_n to a_{n+1} we have to rearrange integrals in Eq. (53) in the following fashion

$$-\frac{1}{\hbar}\int_{b_n}^x|p|\,dx=-\frac{1}{\hbar}\int_{b_n}^{a_{n+1}}|p|\,dx+\frac{1}{\hbar}\int_x^{a_{n+1}}|p|\,dx, \tag{54}$$

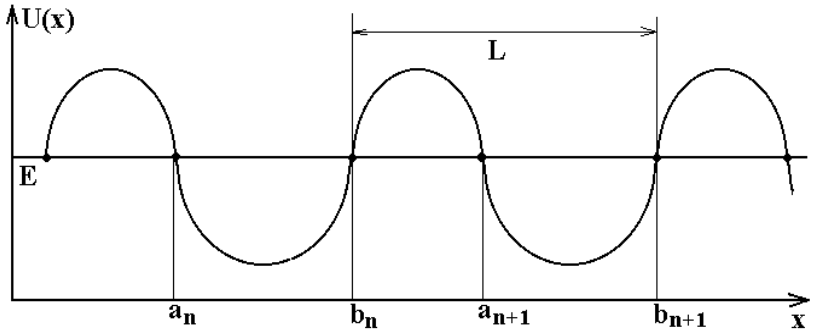

Figure 9: A particle in the periodic quasi-classical potential.

which yields

$$\Psi_n = \frac{C_n}{\sqrt{|p|}} \exp(-\tau) \exp\left(\frac{1}{\hbar}\int_x^{a_{n+1}} |p|\, dx\right) + \frac{D_n}{\sqrt{|p|}} \exp(\tau) \exp\left(-\frac{1}{\hbar}\int_x^{a_{n+1}} |p|\, dx\right), \quad (55)$$

where we introduce the following notation:

$$\tau = \frac{1}{\hbar}\int_{b_{n-1}}^{a_n} |p|\, dx = ... = \frac{1}{\hbar}\int_{b_{k-1}}^{a_k} = ... \quad (56)$$

In fact, τ does not depend on n because all the wells and barriers are identical.

Now we can apply the matching rules of Eqs. (48) and (49) and write the oscillatory wave function within the potential well $a_n \le x \le b_{n+1}$ and then again transfer from a_{n+1} to the turning point b_{n+1} and use the matching rules.

As a result, we have $\left(\int_{a_{n+1}}^{x} \to \int_{a_{n+1}}^{b_{n+1}} - \int_{b_{n+1}}^{x}\right)$

$$\Psi_n = \frac{C_{n+1}}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int_{b_{n+1}}^{x} |p|\, dx\right) + \frac{D_{n+1}}{\sqrt{|p|}} \exp\left(\frac{1}{\hbar}\int_{b_{n+1}}^{x} |p|\, dx\right), \quad (57)$$

where we have introduced the following notations:

$$C_{n+1} = \frac{1}{2} C_n e^{-\tau} \cos\sigma + D_n e^{\tau} \sin\sigma, \tag{58}$$

$$D_{n+1} = -C_n e^{-\tau} \sin\sigma + 2 D_n e^{\tau} \cos\sigma \tag{59}$$

with σ standing for

$$\sigma = \frac{1}{\hbar} \int_{a_{n+1}}^{b_{n+1}} p dx = ... = \frac{1}{\hbar} \int_{a_{k+1}}^{b_{k+1}} |p| \, dx. \tag{60}$$

Equations (58) and (59) can be written in a transfer-matrix form

$$\begin{pmatrix} C_{n+1} \\ D_{n+1} \end{pmatrix} = \hat{T} \begin{pmatrix} C_n \\ D_n \end{pmatrix} \tag{61}$$

with the transfer-matrix defined by

$$\hat{T} = \begin{pmatrix} \frac{1}{2} e^{-\tau} \cos\sigma & e^{\tau} \sin\sigma \\ -e^{\tau} \sin\sigma & 2 e^{\tau} \cos\sigma \end{pmatrix} \tag{62}$$

it is straightforward to check that $\det \hat{T} = 1$. The dispersion equation then is given by the Eq. (20) which yields

$$W \cos qL = \cos\sigma. \tag{63}$$

Here the quantity W^2 is the quasiclassical tunneling probability through the barrier separating adjacent potential wells in Fig. 9, and L is the spatial period of the system in question

$$W = \left(e^{\tau} + \frac{1}{4} e^{-\tau} \right)^{-1}. \tag{64}$$

since in the quasi-classical approximation it is assumed that $\tau \gg 1$, one can write W in a more compact form

$$W \approx e^{-\tau} = e^{-\frac{1}{\hbar} \int_{b_n}^{a_{n+1}} \sqrt{2m|E-U(x)|} dx}. \tag{65}$$

If potential barriers are unpenetrable and $W(E) = 0$, then the dispersion equation (63) yields $\cos\sigma = 0$, i.e.

$$\sigma = \frac{1}{\hbar} \int_{b_{n-1}}^{a_n} p dx = \pi \left(n + \frac{1}{2} \right), \tag{66}$$

which is the Bohr-Sommerfeld quantization rule given by Eq. (52). In this case all the potential wells in a periodic potential are independent, and

the energy spectrum determined by the quantization rule (66) is infinitely degenerated. In the case $W(E) \neq 0$ a particle can walk along the whole chain, the degeneracy is lifted up, and the energy levels broad into the dispersive bands $E(q) = E\left(q + \frac{2\pi}{L}\right)$ which are solutions of the dispersion equation:

$$\frac{1}{\hbar}\int_a^b p dx = \pi\left(n + \frac{1}{2}\right) + (-1)^n \arcsin\left(W \cos qL\right). \tag{67}$$

For small $W \ll 1$ we can find the dispersion relation within the bands as follows. First, put the energy in the form $E_n^{(q)} = E_n^{(0)} + \Delta E(q)$, where $E_n^{(0)}$ is the energy level in a well if it was isolated from the others. This energy level can be found from the Bohr-Sommerfeld quantization rule

$$\frac{1}{\hbar}\int_a^b p\left(E_n^{(0)}\right) dx = \pi\left(n + \frac{1}{2}\right). \tag{68}$$

Next, using the relations

$$2\int_a^b p\left(E_n^{(0)} + \Delta E\right) dx \approx \oint p\left(E_n^{(0)}\right) dx + \Delta E \frac{2\pi}{\omega(E)} \tag{69}$$

we find from Eq. (67)

$$\Delta E(q) = \frac{(-1)^n}{\pi}\hbar\omega(E)\arcsin\left(W\cos qL\right). \tag{70}$$

Here $\omega(E) = 2\pi/T(E)$ is the classical frequency the particle oscillation in the potential well $U(x)$ at the energy E

$$T(E) = \oint\left(\frac{\partial p}{\partial E}\right) dx = \oint \frac{dx}{v(x)} = \frac{2\pi}{\omega(E)}. \tag{71}$$

We see that because of the finite tunneling probability between the wells the energy levels $E_n^{(0)}$ are broaden into the dispersive bands

$$E_n(q) = E_n^{(0)} + \frac{(-1)^n \hbar\omega}{\pi}\arcsin\left(W\cos qL\right). \tag{72}$$

The width of these bands is

$$\delta E = \frac{2\hbar\omega}{\pi}\arcsin W. \tag{73}$$

7 The Landau band in periodic systems

The Landau levels are strongly degenerated on the orbit center position $x_0 = -cp_y/eB$ with the degeneracy factor $g(B) = \Phi/\Phi_0$, as we have shown above. Any spatial inhomogeneity within the plane perpendicular to the magnetic field lifts up this degeneracy making energy levels to be the functions of the quantum number p_y. Thus, the energy levels split up into a series of sub levels of smaller degeneracy. One example of this has been considered above in the previous section, where the degeneracy of the Landau levels have been lifted by the external electric field and both the energy and the wave function became dependent on the complete set of quantum numbers n, p_z and p_y. But periodic external fields are more effective in this sense as well as they are broaden the Landau levels into the dispersive Landau bands. The Landau bands is a very important concept for many problems in the physics of solids and it is the aim of this section to give a concise introduction into this subject.

We will show that periodic perturbations of different nature broaden the Landau levels into the bands. We will discard the p_z degree of freedom since it is irrelevant to the point in question and consider the problem in two dimensions. We begin with the most simple case of the periodic one dimensional potential within the plane and show that the energy $E_n(p_y)$, becomes a periodic function of the momentum p_y with the period $2\pi/a$, where a is the period of the perturbation:

$$E_n(p_y) = E_n\left(p_y + \frac{2\pi}{a}\right). \tag{74}$$

Equation (74), in fact, means that instead of the Landau levels we have a set of dispersive Landau bands. It is self-evident that the dispersion law within these bands depends on the specific form and the nature of the potential but the periodicity of the function $E_n(p_y)$ as we will see is a general property of the Landau bands.

In this section we will consider Landau bands caused by a one dimensional periodicity of the scalar potential and external magnetic field as well as the periodic magnetic breakdown structures, leaving the two-dimensional periodicity to the next section because the energy spectrum in this problem is a fractal in the most general case of irrational flux through a unit cell.

7.1 The perturbative approach

Consider first a one-dimensional periodic potential of the shape $\hat{V}(x) = V_0 \cos(2\pi x/a)$ acting within the plane in addition to the external quantizing magnetic field. The unperturbed values of the energy levels and corresponding eigenfunctions are equal to

$$E_n^{(o)} = \hbar\Omega(n + \frac{1}{2}), \tag{75}$$

$$\Psi^{(0)}_{n,p_y}(x,y) = \varphi_n(x - x_0)\,(L_y)^{-1/2} \exp(ik_y y). \tag{76}$$

Here $\varphi_n(x)$ is the oscillator basis set of functions, $k_y = 2\pi n_y/L_y$ ($n_y = 0, 1, 2..$), and L_y is the size of a specimen the y-direction. Let us assume that the periodic potential is weak to be treated perturbatively. To apply a theory of perturbations we have to calculate first the matrix elements of the potential and then write the secular equation for the first correction to the Landau levels which are degenerated with respect to the quantum number p_y, i.e. on the orbit center position $x_0 = -cp_y/eB$ ($p_y = \hbar k_y$). Calculating the matrix elements we see the they are diagonal in quantum numbers p_y.

$$V_{np_y,np'_y} = \left(\Psi^{(0)}_{np_y}, \hat{V}\Psi^{(0)}_{np'_y}\right) = \left(\varphi_n, \hat{V}\varphi_n\right)\delta_{p_y,p'_y} \tag{77}$$

Because of the diagonality of the matrix element (77) the first correction to the Landau energies $E_n^{(0)}$ caused by $\hat{V}(x)$ is given by

$$E^{(1)}_{n,p_y} = \left(\Psi^{(0)}_{np_y}, \hat{V}\Psi^{(0)}_{np_y}\right) = \frac{V_0}{L_H}\int_{-\infty}^{\infty} dx \mid \varphi_n(x - x_0) \mid^2 \cos\left(\frac{2\pi x}{a}\right). \tag{78}$$

Completing the integration with the help of the formula

$$\int_{-\infty}^{\infty} dq H_n^2(q) e^{-q^2} \cos(Aq) = 2^n n!\sqrt{\pi} e^{-\left(\frac{A}{2}\right)^2} L_n\left(\frac{A^2}{2}\right) \tag{79}$$

we finally have

$$E_n(p_y) = \hbar\Omega\left(n + \frac{1}{2}\right) + V_0 \exp\left(-\frac{Q}{2}\right) L_n(Q) \cos\left(\frac{p_y a(H)}{\hbar}\right) \tag{80}$$

where $Q = 2(\pi L_H/a)^2$ and $a(H) = 2\pi L_H^2/a$.

Thus, each Landau level is broaden into the dispersive band with the cosine dependence on the p_y. The width of these bands is proportional to

the amplitude of the periodic potential V_0 and oscillates with $Q \sim 1/B$ due to the Laguerre polynomial factor $L_n(Q)$. Another typical feature of the Landau bands is the exponential factor $\exp(-Q/2)$ which can be also written in the form

$$\exp(-Q/2) = \exp(-H^*/B) \tag{81}$$

with $H^* = \pi\Phi_0/a^2$. We will see in what follows that the exponent like that in Eq. (81) appears as a factor determining the Landau band width in different periodic systems subjected to the quantizing magnetic field. The oscillations of the band width in case of large $n \gg 1$ becomes periodic function of the inverse square root of the magnetic field $1/\sqrt{B}$ because of the asymptotic form for the Laguerre polynomials in this (quasiclassical) limit

$$\exp\left(-\frac{Q}{2}\right) L_n(Q) \approx J_0\left(\frac{2\pi R_n}{a}\right) \approx \left(\frac{a}{\pi^2 R_n}\right)^{1/2} \cos\left(\frac{2\pi R_n}{a} - \frac{\pi}{4}\right) \tag{82}$$

where $R_n = L_H\sqrt{2n+1}$ is the cyclotron radius of the $n-$th Landau orbit.

7.2 The quasiclassical approach.

As we see from the previous subsection a periodic one-dimensional field broads the Landau levels into the Landau bands. Generally, the periodicity in some direction means that the dispersion relation in this direction is a periodic function of the momentum projection on the corresponding axis. Let it be an x-axis, then the Hamiltonian of a two-dimensional Landau problem can be written in the Landau gauge $\mathbf{A} = (0, Bx)$ as follows:

$$\hat{H} = \mathcal{E}\left(\hat{p}_x\right) + \frac{1}{2m}\left(\hat{p}_y - \frac{e}{c}Bx\right)^2, \tag{83}$$

where $\mathcal{E}\left(\hat{p}_x\right)$ is a periodic function with the period determined by the spatial period a of some external potential $U(x) = U(x+a)$:

$$\mathcal{E}\left(\hat{p}_x\right) = \mathcal{E}(\hat{p}_x + \frac{2\pi\hbar}{a}). \tag{84}$$

In principle, one can calculates $\mathcal{E}\left(\hat{p}_x\right)$ directly from the Schrödinger equation in the coordinate representation with the periodic potential energy $U(x)$. Generally, this problem can not be solved for the arbitrary shape of the periodic function $U(x)$. We can avoid this difficulty by assuming $\mathcal{E}\left(\hat{p}_x\right)$ to be an arbitrary periodic function with the only reservation that it can be

treated quasiclassically in the momentum representation of the Schrödinger equation. This is along the lines of the Lifshitz-Onsager approach known as a "Fermiology" to the electron theory of metals which is based completely on the ideology of the arbitrary electron dispersion function. We also ignore a trivial free motion of a particle along the magnetic field resulting only in the shift of the energy Landau levels by the kinetic term $p_z^2/2m$.

Since $\hat{p}_y$ commutes with the Hamiltonian of Eq. (83), i.e. $[\hat{H}, \hat{p}_y] = 0$, we can separate variables in the Schrödinger equation

$$\hat{H}\Psi_E(x,y) = E\Psi_E(x,y) \tag{85}$$

by factorizing the eigenfunctions

$$\Psi_E(x,y) = \varphi_E(x)\exp(i\frac{p_y y}{\hbar}). \tag{86}$$

Taking this into account and shifting the x-coordinate by the orbit centre position $q = x - x_0$ ($x_0 = -cp_y/eB$) one can rewrite the Schrödinger equation in the momentum representation

$$\left[\mathcal{E}(p) - \frac{m}{2}\left(\hbar\Omega\right)^2\frac{d^2}{dp^2}\right]\varphi_E(p) = E\varphi_E(p), \tag{87}$$

where

$$\varphi_E(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\varphi_E(q)\exp(i\frac{qp}{\hbar})dq. \tag{88}$$

One can not solve Eq. (87) before the dispersion $\mathcal{E}(p)$ is not specified, and even so, the exact solutions are known only for a few specific functions $\mathcal{E}(p)$. On the other hand, the quasiclassical solution of the differential equation (87) can be obtained for arbitrary type of the dispersion $\mathcal{E}(p)$ provided it satisfies the quasiclassical condition

$$\left|\frac{dk}{dp}\right| \ll k^2, \tag{89}$$

where

$$k(p) = \frac{1}{\hbar\Omega}\sqrt{\frac{2}{m}\left(E - \mathcal{E}(p)\right)}. \tag{90}$$

The equation (87) in terms of the function $k(p)$ reads

$$\frac{d^2\varphi_E(p)}{dp^2} + k^2(p)\varphi_E(p) = 0. \tag{91}$$

Solutions of this equation taken for some energy E oscillate , as a function of p, within the "potential wells" defined by condition $k^2(p) > 0$ (i.e. for $a_n < p < b_n$) and displays an exponential behavior under the "potential barriers", i.e. within the intervals $b_n < p < a_n$ where $k^2(p) < 0$ .The quasiclassical solution within the $n-$th barrier can be written in the form

$$\varphi_E(p) = \frac{C_n}{\sqrt{|k|}} e^{-\int_{b_n}^{p} |k| dp} + \frac{D_n}{\sqrt{|k|}} e^{\int_{b_n}^{p} |k| dp} \tag{92}$$

Using the standard matching conditions of the quasiclassical approach, relating the coefficients C in the neighboring regions with the different signs of the function $k^2(p)$

$$\frac{C}{\sqrt{|k|}} e^{-\int_{p}^{a} |k| dp} \leftrightarrow \frac{2C}{\sqrt{k}} \cos\left(\int_{a}^{p} k dp - \frac{\pi}{4} \right), \tag{93}$$

$$\frac{C}{\sqrt{|k|}} e^{\int_{a}^{p} |k| dp} \leftrightarrow \frac{C}{\sqrt{k}} \cos\left(\int_{p}^{a} k dp + \frac{\pi}{4} \right) \tag{94}$$

we can obtain the relationship between coefficients C_n and D_n of the neighboring cells

$$C_{n+1} = \frac{1}{2} C_n e^{-\tau} \cos\sigma + D_n e^{\tau} \sin\sigma, \tag{95}$$

$$D_{n+1} = -C_n e^{-\tau} \sin\sigma + 2 D_n e^{\tau} \cos\sigma. \tag{96}$$

Here we have denoted

$$\tau = \int_{b_{n-1}}^{a_n} |k(p)| \, dp, \tag{97}$$

$$\sigma = \int_{a_n}^{b_n} k(p) dp. \tag{98}$$

Constants a_n and b_n stand for the turning points of a "particle" moving in the "potential" $\mathcal{E}(p)$ (i.e. the roots of equation $E - \mathcal{E}(p) = 0$

To obtain the energy spectrum it is convenient to introduce a transfer-matrix

$$\hat{T} = \begin{pmatrix} \frac{1}{2} e^{-\tau} \cos\sigma & e^{\tau} \sin\sigma \\ -e^{-\tau} \sin\sigma & 2 e^{\tau} \cos\sigma \end{pmatrix}. \tag{99}$$

The important property of this matrix is that its determinant equals unity

$$\det \hat{T} = 1. \tag{100}$$

With the help of the transfer matrix a couple of equations (95) and (96) can be rewritten in the matrix form

$$\begin{pmatrix} C_{n+1} \\ D_{n+1} \end{pmatrix} = \hat{T} \begin{pmatrix} C_n \\ D_n \end{pmatrix}. \tag{101}$$

Since the spatial period in the problem in question equals a, one can try to find a solution of the equation (101) with the help of the following substitution

$$\begin{pmatrix} C_n \\ D_n \end{pmatrix} = e^{iqan} \begin{pmatrix} C_0 \\ D_0 \end{pmatrix} \tag{102}$$

which yields a couple of uniform and linear equations for two unknown quantities C_0 and D_0. These equations have nontrivial solution $C_0 \neq 0, D_0 \neq 0$ under the condition that

$$\det \left(\hat{T} - e^{iqa} \hat{I} \right) = 0. \tag{103}$$

($\hat{I}$ is the unit 2×2 matrix).

Using Eq. (100) one can remold the dispersion equation (103) in the form

$$\cos qa = \frac{1}{2} \mathrm{Sp} \hat{T}(E). \tag{104}$$

The dispersion equation (104) determines a set of periodic functions $E_k(q) = E_k(q + 2\pi/a)$ $(k = 0, 1, 2...)$ which are nothing but the dispersive energy bands whose derivatives are also periodic functions of the quasimomentum q vanishing at the points $q = 0, \pm\pi/a, \pm 2\pi/a$, where $dE_k/dq = 0$.

In fact, equations (100)-(104) holds for arbitrary transfer-matrix $\hat{T}$ and we will address them time and again in the next chapters.

Turning back to our problem we can write down the dispersion equation (104) with the transfer-matrix (99) in an explicit form:

$$\cos qa = W \cos \sigma. \tag{105}$$

The quantity W here stands for the quasiclassical tunneling probability for a particle to transfer from the one classically permitted region $a_n \leq p \leq b_n$ to the another neighboring "potential well" $a_{n+1} < p < b_{n+1}$.

$$W = \left(\frac{1}{4}e^{-\tau} + e^{\tau}\right)^{-1} \approx e^{-\tau}. \tag{106}$$

(Note that in the quasiclassical approach $\tau \gg 1$).

Solving then equation (105) and using Eqs.(90), (98) for σ, we arrive at the following quantization rule:

$$\frac{1}{2\pi}\oint\left[\frac{2}{m}\left(E-\mathcal{E}(p)\right)\right]^{1/2}dp = \hbar\Omega\left(n+\frac{1}{2}\right)+(-1)^n\frac{\hbar\Omega}{\pi}\arcsin\left[\sqrt{W}\cos\left(\frac{qa}{\hbar}\right)\right]. \tag{107}$$

Let us analyze the energy spectrum determined by this quantization rule. Consider first the limit when the probability of tunneling between the adjacent "potential wells" of the "potential" $\mathcal{E}(p)$ equals zero $W \equiv 0$. If we also take the shape of the "potential" $\mathcal{E}(p)$ within the well to be parabolic $\mathcal{E}(p) = p^2/2m$, then calculating the integral in the left-hand-side of Eq. (107) we obtain the standard Landau spectrum $E_n = \hbar\Omega(n + 1/2)$. Nonzero tunneling probability means that the particle can move along the periodic "potential" $\mathcal{E}(p)$ which itself appears due to the spatial periodicity of the true potential $U(x) = U(x+a)$. Periodicity lifts up the degeneracy of the Landau levels E_n on the orbit center position and thereby broads them into the Landau bands of the width

$$\Delta E = \frac{\hbar\Omega}{\pi}\arcsin W, \tag{108}$$

which is determined by the second term in the right-hand-side of Eq. (107). The tunneling probability $W \simeq \exp(-\tau)$ being written in terms of the external magnetic field B has a standard exponential form

$$W = \exp\left(-\frac{H^*}{B}\right) \tag{109}$$

with the "breakdown" field

$$H^* = \frac{\Phi_0}{2\pi\hbar^2}\int_a^b\sqrt{2m\left(E-\mathcal{E}(p)\right)}dp. \tag{110}$$

Near the bottom of the energy band the function $\mathcal{E}(p)$ has a minimum and can be expanded in the power series in p which yields in the second order (provided that both the energy and momentum are counted from the minimum)

$$\mathcal{E}(p) \approx \frac{p^2}{2M}, \tag{111}$$

where the effective mass of a particle is given by

$$M^{-1} = \frac{\partial^2 \mathcal{E}(p)}{\partial p^2} \mid_{p=0} . \tag{112}$$

The quantization rule (107) then yields immediately the Landau bands

$$E_n(q) = \hbar\Omega \left(n + \frac{1}{2}\right) + (-1)^n \frac{\hbar\Omega}{\pi} \arcsin\left[\exp\left(-\frac{H^*}{B}\right) \cos\left(\frac{qa}{\hbar}\right)\right] \tag{113}$$

with

$$H^* = \frac{\Phi_0}{2\pi\hbar^2} \int_a^b \sqrt{2m\mathcal{E}(p)} dp. \tag{114}$$

It is well known that for the nonsingular "potential" $\mathcal{E}(p)$ the quasiclassical approach is valid far beyond the formal limitations given by the condition of Eq. (89). In particular, Eq. (113) holds for a wide class of arbitrary (but quasiclassical) periodic functions $\mathcal{E}(p)$. This makes our approach ideologically similar to the one developed by I. Lifshitz and Onsager for electrons in conventional metals where the arbitrary three dimensional dispersion function $\mathcal{E}(\mathbf{p})$ is the basic quantity of their theory. In principle, $\mathcal{E}(p)$ can be calculated from the Schrödinger equation with the periodic potential $U(x)$, but in practice this difficult problem was solved exactly only for a few specific one dimensional periodic potentials. In this connection, it is worthwhile to note that both the perturbative (Eq. (80)) and quasiclassical (Eq. (113)) spectra yield Landau bands of the width proportional to the same exponent $\exp(-H^*/B)$. We will see in the section, devoted to the energy spectrum of the periodic magnetic breakdown systems, that the very same exponent determines the Landau band width in such systems too.

8 A two-dimensional electron in a one-dimensional periodic magnetic field

In this section we will consider an electron moving within a 2D plane (X,Y) in the presence of a perpendicular magnetic field which we assume to be homogeneous along the Y axis and periodic in the X direction. In the Landau gauge, this means that the vector potential takes the form $\mathbf{A} =$

$[0, -A(x), 0]$, where $A(x) = A(x + L)$ is a periodic function with the period L.

The Hamiltonian of the system is

$$\hat{H} = \frac{1}{2m}\left(\hat{P}_x^2 + \left[\hat{P}_y + \frac{e}{c}A(x)\right]^2\right). \tag{115}$$

Since the y-component of the momentum, $\hat{P}_y$, commutes with the Hamiltonian, $\left[\hat{H}, \hat{P}_y\right] = 0$, the wave function can be written as a product of the eigenfunction of the operator $\hat{P}_y$ (i.e. the plane wave $\exp(ik_y y)$) and some unknown function $\psi(x)$ which have to be found:

$$\psi(x, y) = e^{ik_y y}\psi(x). \tag{116}$$

It follows from the eigenvalue equation $\hat{H}\ \psi(x, y) = E\psi(x, y)$ and Eqs. (115)-(116) that the wave function $\psi(x)$ satisfies the one-dimensional Schrödinger equation

$$\left\{\frac{d^2}{dx^2} - \left[k_y + \frac{e}{\hbar c}A(x)\right]^2 + \frac{2mE}{\hbar^2}\right\}\psi(x) = 0. \tag{117}$$

To go ahead with the problem in question we have to resort to some model approximations in as much as one can not solve Eq. (117) for an arbitrary periodic function $A(x)$.

We consider first the magnetic Kronig-Penny model, which means that the function $A(x)$ has the shape of periodic array of rightangle steps. Since the magnetic $H(x)$ and the function $A(x)$ are related through the equation $H(x) = dA(x)/dx$, we see that the profile of the $A(x)$ corresponds to the $H(x)$ which has the form of the periodic array of δ-functions with the alternating signs at the neighboring δ-peaks. The magnetic Kronig-Penny (KP) model, therefore, describes the magnetic field of the profile $H(x)$ which total flux through the 2D sample equals zero.

It is useful for the following consideration to introduce a "potential energy" which we determine by the equation

$$V(x, k_y) = \frac{\hbar^2}{2m}\left(k_y + \frac{e}{\hbar c}A(x)\right)^2. \tag{118}$$

Note that this "potential energy" parametrically depends on the particle momentum component k_y.

In the periodic step-like magnetic KP model this quantity takes two values corresponding to the maximum and minimum of the potential $V(x, k_y)$:

$$V_{\max} = \frac{\hbar^2}{2m}\left(k_y + \frac{e}{\hbar c}A_0\right)^2, \tag{119}$$

$$V_{\min} = \frac{\hbar^2}{2m}{k_y}^2. \tag{120}$$

The Schrödinger equation (117) then may be rewritten in the standard fashion

$$\frac{d^2\psi(x)}{dx^2} + K^2(x)\psi(x) = 0, \tag{121}$$

where the quantity

$$K^2(x) = \frac{2m}{\hbar^2}\left[E - V\left(x, k_y\right)\right]$$

takes only two possible values:

$$\kappa^2 = \frac{2m}{\hbar^2}\left[E - V_{\max}\right], k^2 = \frac{2m}{\hbar^2}\left[E - V_{\min}\right]. \tag{122}$$

The solutions of the Eq. (121) differ for $E > V_{\max}$ and $E < V_{\max}$. We begin our analysis with the case $E > V_{\max}$. The solutions for the three neighboring regions I-III may be written in this case as follows :

$$\psi_1(x) = C_1 e^{ikx} + D_1 e^{-ikx}, \tag{123}$$

$$\psi_2(x) = B_1 e^{i\kappa x} + B_2 e^{-i\kappa x}, \tag{124}$$

$$\psi_3(x) = C_2 e^{ik(x-L)} + D_2 e^{-ik(x-L)}. \tag{125}$$

We have shifted the origin of the X-coordinate by the period $L = a + b$ in Eq. (125) which simply means a standard choice of the phase factors, $\exp(\pm ikL)$, according to the Flouquet theorem.

Using then the boundary conditions for the wave functions and their derivatives

$$\psi_1(a) = \psi_2(a), \psi_1'(a) = \psi_2'(a), \tag{126}$$

$$\psi_2(L) = \psi_3(L), \psi_2'(L) = \psi_3'(L), \tag{127}$$

we arrive at a set of linear equations relating the coefficients B_n, C_n, and D_n which is convenient to present in the matrix form

$$\begin{pmatrix} C_2 \\ D_2 \end{pmatrix} = \hat{V} \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}, \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \hat{M} \begin{pmatrix} C_1 \\ D_1 \end{pmatrix}. \tag{128}$$

Matrices $\hat{V}$ and $\hat{M}$ are given by:

$$\hat{V} = \begin{pmatrix} e^{i\kappa L}(1+\kappa/k) & e^{-i\kappa L}(1-\kappa/k) \\ e^{i\kappa L}(1-\kappa/k) & e^{-i\kappa L}(1+\kappa/k) \end{pmatrix}, \tag{129}$$

$$\hat{M} = \begin{pmatrix} e^{i(k-\kappa)a}(1+k/\kappa) & e^{-i(k+\kappa)a}(1-k/\kappa) \\ e^{i(k+\kappa)a}(1-k/\kappa) & e^{i(\kappa-k)a}(1+k/\kappa) \end{pmatrix}. \tag{130}$$

Having at hand the matrix equations (128) one can calculate the transfer-matrix (which was introduced and discussed in detail in Section 9) as a product of two matrices: $\hat{T} = \hat{V}\hat{M}$. Then Eqs. (128) may be rewritten in the form

$$\begin{pmatrix} C_{n+1} \\ D_{n+1} \end{pmatrix} = \hat{T} \begin{pmatrix} C_n \\ D_n \end{pmatrix}. \tag{131}$$

The dispersion equation now reads

$$\cos qL = \frac{1}{2}\mathrm{Sp}\hat{T}(E), \tag{132}$$

where

$$\frac{1}{2}\mathrm{Sp}\hat{T}(E) = \cos ka \cos \kappa b - \frac{\kappa^2 + k^2}{2\kappa k} \sin ka \sin \kappa b. \tag{133}$$

Thus, equations (132) and (133) determine the energy E as a function of the three quantum numbers: n, k_y, q. Where n denotes the energy band number and q stands for the Bloch index related to the electron motion within the bands. It is instructive to recast the dispersion equation (132) in the form

$$\sqrt{W} \cos qL = \cos(ka + \varphi) \tag{134}$$

where W is the transition probability through the rectangular potential barrier separating two adjacent wells in periodic magnetic KP potential

$$W = \frac{1}{1 + \left(\frac{\kappa^2 - k^2}{2\kappa k}\right)^2 \sin^2 \kappa b}. \tag{135}$$

This parameter determines the widths of the bands in the case $E > V_{\max}$
The phase φ entering Eq. (134) is determined by the relation

$$\mathrm{tg}\varphi = \frac{\kappa^2 + k^2}{2k\kappa}\mathrm{tg}\kappa b. \tag{136}$$

The energy spectrum of the problem in question consists of a discrete set of bands permitted for a free electron motion and gaps between them. The widths of these bands can be obtained from the inequality

$$\sqrt{W} \geq |\cos(ka - \varphi)|. \tag{137}$$

The bands grow narrower with the decrease of the transmission probability and vanish (become a sharp energy levels) if $W \to 0$. On the other hand, the energy gaps between the bands decrease with the enhancement of the transparency coefficient T and collapse when $W = 1$ and the barrier becomes absolutely transparent. This happens each time when $\sin^2 \kappa b = 0$ as one can see from Eq. (135). The transition probability W, as well as, the quantities φ and k are the functions of the parameter k_y.

To discuss some specific features of the results obtained, let us introduce a vector potential amplitude entering the equation (119) by the relation $A_0 = BL$, where , B is the magnetic field amplitude and L being some length. The quantity $V_{\max}$ then reads

$$V_{\max} = \frac{\hbar\Omega}{2}\left(L_H k_y + \frac{L}{L_H}\right)^2. \tag{138}$$

Here $L_H = (\hbar c/eB)^{1/2}$ is the magnetic length, and $\Omega = eB/mc$ is the cyclotron frequency.

The transparency coefficient W becomes equal to unity under the condition $\sin \kappa b = 0$, which yields

$$\sqrt{\frac{2m}{\hbar^2}(E - V_{\max})}b = \pi\left(n + \frac{1}{2}\right) \tag{139}$$

where n stands for the integer. Therefore, at energies

$$E_n(k_y) = \frac{\hbar^2\pi^2}{2mb^2}\left(n + \frac{1}{2}\right)^2 + \frac{\hbar\Omega}{2}\left(\frac{L}{L_H} + L_H k_y\right)^2, \tag{140}$$

the resonant transition through the barriers holds i.e. the energy bands merge and the energy spectrum becomes continuous.

For energies less than the barrier height $V_{\min} < E < V_{\max}$ the transparency coefficient becomes

$$W = \frac{1}{1 + |\frac{\kappa^2+k^2}{2\kappa k}|^2 \sinh(|\kappa|b)}. \tag{141}$$

The transparency coefficient behaves rather unusual as a function of B and k_y.To see this more clearly, consider the case $|\kappa|b \gg 1$, when T is exponentially small

$$W \sim e^{-|\kappa|b}. \tag{142}$$

Putting in Eq. (142) $E = 0$ for simplicity, we have

$$T \sim \exp\left(-\frac{B}{H_*}\right) \exp(-k_y b). \tag{143}$$

The quantity $H_* = \Phi_0/2\pi Lb$ determines the magnetic-field scale in the tunneling problem. The decrease of the tunneling probability with the enhancement of B is clear since the magnetic field intensity determines the height of the barrier. More exotic is the strong exponential suppression of the tunneling probability by the factor $\exp(-k_y b)$. This is a specific feature of the magnetic barrier, because its effective height, $V_{\max} - V_{\min}$, according to the Eq. (138), depends both on k_y and B.

We conclude this section by the quasiclassical approach to the problem which makes a whole consideration of the electron motion in periodic magnetic field more general. To do this we note first that equation (121), after the substitution variable x instead of p, has the very same shape as Eq. (41) which is convenient for the quasiclassical calculations. Thus, we can proceed in the same fashion as in the section 4.4, to obtain a quasiclassical transfer-matrix of the equation (62) with τ and σ given by

$$\tau = \int_{b_{n-1}}^{a_n} |K(x)|dx, \tag{144}$$

$$\sigma = \int_{a_n}^{b_n} |K(x)|dx, \tag{145}$$

where

$$K^2(x) = \frac{2m}{\hbar^2}\left[E - \frac{\Omega^2 m}{2}\left(x_0 + L\tilde{A}(x)\right)^2\right] \tag{146}$$

and the Landau orbit center coordinate equals to its standard value

$$x_0 = -\frac{cP_y}{eH}. \tag{147}$$

We imply the dimensionless vector potential $\tilde{A}(x)$ to be a periodic function $\tilde{A}(x) = \tilde{A}(x+L)$ related to the true vector potential $A(x)$ according to the equation

$$A(x) = BL\tilde{A}(x). \tag{148}$$

The shape of the effective potential which "a particle" feels $V(x_0, x)$ depends on the shape of the function $\tilde{A}(x) = \tilde{A}(x+L)$ as well as on the value and sign of the coordinate x_0. The quasiclassical tunneling probability through the potential barrier is given then by the following relation

$$W = e^{-\tau} \tag{149}$$

with

$$\tau = \frac{m\Omega}{\hbar} \int\limits_{b_{n-1}}^{a_n} \sqrt{|\frac{2E}{m\Omega^2} - \left(x_0 + L\tilde{A}(x)\right)^2}\,|dx \tag{150}$$

and the quantization rule is given by

$$\begin{aligned} &\frac{1}{\pi} \int\limits_{a_n}^{b_n} \frac{m\Omega}{\hbar} \sqrt{\frac{2E}{m\Omega^2} - \left(x_0 + L\tilde{A}(x)\right)^2}\,dx \\ = \quad &\hbar\Omega\left(n + \frac{1}{2}\right) + (-1)^n \frac{\hbar\Omega}{\pi} \arcsin\left(\sqrt{W}\cos\left(\frac{qa}{\hbar}\right)\right) \end{aligned} \tag{151}$$

In case when $E = 0$ the tunnel probability equals to

$$W = \exp\left(-\frac{m\Omega L}{\hbar} \int_b^a \mid \frac{x_0}{L}\tilde{A}(x) \mid dx\right). \tag{152}$$

This equation can be recast to the form

$$W = \exp\left(-\frac{B}{H_*}\right), \tag{153}$$

where the characteristic field H_* is determined by

$$H_* = \frac{\Phi_0}{2\pi Ll} \tag{154}$$

with

$$l = \int_b^a |\frac{x_0}{L}\tilde{A}(x)|dx. \tag{155}$$

We see again that as in Eq. (143)the tunneling probability through a magnetic barrier depends both on the B (the height of the barrier) and p_y, the momentum component along the barrier.

9 The magnetic breakdown in metals

The dynamics of electrons in conventional metals in external magnetic fields is described within the quasiclassical Lifshitz-Onzager approach based on the smallness of the parameter $\kappa = a/R \ll 1$ which is the ratio of the lattice constant a and the Larmor radius R. Since in conventional metals the lattice constant is of the order of $a = \hbar/p_F$, and $R = cp_F/eB$ the parameter $\kappa \simeq \hbar\Omega/E_F$ is very small in experimentally attainable fields because $\hbar\Omega << E_F$ (E_F is the Fermi energy and p_F stands for the Fermi momentum). Under these conditions the crystal lattice does not influence the electron dynamics directly but only through the shape of the Fermi surface which is determined by the dispersion relation within the m-th band $\mathcal{E}_m(\mathbf{p})$. In the zero approximation on parameter κ the conducting electrons may be considered as classical particles which obey the Newton's mechanics. The equations of motion, hence, are given by

$$\frac{d\mathbf{p}}{dt} = \frac{e}{c}[\mathbf{v}_m\mathbf{B}], \quad \mathbf{v}_m = \frac{\partial\mathcal{E}_m(\mathbf{p})}{\partial\mathbf{p}}, \frac{d\mathbf{r}}{dt} = \mathbf{v}_m(\mathbf{p}),$$

where $\mathbf{p}$ is the quasimomentum, $\mathbf{v}_m(\mathbf{p})$ is the velocity of the electron and $\mathbf{r}$ stands for its coordinate. The above equations determine a classical trajectory of the electron in the momentum space which has the following geometrical interpretation: the trajectory is the contour line along the cross-section of the constant energy surface $\mathcal{E}_m(\mathbf{p}) = E$ by the plane perpendicular to the external magnetic field. This trajectory is determined by relations:

$$\mathcal{E}_m(\mathbf{p}) = E, p_z = const \tag{156}$$

where E is the energy of the electron and it is assumed that the magnetic field directed along the z-axis. In real metals, because of the anisotropy and periodicity of the dispersion relation $\mathcal{E}_m(\mathbf{p})$ in the momentum space the trajectory (156) may be rather complex in shape. Two types of trajectories

are possible in general: the open and closed ones. In case of closed trajectories the quasiclassical quantization yields discrete energies E_n (for fixed p_z values) according to the Lifshitz-Onzager quantization rule

$$S_m(E, p_z) = \frac{2\pi\hbar eB}{c}(n + \gamma), \tag{157}$$

which has a simple geometric meaning: the cross-section area $S_m(E, p_z)$ of the constant energy surface by the plane $p_z = const$ is quantized. It is assumed that the integer n is large $n \gg 1$ and constant γ is less than unity. We have considered this quantization in detail in the previous section and have shown that the Lifshitz-Onzager relation (157) is a direct consequence of the commutation rules between the momentum components in the magnetic field.

In many metals classical trajectories of electrons may go very close to each other in some places (usually near the Brilouin zone boundaries) so that electrons may tunnel from one trajectory to another.

This phenomenon known in the literature as the magnetic breakdown (MB) is very similar to the Landau problem for the electron moving in a chain of rings connected by the tunneling centers we have considered in the subsection 3.4.2. In what follows we will see that the mathematical approaches to both problems are very similar too. The main difference is in that, contrary to the case of chain of rings, we can not consider the tunneling probability independent on the magnetic field. Here we do not intent to calculate the MB tunneling probability$W(B)$, but note that physically it is clear that it should depend on B in the same fashion like the probability (109) to tunnel from one potential well to another in the presence of the external magnetic field. We will see and discuss below the analogy between the coherent magnetic breakdown in periodic structures and the Landau problem in the periodic potential. Now let us take for granted that the tunneling probability W for electron transition between close trajectories is given by the exponent like that of

$$W = \exp\left(-\frac{H^*}{B}\right). \tag{158}$$

The breakdown field H^* can be estimated as follows. Let Δ be the energy gap which separates trajectories near the MB center. Then the distance (in the momentum space) between the trajectories near the MB center may be estimated as $\delta p \sim \Delta/v_F$ (v_F is the Fermi velocity). The tunneling takes place if δp^2 is of the order of the uncertainties product $\delta p_x \delta p_y$ which is

determined by the commutation rule

$$[\hat{p}_x, \hat{p}_y] = \frac{e\hbar}{c} B.$$

Thus, equating δp to $\delta p_x \delta p_y$, we have

$$\delta p_x \delta p_y \sim \frac{e\hbar}{c} H^* \sim \delta p^2 \simeq \left(\frac{\Delta}{v_F}\right)^2,$$

so that the MB field is given by

$$H^* \simeq \frac{c}{e\hbar} \left(\frac{\Delta}{v_F}\right)^2. \tag{159}$$

In conventional metals the gap between the neighboring two zones is of the order $\Delta \simeq 10^{-2}$ eV, $v_F \simeq 10^8$ cm/sec and $H^* \simeq 10^4 - 10^5$ Gauss. In the limit of large fields $B \to \infty$ the tunneling probability approaches unity and $W(B) \to 1$. (We do not consider here the case of self-crossing trajectory for which the MB point is also the stopping point and the corresponding tunneling probability has different dependence on B so that $W(B) \to 1/2$ in this case when $B \to \infty$).

Theory of the MB is rather complex and sophisticated matter which we do not intent to consider here in general, addressing the reader for more details to some review articles given in the literature. To be more specific, we will discuss below the main features of the coherent MB in the case of a chain of closed orbits coupled by centers of MB, as shown in the Fig. 10.

Outside the MB-center, where the quasiclassical approach holds, the motion of an electron obey the Schrödinger equation with the Hamiltonian $\hat{H}$ which comes out of the dispersion relation $\mathcal{E}_m(p_x, p_y, p_z)$ after the substitution

$$p_x \to \hat{P}_x + \frac{eB}{c}\hat{y}, \quad p_y \to \hat{P}_y, \quad p_z \to \hat{P}_z. \tag{160}$$

Another words, in the Landau gauge we have

$$\hat{H} = \mathcal{E}_m \left(\hat{P}_x + \frac{eB}{c}\hat{y}, \hat{P}_y, \hat{P}_z\right) \tag{161}$$

where the generalized momentum operator $\hat{\mathbf{P}}$ is canonically conjugate of the coordinate operator $\hat{r}$. It follows from the Eq. (161) that $\hat{P}_x$ and $\hat{P}_z$ are the quantum integrals of motion since $\left[\hat{H}, \hat{P}_x\right] = \left[\hat{H}, \hat{P}_z\right] = 0$. Taking this

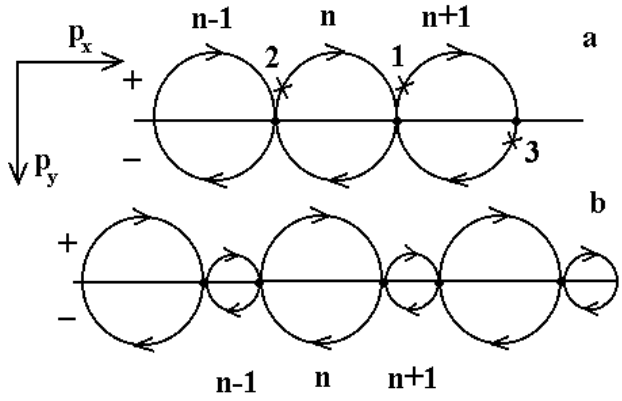

Figure 10: The coherent magnetic breakdown in the case of a chain of closed orbits coupled by centers of MB.

into account one can write down a quasiclassical solution of the Schrödinger equation

$$\hat{H}\Psi_m(\mathbf{P}) = E\Psi_m(\mathbf{P}) \tag{162}$$

in the standard quasiclassical form

$$\Psi_m(\mathbf{P}) = \frac{C_m}{\sqrt{\left|v_x^{(m)}\right|}} \exp\left(\frac{ic}{e\hbar B}\left(P_x p_y - \int_p^{p_y} p_x(p_y')dp_y'\right)\right)\delta p_x p_{xo}\delta p_z p_{zo}. \tag{163}$$

Here $P_x = P_x^{(m)}(p_y, E, p_{zo})$ is a solution of the classical equation (156); p_{xo} and p_{zo} are the constants of motion, $v_x^{(m)} = \partial\mathcal{E}_m/\partial p_x$ is the electron's velocity, and C_m is an arbitrary constant which should be found from the appropriate boundary conditions.

The MB-center may be considered as a two-channel quantum scattering center connecting four quasiclassical trajectories as it is shown in Fig. 11. The inside electronic state $|\alpha\rangle$ splits up by the MB center into two states $|\alpha'\rangle$ and $|\beta'\rangle$. The appropriate amplitudes are related by the scattering matrix $\hat{S}$ which is the major characteristic of the MB center:

$$\begin{pmatrix} |\alpha\rangle \\ |\beta\rangle \end{pmatrix} = \begin{pmatrix} S_{\alpha\alpha'} & S_{\alpha\beta'} \\ S_{\beta\alpha'} & S_{\beta\beta'} \end{pmatrix} \begin{pmatrix} |\alpha'\rangle \\ |\beta'\rangle \end{pmatrix}. \tag{164}$$

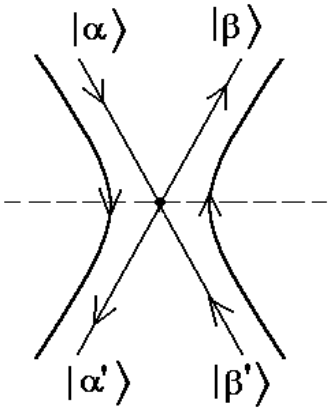

Figure 11: The MB-center may be considered as a two-channel quantum scattering center connecting four quasiclassical trajectories.

The $\hat{S}$-matrix components are given by

$$S_{\alpha\alpha'} = \sqrt{1-W},\ \ S_{\alpha\beta'} = \sqrt{W},\ \ S_{\beta\alpha'} = -S_{\beta'\alpha},\ \ S_{\beta\beta'} = S_{\alpha'\alpha}\ \ . \qquad (165)$$

They can be found directly from the matching condition for the quasiclassical wave functions (163) if one applies them to the Ψ-functions on both sides of the MB-center. Thus, we arrive at the following picture. Electron moves classically along the trajectory fixed by the external magnetic field up to the MB-center where two classical trajectories from the neighbouring Briloin zones come close to the zone boundary (see Fig. 11) and electron can either tunnel to the adjacent trajectory with the probability W, or stay at the same trajectory with the probability $1-W$. Another words, each of the two states $|\alpha\rangle$ and $|\beta\rangle$ split at the MB-center into another two:

$$|\alpha\rangle = \sqrt{1-W}\,|\alpha'\rangle + \sqrt{W}\,|\beta\prime\rangle\,,\ \ |\beta\rangle = -\sqrt{W}\,|\alpha'\rangle + \sqrt{1-W}\,|\beta\prime\rangle\,. \qquad (166)$$

It is convenient for the further consideration to introduce quantum amplitudes ρ and τ defining them as $W=\rho^2$ and $\tau^2 = 1-\rho^2$. These amplitudes have a clear physical meaning: ρ is the quantum amplitude for electron to break down from one trajectory to another, while τ is the quantum amplitude to stay at the same trajectory after the scattering at the MB center.

10 The transfer-matrix and the quantization rules for a chain of a coherent MB-coupled closed orbits

Consider a chain of MB-coupled closed orbits shown in Fig. 10a. Let us denote by symbols $C_+(n)$ and $C_-(n)$ the quantum amplitudes to find an electron at the upper (+) and lower (-) sections of the classical orbit n in the immediate vicinity of the MB-center. Now we can write down the balance equation for these amplitudes in a closed and simple form

$$\begin{aligned} C_+(n+1) &= \rho e^{i\varphi(n)} C_+(n) + \tau e^{i\varphi(n+1)} C_-(n+1), \\ C_-(n) &= -\tau e^{i\varphi(n)} C_+(n) + \rho e^{i\varphi(n+1)} C_-(n+1). \end{aligned} \tag{167}$$

To obtain, for example, the first equation consider points marked by cross in Fig. 10a. The amplitudes $C_+(n+1)$, $C_+(n)$ and $C_-(n+1)$ corresponds to the points 1,2 and 3. Provided that $C_+(n)$ and $C_-(n+1)$ are known we can write $C_+(n+1)$ as a Feyman sum of amplitudes along the two classical paths: $2 \to 1$, with the amplitude $\exp(iS_{21}/\hbar)\,\rho C_+(n)$, and $3 \to 1$, with the amplitude $\exp(iS_{31}/\hbar)\,\tau C_-(n+1)$. Here $\hat{S}$ is the classical action given by

$$S = \frac{c}{eB}\int_0^{p_y} p_x(p_y')dp_y' = \frac{c}{2eB} S_n(E, p_z), \tag{168}$$

where $S_n(E, p_z)$ is the area inside the n-th orbit. Thus, the phases in Eqs. (167) are equal to

$$\varphi(n) = \frac{c}{2eB\hbar} S_n(E, p_z). \tag{169}$$

(Note that we assume an axial symmetry of the orbits with respect to the MB-centers axis). In the second equation of Eqs. (167) can be obtained in the same fashion. The above equations are very similar to the ones we dealed with when considered the Landau problem of electron in a chain of rings. The difference is that in the problem in question a chain of closed orbits is in the momentum space.

Let us introduce a two-component vector

$$\bar{C}(n) = \begin{pmatrix} C_+(n) \\ C_-(n)e^{i\varphi(n)} \end{pmatrix} \tag{170}$$

in terms of which Eqs.(167) may be rewritten in the matrix form

$$\bar{C}(n+1) = \hat{T}(n)\bar{C}(n), \tag{171}$$

where $\hat{T}(n)$ stands for the transfer-matrix

$$\hat{T}(n) = \frac{1}{\rho}\begin{pmatrix} e^{i\varphi(n)} & \tau e^{-i\varphi(n)} \\ \tau e^{i\varphi(n)} & e^{-i\varphi(n)} \end{pmatrix}. \tag{172}$$

Because of the relation $\rho^2 + \tau^2 = 1$ the determinant of $\hat{T}(n)$ is equal to unity: $\det \hat{T}(n) = 1$.

Consider first the case of a chain composed of identical orbits with ρ and φ independent of n. Then, the dispersion relation of the transfer-matrix approach

$$\cos qL = \frac{1}{2}\mathrm{Sp}\hat{T} \tag{173}$$

yields

$$\rho \cos qL = \cos\varphi. \tag{174}$$

Solving this equation with the help of the Eq. (169) we have

$$S(E, p_z) = \frac{2\pi e\hbar B}{c}\left[n + \frac{1}{2} + \frac{(-1)^n}{\pi}\arcsin\left(\rho\cos qL\right)\right], n = 0, 1, 2... \tag{175}$$

L- is the spatial period of the MB-chain.

This equation generalizes the Lifshitz-Onzager quantization rule (see Eq. (157)) to the case of the coherent magnetic breakdown in the chain of coupled orbits. If these orbits have a shape of a circle, then

$$S(E, p_z) = \pi\left(2mE - p_z^2\right) \tag{176}$$

The insertion of the Eq. (176) into the quantization rule yields the Landau equidistant spectrum broaden into bands due to the coherent motion of electrons along the periodic and regular MB-chain

$$E_n(p_z, q) = \hbar\Omega\left(n + \gamma\right) + \frac{p_z^2}{2m} + (-1)^n\frac{\hbar\Omega}{\pi}\arcsin\left(\rho\cos qL\right) \tag{177}$$

where $\gamma = 1/2$.

The band width is equal to

$$\Delta E = \frac{2\hbar\Omega}{\pi}\arcsin\rho. \tag{178}$$

We see that this quantity as well as the energy spectrum $E_n(p_z, q)$ are very similar to the appropriate quasiclassical equations (114) and (108) which is no wonder since our approach is quasiclassical in essence as well.

Consider now the case of a chain composed of two different types of closed orbit coupled by the MB-centers. In this case a transfer-matrix entering the dispersion equation (173) is a product of the two matrices (172) with the two different phases $\varphi = \varphi_1(E, p_z)$ and $\varphi = \varphi_2(E, p_z)$

$$\hat{T} = \hat{T}(\varphi_1)\hat{T}(\varphi_2) \tag{179}$$

because the period of a chain now consists of the two closed orbits with the areas S_1 and S_2 inside them. A simple calculation then yields the dispersion equation

$$\cos qL = \cos(\varphi_1 + \varphi_2) - 2\tau^2 \cos\varphi_1 \cos\varphi_2. \tag{180}$$

The right-hand-side of the Eq. (180), considered as a function of the energy E, is determined by two periodic functions of E. If the periods of these functions, given by the quantities $S_{1,2}(E, p_z)$, are noncomensurate, then the right-hand-side of Eq. (180) is aperiodic function of E. The energy spectrum in this case is quasirandom in the sense that the Landau bands are distributed quasiregular on the energy scale.

In fact, this is a general property of the energy spectrum for the MB configurations composed of the orbits of different types. In some metals the areas inside closed orbits are strongly differs in magnitude, i.e. $S_1 \ll S_2$. The latter means that cosine periods in Eq. (180), also differs strongly and locally the energy spectrum is nearly equidistant. In as much as the electronic properties of conductors are determined by the electrons near the Fermi level, E_F, we can approximate the small phase by

$$\varphi_1\left(\frac{1}{B}\right) = \frac{c}{2\pi e\hbar B} S_1(E_F, p_z). \tag{181}$$

Since the phase φ_1 in this approximation does not depend on E, we can reorganize Eq. (181) to the shape of Eq. (174) with respect to the phase $\varphi_2(E, p_z)$. Solving this trigonometric equation, we obtain the following quantization rule for the large orbit:

$$S_2(E, p_z) = \frac{2\pi e\hbar B}{c}\left[n + \gamma_{eff} + \frac{(-1)^n}{\pi}\arcsin\left(\rho_{eff}\cos qL\right)\right]. \tag{182}$$

Here the following parameters have been introduced:

$$\rho_{eff} = \rho^2 \left[\rho^4 + 4(1-\rho^2)\cos^2\varphi_1\right]^{-1/2}, \tag{183}$$

and

$$\gamma_{eff} = \frac{1}{\pi}\arctan\left[\left(\frac{2}{\rho^2} - 1\right)\cot\varphi_1\right]. \tag{184}$$

Comparing Eqs. (182) and (175) we arrive at the conclusion that the quantity ρ^2_{eff} plays a role of the effective tunneling probability through the small orbit. According to the Eq. (183) ρ_{eff} is periodic function of the phase of a small orbit (181), i.e. ρ_{eff} is periodic in inverse field $1/B$ with the amplitude of the order of unity for small $\rho \ll 1$. The effective probability $\rho_{eff} = 1$ in the fields which satisfy the equation $\cos\varphi_1(1/B) = 0$. The Landau bandwidth oscillate together with $\rho_{eff}(1/H)$:

$$\Delta E = \frac{2\hbar\Omega}{\pi}\arcsin\rho_{eff}(1/B). \tag{185}$$

At the same time positions of the Landau bands depend on the γ_{eff} which is also an oscillating function of the phase $\varphi_1(1/B)$. Both these effects contribute into the diverse quantum oscillation phenomena in metals.

11 The energy spectrum and the density of states in periodic coherent MB structures

The density of states (DOS) is an important characteristics of the energy spectrum. For one-dimensional periodic structures (1D) it is defined by the following equation

$$g(E) = \frac{1}{\pi}\left|\frac{dq}{dE}\right|, \tag{186}$$

where q and E are related by the transfer-matrix dispersion equation

$$\cos qL = \frac{1}{2}\mathrm{Sp}\hat{T}(E) = f(E). \tag{187}$$

Hence,

$$g(E) = \frac{1}{\pi L}\frac{\left|\frac{df(E)}{dE}\right|}{\sqrt{1-f^2(E)}}. \tag{188}$$

In case of a simple chain with the energy spectrum of Eq. (174) the function $f(E)$ is given by

$$f(E) = \cos\varphi(E)/\rho \tag{189}$$

and for MB-chain composed of alternating small and large orbits, according to Eq. (180) we have

$$f(E) = \cos\left[\varphi_1(E) + \varphi_2(E)\right] - 2\tau^2 \cos\varphi_1(E)\cos\varphi_2(E). \tag{190}$$

The function $g(E)$, given by the equation (188) determines the DOS inside the Landau bands. The boundaries of the Landau bands are determined by the condition

$$1 - f^2(E) = 0. \tag{191}$$

Outside the Landau bands $g(E) \equiv 0$. As we have discussed it above, the energy spectrum is periodic in case (189) and quasiperiodic in case (190). Inserting the function $f\,(E)$ of Eq. (189) into the definition Eq. (186) we have

$$g(E) = G_\rho(E)\left|\frac{d\varepsilon}{dE}\right|, \tag{192}$$

where

$$G_\rho(\varepsilon) = \frac{1}{\pi L}\frac{1}{\sqrt{4\rho^2 - \varepsilon^2}} \tag{193}$$

is the DOS of a 1D chain of atoms with energies $\varepsilon = 2\cos\varphi(E)$ and "hopping integrals" ρ. The analogy between the right-binding chain of atoms and the chain of coupled MB orbits makes it possible to calculate the DOS of two-dimensional MB structure shown in Fig.11.

To make this analogy more clear it is instructive to rewrite Eqs.(167) in the case when $\varphi(n)$ is independent on the orbit number n in the form

$$\rho\left[C_+(n+1) + C_+(n-1)\right] = 2\cos\varphi C_+(n). \tag{194}$$

This is exactly the tight-binding Schrödinger equation for the particle moving along the chain of atoms with the site energies $\varepsilon = 2\cos\varphi(E)$ and hopping integrals ρ between them. The DOS for this chain equals to the function $G_\rho(\varepsilon)$ (193).

The DOS of a 2D lattice shown in Fig. 12 is given then by the convolution of the two 1D densities of states

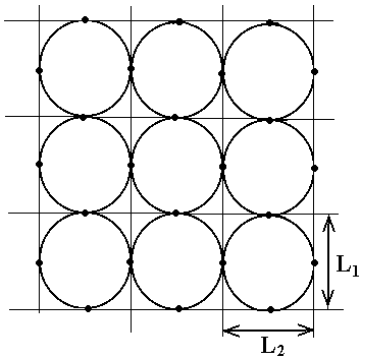

Figure 12: The DOS of a 2D lattice is given then by the convolution of the two 1D densities of states.

$$G_{\rho_1\rho_2}(\varepsilon) = \int_{-\infty}^{\infty} G_{\rho_1}(\varepsilon) G_{\rho_2}(\varepsilon - \omega) d\omega. \tag{195}$$

Completing integration in the Eq. (195) we find

$$G_{\rho_1\rho_2}(\varepsilon) = \frac{2}{\pi^2 L_1 L_2} \begin{array}{l} \left(a^2 - \varepsilon^2\right)^{-1/2} K\left[\frac{4(\rho_1\rho_2)^{1/2}}{(a^2-\varepsilon^2)^{1/2}}\right], |\varepsilon| \le 2b \\ \rho_1\rho_2^{-1/2} K\left[\frac{(a^2-\varepsilon^2)^{1/2}}{4(\rho_1\rho_2)^{1/2}}\right], 2b < |\varepsilon| \le 2a \\ 0, |\varepsilon| > 2a \end{array}, \tag{196}$$

where $a = 2(\rho_1 + \rho_2), b = 2|\rho_1 - \rho_2|$ and K stands for the complete elliptic integral of the first kind.

In the case of a square lattice $L_1 = L_2 = L, \rho_1 = \rho_2 = \rho$ and the DOS becomes

$$G_{\rho_1\rho_2}(\varepsilon) = \frac{2}{\pi^2 L^2 \rho} K\left[1 - \left(\frac{\varepsilon}{4\rho}\right)^2\right]. \tag{197}$$

The DOS's given by Eqs. (196) and (197) have logarithmic singularities at energies $\varepsilon = \pm 2b$ and $\varepsilon = 0$ correspondingly. Note that the 1D density of states $G_\rho(\varepsilon)$ (193) has a square root singularities at $\varepsilon = \pm 2\rho$.

So far we have obtained the DOS's of a MB-coupled networks as a function of the "energy" $\varepsilon = 2\cos\varphi(E)$. In terms of the real energy the DOS in all above cases is given by

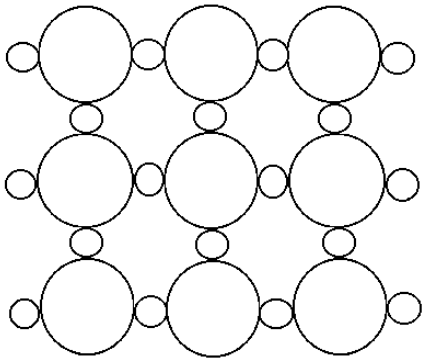

Figure 13: A 2D lattice composed of a small and large orbits.

$$g(E) = G_{\rho_1\rho_2}\left(2\cos\varphi(E)\right) 2\left|\sin\varphi(E)\right| \left|\frac{d\varphi(E)}{dE}\right| \tag{198}$$

with $\varphi(E)$ depending on the $S(E, p_z)$ according to the Eq. (169). In the case of a 2D lattice composed of a small and large orbits, as shown in Fig. 13, the density of states is given by Eq. (197) with $\rho = \rho_{eff}$ determined by Eq. (186).

The physical origin of the fact that a small orbit plays a role of the quantum gate with the effective tunneling probability $W_{eff} = \rho_{eff}^2$ is absolutely clear. To see this let us calculate the amplitude of probability for electron to transfer from a large orbit to the neighboring one via the small orbit. The result placed between them is given by the sum

$$\rho_{eff} = \rho e^{i\varphi}\rho - \rho e^{i\varphi}\tau e^{i\varphi}\tau e^{i\varphi}\rho + \rho e^{i\varphi}\tau e^{i\varphi}\tau e^{i\varphi}\tau e^{i\varphi}\tau e^{i\varphi}\rho... \tag{199}$$

Each term in this sum corresponds to transitions along the different paths. For example, the first term $\rho e^{i\varphi}\rho$ is the amplitude to tunnel from the large to small orbit (ρ) and after traveling along the semicircle ($e^{i\varphi}$) tunnel to the next large orbit (ρ). The following terms differ only by the number of windings around the small orbit. Every complete revolution around the small orbit yields a factor $-\tau e^{i\varphi}\tau e^{i\varphi}$ to the quantum amplitude ρ_{eff}. The negative sign in the amplitude $-\tau e^{i\varphi}\tau e^{i\varphi}$ is because of the our choice of the S-matrix (see Eq. (165)). Thus, the amplitude τ corresponds to the transition from the upper (+) semicircle of the small orbit to the lower (-) one, whereas for the transition in the opposite direction it equals $-\tau$.

Because of that terms with even and odd numbers of revolutions contribute to the ρ_{eff} with different signs. Summing the series (199) we have

$$W_{eff} = \left|\rho_{eff}\right|^2 = \frac{\rho^4}{\left|1+\tau^2 e^{i2\varphi}\right|^2} \tag{200}$$

One can see that equation (200) yields exactly ρ_{eff} of the Eq. (183) which oscillate because of the phase interference in full analogy with the interference optic devices.

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References

[1] V.M. Gvozdikov, A.G.M. Jansen, D.A. Pesin, I.D. Vagner, and P. Wyder, Phys. Rev B **68**, 155107 (2003); *ibid* **70**, 245114 (2004).

[2] I. Vagner, P. Wyder, and T. Maniv (Eds.), *Recent Trends in Theory of Physical Phenomena in High Magnetic Fields*, Proc. NATO Advanced Research Workshop, Les Houches, France, February 25 - March 1, 2002. NATO Science Series, v. **106**, pp.255-263 (Kluwer Academic Publishers, 2003).

[3] M. Taut, Phys. Rev. B **62**, 8126, (2000); *ibid* **63**, 115319 (2001).

[4] M. Taut, H. Eshrig, and M. Richter, Phys. Rev B **74**, in press (2005).

[5] F.A. Meyer, E. Steep, W. Biberacher, P. Christ, A. Lerf, A.G.M. Jansen, W. Joss, and P. Wyder, Europhys. Lett. **32**, 681 (1995).

[6] S. Uji, M. Chaparala, S. Hill, P.S. Sandhu, J. Qualls, L. Seger, and J.S. Brooks, Synth. Met. **85**, 1573 (1997).

[7] E. Steep, L.H. Nguyen, W. Biberacher, H. Muller, A.G.M. Jansen, and P. Wyder, Physica B **259-261**, 1079 (1999).

[8] C.P. Heidmann, H. Mueller, W. Biberacher, K. Neumaier, C. Probst, K. Andres, A.G.M. Jansen, and W. Joss, Synth. Met. **41-43**, 2029 (1991).

[9] T. Sasaki, H. Sato, and N. Toyota, Solid State Commun. **76**, 507 (1990).

[10] J. Caulfield, J. Singleton, F.L. Pratt, M. Doporto, W. Lubczynski, W. Hayes, M. Kurmoo, P. Day, P.T.J. Hendriks, and J.A.A.J. Perenboom, Synth. Met. **61**, 63 (1993).

[11] M.V. Kartsovnik, G.Yu. Logvenov, T. Ishiguro, W. Biberacher, H. Anzai, and N.D. Kushch, Phys. Rev. Lett. **77**, 2530 (1996).

[12] N. Harrison, J. Caulfield, J. Singleton, P.H.P. Reinders, F. Herlach, W. Hayes, M. Kurmoo, and P. Day, J. Phys. Cond. Matter **8**, 5415 (1996).

[13] E. Steep, L.H. Nguyen, W. Biberacher, H. Muller, A.G.M. Jansen, and P. Wyder, Physica B **259-261**, 1079 (1999).

[14] I.M. Lifshitz and A.M. Kosevich, Zh. Eksp. Teor. Fiz. **29**, 730 (1956).

[15] M. Nakano, J. Phys. Soc. Jpn. **66**, 19 (1997).

[16] A.S. Alexandrov, and A.M. Bratkovsky, Phys. Rev. Lett. **76**, 1308 (1986)

[17] P.D. Grigoriev and I.D. Vagner, Pis'ma Zh. Exp. Teor. Fiz. **69**, 139 (1999) [JETP Lett. **69**, 156 (1999)

[18] P. Grigoriev, Zh. Exp. Teor. Fiz. **119**, 1257 (2001) [JETP **92**, 1090 (2001)

[19] T. Champel, Phys. Rev. **B64**, 054407 (2001)

[20] T. Champel and V.P. Mineev, Philos. Mag. B **81**, 55 (2001)

[21] L.D. Landau, Z. Phys. **64**, 629 (1930).

[22] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, (Pergamon Press, New York, 1976).

[23] S. Flugge, *Practical Quantum Mechanics* (Springer, 1974).

[24] J.M. Ziman, *Principles of the Theory of Solids* (Cambridge Univ. Press, Cambrigde, 1972).

[25] M.H. Johnson and B.A. Lippmann, Phys. Rev. **76**, 828 (1949).

[26] A. Feldman and A.H. Kahn, Phys. Rev. B **1**, 4584 (1970).

[27] P. Carruthers and M.N. Nieto, Rev. Mod. Phys. **40**, 411 (1968). (1979).

[28] M.Ya. Azbel', Sov. Phys. JETP **19**, 634 (1964).

[29] D. Hofstadter, Phys. Rev. B **14**, 2239 (1976).

[30] Ju.H. Kim and I.D. Vagner, Phys. Rev. B **48**, 16564 (1993).

[31] M. Azbel, Solid State Commun. **53**, 147 (1985).

[32] L.E. Gurevich and A.Ya. Shik, Sov. Phys. - JETP **27**, 1006 (1968).

[33] V.M. Gvozdikov, Sov. Phys. - Solid State **26**, 1560 (1984).

[34] V.M. Polyanovskii, Sov. Phys. - Semicond. **21**, 783 (1987).