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The Landau problem in a two-band model

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Abstract

The Landau problem is a quantization of the motion of a charged particle in an external magnetic field on a basis of the standard Schrödinger equation. In this paper the Landau quantization is generalized to the case of a two-component wave function which obeys to the Bogoliubov-de Gennes equations.

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1 Introduction

This paper is devoted to the memory of my untimely deceased friend Professor Israel Vagner. His main scientific achievements have been related to the field of quantum magnetic oscillations in the low-dimensional conductors and superconductors. The latter are summarized in a well-known to experts review article [1].

In superconductors the energy spectrum and the two-component wave functions of the quasiparticles is governed by the Bogoliubov-de Gennes equations. Correspondingly, to calculate the energy spectrum and the wave functions in this case is much more difficult than to solve a standard Landau problem of the electron in an external magnetic field on a basis of the Schrödinger equation within the one band approach. In semiconductors the band effects are important. The most simple generalization is a two-band model with the gap due to the periodicity of the lattice or superlattice potential. In superconductors the gap is due to the correlations between electrons which brings an additional complication related to the self-consistency of the gap function $\Delta(\mathbf{r})$ which is very difficult to calculate because of the vortex-lattice formation in external magnetic field. The vortices make the effective magnetic field also a periodic function of coordinates. These effects are small near the upper critical magnetic field but in general even numerical calculations of the energy spectrum are rather difficult in superconductors [1, 2, 3]. In view of the above reasoning we will consider a more simple case assuming that $\Delta(\mathbf{r})$ is a known function of coordinate and neglecting the spatial dependence of the magnetic field. The latter in the Landau problem was studied in [4, 5]. We will call a model we use below for the Landau energy spectrum calculations "a two-band model".

2 Basic equations

The wave function in the two-band model has two components

$$\psi(\mathbf{r}) = \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix}, \tag{1}$$

which are normalized by the condition

$$|u(\mathbf{r})|^2 + |v(\mathbf{r})|^2 = 1. \tag{2}$$

The Schrödinger equation for the two-component wave function reads

$$\hat{H} \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix}. \tag{3}$$

A specific form of the matrix-Hamiltonian $\hat{H}$ depends on the physics behind the two-band model as we have discussed it in the Introduction. The gap may be due to the periodicity of the lattice or superlattice potential or due to the correlations between the charged particles (electrons, in superconductors). We do not go into these details here and just adopted the Hamiltonian $\hat{H}$ in the Bogoliubov-de Gennes form

$$\hat{H} = \begin{pmatrix} \hat{H}_A & \Delta \\ \Delta & -\hat{H}_A \end{pmatrix}, \tag{4}$$

where

$$\hat{H}_A = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}\right)^2 - E_F. \tag{5}$$

Here E_F is the Fermi energy, m and e stand for the electron mass and charge, c is the speed of light.

We assume here for more generality that Δ is a function of the spatial coordinate $\mathbf{r}$, i.e. $\Delta = \Delta(\mathbf{r})$. In the basis of the eigenfunctions of the Hamiltonian (5) which satisfy an equation

$$\hat{H}_A \varphi_n(\mathbf{r}) = \varepsilon_n \varphi_n(\mathbf{r}) \tag{6}$$

the equations for the $u - v$ functions can be written as follows

$$u(\mathbf{r}) = \sum_n u_n \varphi_n(\mathbf{r}),\; v(\mathbf{r}) = \sum_n v_n \varphi_n(\mathbf{r}), \tag{7}$$

$$(\varepsilon_n - E)\, u_n + \sum_m \Delta_{nm} v_m = 0, \tag{8}$$

$$\sum_m \Delta_{nm} u_m - (\varepsilon_n + E)\, v_n = 0.$$

The specific form of the $\varphi_n(\mathbf{r})$ depends on the gauge choice, whereas the Landau spectrum, $\varepsilon_n = \hbar\Omega(n + 1/2) - E_F$ is the gauge invariant ($\Omega = eB/mc$ is the cyclotron frequency).

The matrix element of Δ is equal to

$$\Delta_{nm} = \int \varphi_n^*(\mathbf{r})\, \Delta(\mathbf{r})\, \varphi_n(\mathbf{r})\, d\mathbf{r}. \tag{9}$$

We consider here a two-dimensional case in the Landau gauge $\mathbf{A} = (0, Bx)$ so that the basis functions are

$$\varphi_n(\mathbf{r}) = \psi_{NX}(\mathbf{r}) = L^{-1/2} \exp\left(-i\frac{Xy}{L_H^2}\right) \psi_N\left(\frac{x - X}{L_H}\right), \tag{10}$$

where

$$\psi_N(q) = \frac{H_N(q)}{\sqrt{2^N N! \pi^{1/2}}} \exp\left(-\frac{q^2}{2}\right) \tag{11}$$

is the wave function of the oscillator, $H_N(q)$ is the Hermitian polynomial of the order N, $L_H^2 = \hbar c/eB$ is the magnetic length. We also employ a complex index ($n \equiv N, X$) composed of the two quantum numbers: the Landau level number N, and the coordinate of the Landau orbit center, $X = -(cp_y/eB)$; L is the size of a sample along the Y-axis.

Equations (8) can not be solved without additional assumptions with resect to the function $\Delta(\mathbf{r})$ and the corresponding matrix element Δ_{nm} which in general is a complex function of the two quantum numbers decreasing exponentially with the enhancement of the parameter $|n-m|$. Fortunately, for some physical applications (vortex lattice in superconductors, for example) Δ_{nm} can be taken in the following approximate form [6]

$$\Delta_{nm} \approx \Delta_{N-m}. \tag{12}$$

We will use this equation as a model approach which makes possible analytical calculations. Another option is the perturbation theory.

3 The perturbative approach

To develop a perturbation theory on a basis of Eqs.(8) we first exclude one of the two components (u_n or v_n) from these equations. Excluding v_n, we have

$$(E-\varepsilon_n)\,u_n - \sum_k \sigma_{nk}(E)\,u_k = 0. \tag{13}$$

This equation has a form of the Schrödinger equation for some fictitious "particle on a lattice" with the hopping integrals

$$\sigma_{nk}(E) = \sum_m \frac{\Delta_{nm}\Delta_{mk}}{E+\varepsilon_m}. \tag{14}$$

The Green's function of Eq.(13) satisfies the following equation

$$\sum_m \left[(E-\varepsilon_n)\,\delta_{nm} - \sigma_{nm}(E)\right] G_{mk}(E) = \delta_{nk}. \tag{15}$$

The diagonal element of the Green's function can be written in the form:

$$G_{nn}(E) = \left[E-\varepsilon_n - \Sigma_n(E)\right]^{-1}, \tag{16}$$

where the self-energy $\Sigma_n(E)$ is given by

$$\Sigma_n(E) = \sigma_{nn}(E) + \sum_{k\neq n} \frac{\sigma_{nk}\Gamma_{kn}}{E-\varepsilon_k-\sigma_{kk}}. \tag{17}$$

The function Γ_{nm} here satisfies the integral equation

$$\Gamma_{nm} = \sigma_{nm} + \sum_{k\neq n,m} \frac{\sigma_{nk}\Gamma_{km}}{E-\varepsilon_k-\sigma_{kk}}, \tag{18}$$

which is equivalent to an infinite series in powers of σ_{nm} in the right-hand-side of this equation.

The energy spectrum of the system under consideration is determined by poles of the diagonal matrix element of the Green's function (16). In general this is a difficult problem, which nonetheless, can be solved for some specific cases. In case of $\Delta = const$ the matrix element Δ_{nm} (9) has only diagonal terms $\Delta_{nm} = \Delta\delta_{nm}$ and the self-energy

$$\Sigma_n(E) \equiv \sigma_{nn} \equiv \frac{\Delta^2}{E + \varepsilon_n} \tag{19}$$

since all the other terms in the series (17) are equal to zero. The energy spectrum in this case equals to

$$E_n = \sqrt{\left(\hbar\Omega\left(n + \frac{1}{2}\right) - E_F\right)^2 + \Delta^2}. \tag{20}$$

When Δ_{nm} is small, i.e. $|\Delta_{nm}| \ll |\varepsilon_n - \varepsilon_m|$, Eqs.(16)-(18) yield a perturbation series corrections for the Landau level ε_n:

$$E_n = \varepsilon_n + \sum_m \frac{|\Delta_{nm}|^2}{\varepsilon_n + \varepsilon_m} + ... \tag{21}$$

Now turn to the case of Eq.(12) for which a quasiclassical approach can be developed.

4 The quasiclassical approach

To develop a quasiclassical approach to the problem in question we first put the matrix elements Δ_{nm} in the form given by Eq.(12) into the Eq.(8) to obtain

$$[\hbar\Omega\,(N - N_0) - \delta - E]\, u_{NX} + \sum_{M,X'} \Delta_{N-M} v_{MX'} = 0,$$

$$\sum_{M,X'} \Delta_{N-M} u_{MX'} - [\hbar\Omega\,(N - N_0) - \delta + E]\, v_{NX} = 0, \tag{22}$$

where N_0 is the integer part of the ratio $E_F/\hbar\Omega$ so that $E_F = \hbar\Omega N_0 + \delta$.

The summation on the Landau orbit position X, in fact, is an integration over the variable X: $\sum_X \equiv \frac{1}{L_x}\int_0^{L_x} dx$, where L_x stands for the sample size in the X direction.

Taking this into account and counting N from the $N_0 \gg 1$, we have

$$\left(\hbar\Omega N-\delta-E\right)\tilde{u}_N+\sum_M \Delta_{N-M}\tilde{v}_M=0,$$

$$\sum_M \Delta_{N-M}\tilde{u}_M-\left(\hbar\Omega N-\delta+E\right)\tilde{v}_N=0, \tag{23}$$

where

$$\tilde{u}_N=\sum_X u_{NX},\ ,\tilde{v}_N=\sum_X v_{NX}. \tag{24}$$

One can rewrite Eq.(23) in the form of the differential equations with the help of the Fourier transform

$$f\left(\varphi\right)=\sum_N e^{-iN\varphi}f_N,\ ,f_N=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{iN\varphi}f\left(\varphi\right)d\varphi. \tag{25}$$

Applying this transform to Eq.(23) we obtain

$$\left(i\hbar\Omega\frac{d}{d\varphi}-E-\delta\right)u\left(\varphi\right)+\Delta\left(\varphi\right)v\left(\varphi\right)=0,$$

$$\Delta\left(\varphi\right)u\left(\varphi\right)-\left(i\hbar\Omega\frac{d}{d\varphi}+E-\delta\right)v\left(\varphi\right)=0, \tag{26}$$

where

$$\begin{cases} u\left(\varphi\right)=\sum_N e^{-iN\varphi}\tilde{u}_N, \\ v\left(\varphi\right)=\sum_N e^{-iN\varphi}\tilde{v}_N, \end{cases} \tag{27}$$

and

$$\Delta\left(\varphi\right)=\sum_N e^{iN\varphi}\Delta_{N.} \tag{28}$$

All these functions are 2π-periodic since a substitution $\varphi\to\varphi+2\pi$ does not change them.

A transformation

$$\begin{aligned} u\left(\varphi\right) &= e^{-i\frac{\delta}{\hbar\Omega}\varphi}\bar{u}\left(\varphi\right), \\ v\left(\varphi\right) &= e^{-i\frac{\delta}{\hbar\Omega}\varphi}\bar{v}\left(\varphi\right) \end{aligned} \tag{29}$$

helps to rid of the quantity δ in Eqs.(26) and a substitution

$$\begin{aligned} \bar{u}\left(\varphi\right) &= \frac{1}{2}\left(P\left(\varphi\right)-iQ\left(\varphi\right)\right), \\ \bar{v}\left(\varphi\right) &= \frac{1}{2}\left(Q\left(\varphi\right)-iP\left(\varphi\right)\right) \end{aligned} \tag{30}$$

yields the following equations for the new functions $P(\varphi)$ and $Q(\varphi)$:

$$-\hbar^2\Omega^2\frac{d^2P}{d\varphi^2}+W(\varphi)P=E^2P, \tag{31}$$

$$Q=\frac{1}{E}\left(-\hbar\Omega\frac{dP}{d\varphi}+\Delta(\varphi)P\right). \tag{32}$$

The equation for $P(\varphi)$ can be written then in the standard Schrödinger form

$$\hat{H}_W P(\varphi)=E^2P(\varphi) \tag{33}$$

with the Hamiltonian

$$\hat{H}_W=-\hbar^2\Omega^2\frac{d^2}{d\varphi^2}+W(\varphi), \tag{34}$$

where $W(\varphi)$ is periodic potential

$$W(\varphi)=\Delta^2(\varphi)+\hbar\Omega\frac{d\Delta(\varphi)}{d\varphi}. \tag{35}$$

The hamiltonian $\hat{H}_W$ has the very same "superpotential" form as the Hamiltonian of the Wittens supersymmetric quantum mechanics. The periodicity of the potential $W(\varphi)$ is a consequence of the periodicity of the function $\Delta(\varphi)=\Delta(\varphi+2\pi)$ which is periodic because of the model approach adopted by Eq.(12). It was shown in [6] that this approximation for the matrix elements holds for the spatially periodic "off diagonal" potential $\Delta(\mathbf{r})$ due to the vortex-lattice. This periodicity lifts up the Landau levels degeneracy on the orbit center position and broaden them into the dispersive Landau bands.

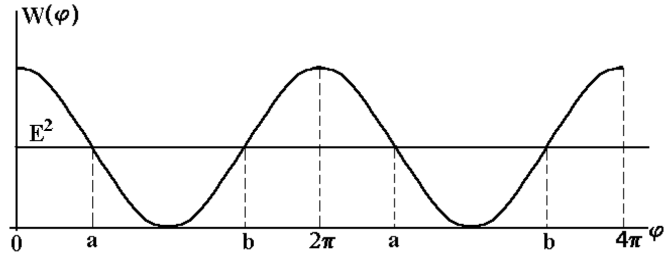

Figure 1: The band formation by periodic superpotential $W(\varphi)$. See text for more details.

Consider how these bands appear within the quasiclassical approach to the Schrödinger equation (33) in case when $E^2 < \max W(\varphi)$ as it is shown in Fig.1.

Eq.(33) can be written in a form suitable for the quasiclassical solution

$$\frac{d^2P}{d\varphi^2} + k^2(\varphi)\,P = 0, \tag{36}$$

where

$$k(\varphi) = \frac{1}{\hbar\Omega}\sqrt{E^2 - W(\varphi)}. \tag{37}$$

The standard quasiclassical quantization rule then yields

$$\oint k(\varphi)\,d\varphi = 2\pi\left(n + \frac{1}{2}\right) + \frac{(-1)^n}{\pi}\arcsin\left[\rho\cos(2\pi q)\right]. \tag{38}$$

The quantity

$$\rho = \exp\left(-\frac{B_0}{B}\right) \tag{39}$$

is a tunneling probability between the two adjacent potential wells in Fig. 1. It has the same exponential dependence on the magnetic field B as the magnetic breakdown probability [7]. The "breakdown magnetic field" is given by

$$B_0 = \frac{mc}{e\hbar}\int_a^b \sqrt{W(\varphi) - E^2}\,d\varphi. \tag{40}$$

The Bloch index q vary within the interval $[0,1]$. We can write the quantization rule (38) in the form

$$\frac{1}{2\pi}\oint \sqrt{E^2 - W(\varphi)}\,d\varphi = \hbar\Omega\left(n + \frac{1}{2}\right) + \varepsilon(\rho, q), \tag{41}$$

where $\varepsilon(\rho, q)$ is a dispersion within the Landau band

$$\varepsilon(\rho, q) = \frac{(-1)^n}{\pi}\hbar\Omega\arcsin\left[\rho\cos(2\pi q)\right]. \tag{42}$$

Within the quasiclassical approximation the Landau bands in our problem have the same structure as in the case of coherent magnetic breakdown in organic superconductors [7]. They appear as a result of the lifting up a degeneracy of the Landau levels by the periodic gap function $\Delta(\mathbf{r})$ which makes possible to approximate the matrix elements by $\Delta_{nm} \approx \Delta_{n-m}$ [6]. In a general case Δ_{nm} is not a function of the difference $n-m$ and the problem became untractable analytically. As we see, our model approach yields a simple analytic solution for the energy spectrum compatible qualitatively with the Landau band spectrum obtained numerically [1, 2, 3].

The width of the Landau bands is equal to

$$\Delta\varepsilon = \frac{2\hbar\Omega}{\pi} \arcsin \rho. \tag{43}$$

In case $B \gg B_0$ when $\rho \to 1$ and $\Delta\varepsilon \to \hbar\Omega$ the gap between the Landau bands vanishes as it is shown in Fig.2.

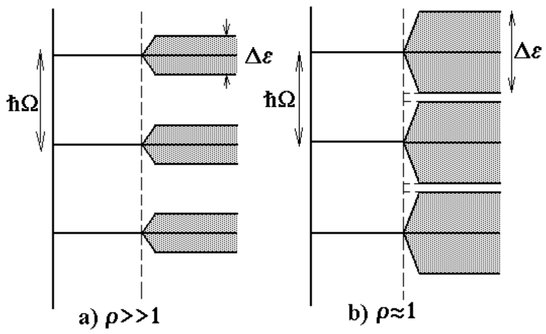

Figure 2: The Landau bands for small (a) and strong (b) magnetic breakdown effect. These bands appear as a result of the lifting up of the Landau levels degeneracy by the periodic gap potential $\Delta(\mathbf{r})$.

The Landau bands produces a special magnetic-breakdown factors in de Haas-van Alphen oscillations which strongly modulates the magnetic field dependence of oscillations in the superconducting vertex state [5].

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