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Impurity levels of electrons in 2D structures formed by magnetic edge states

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The bound states at the impurity center arising in a two-dimensional electron gas in a strong transverse magnetic field, taking into account the influence of the sample boundaries, are theoretically investigated. In the edge states, one component of the electron momentum is preserved, i.e. the motion becomes effectively one-dimensional. Using the example of a band of finite width, an equation is obtained that determines the energy of the impurity state and is a generalization of the known result for a shallow potential well in a one-dimensional system in the case of an arbitrary law of dispersion. The energies of the impurity levels belonging to the zero magnetic subzone are numerically found.

Keywords: two-dimensional electron gas, quantizing magnetic field, edge states, impurity levels.

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1. Introduction

In a bulk sample a strong magnetic field effectively „one-dimensionalizes“ the particle motion along the field direction. Since in the one-dimensional case any symmetric potential well has at least one bound level, the magnetic field creates a bound state even in a shallow and narrow attractive potential (Bychkov, 1960, see [1]).

In infinite two-dimensional system placed in a magnetic field normal to it, the electron spectrum is discrete with a degeneracy multiplicity proportional to the area of the system, and the wave functions, depending on the choice of calibration of the vector potential, can describe either state localized in the plane with a conserved moment projection onto the normal to the plane, or (Landau gauge) states delocalized along one axis (plane wave with momentum p) and localized in the perpendicular direction. The localization point X(oscillator suspension point) is determined by the value p: $X = pl^2$, where l — magnetic length.

The presence of an edge (boundary) of the sample violates the moment conservation, „skipping orbits“ arise, and only one type of states remains, it is described in the Landau gauge — magnetic edge states (MES). The degeneracy of Landau levels is removed, they turn into subbands $E_n(p)$ (or $E_n(X)$, $n = 0, 1, 2 \ldots$), i.e. the spectrum becomes similar to the spectrum of a quantum well, there is only free motion along one axis — along the edge of the sample. Thus, in a strong magnetic field, when transitions with change n are suppressed, the problem of the impurity center spectrum becomes similar to that in a one-dimensional system. Note that, in contrast to Bychkov's case, here the infinite motion occurs across the magnetic field, and the localization point of the wave function of the motion transverse to the edge depends on the momentum of this motion. Therefore, the energy of the bound state on the impurity depends significantly on the distance of the impurity center to the sample boundary. This paper relates to finding the energy of the impurity state in 2D system taking into account the existence of the MES.

2. Equivalent Hamiltonian method

We will apply an approach similar to the Vanier method in the theory of impurity states of 3D semiconductors. Let's consider a strip of 2D electron gas with width L ($-L/2 \le x \le L/2$), the edges of which specify the direction Oy. The boundary conditions correspond to impenetrable „walls“ i.e. the wave function $\Psi(x, y)$ goes to zero $x = \pm L/2$. In the Landau gauge Ψ has the form

$$\Psi_{np} = \frac{e^{ipy}}{\sqrt{2\pi}} \phi_n(x - pl^2),$$

where $n = 0, 1, 2 \ldots$, $-\infty < p < \infty$, ϕ_n normalized to one in the interval $[-L/2, L/2]$, and ϕ — to δ-function of momentum p along axis y (hereinafter $\hbar = 1$). The transverse motion function ϕ_n is expressed through degenerate hypergeometric functions F:

$$\phi_n = AD_q\left(\frac{x - X}{l/\sqrt{2}}\right) + BD_q\left(-\frac{x - X}{l/\sqrt{2}}\right), \qquad (1)$$

$$D_q(Z) = \frac{2^{q/2}\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1-q}{2}\right)} e^{-z^2/4} F\left(-\frac{q}{2}, \frac{1}{2}, \frac{z^2}{2}\right) - \frac{2^{q/2}\sqrt{2\pi}}{\Gamma\left(-\frac{q}{2}\right)} z e^{-z^2/4} F\left(\frac{1-q}{2}, \frac{3}{2}, \frac{z^2}{2}\right),$$

$$q = \frac{E}{\omega} - \frac{1}{2}.$$

Index n arises when solving the equation to eigen energies $E_n(p)$ resulting from the boundary conditions

$$\frac{D_q\left(\frac{L/2-X}{l/\sqrt{2}}\right)}{D_q\left(-\frac{L/2+X}{l/\sqrt{2}}\right)} - \frac{D_q\left(\frac{L/2-X}{l/\sqrt{2}}\right)}{D_q\left(\frac{L/2+X}{l/\sqrt{2}}\right)} = 0. \quad (2)$$

Let us introduce the Fourier transform Ψ_{np} with respect to the variable p:

$$\Psi_{np} = \frac{1}{\sqrt{2\pi}} \int e^{ipu} \varphi_n(u) du. \quad (3)$$

Accordingly, we have

$$\varphi_n(u; x, y) = \frac{1}{2\pi} \int e^{-ipu} \Psi_{np}(x, y) dp.$$

Then the functions φ are normalized by the condition

$$\left\langle \varphi_m^*(v) \varphi_n^*(u) \right\rangle = \delta_{nm} \delta(u - v).$$

The action of the undisturbed, i.e. without impurity, Hamiltonian $\hat{H}_0$ to the function $\varphi_n(u)$ leads to the result

$$\hat{H}_0 \varphi_n(u) = \int E_n(u - v) \varphi_n(v) dv, \quad (4)$$

where $E_n(w)$ is the Fourier image of the energy $E_n(p)$:

$$E_n(w) = \frac{1}{2\pi} \int e^{-ipw} E_n(p) dp. \quad (5)$$

In the presence of the impurity center, the solution is sought in the form of a series in n and an integral in u of the functions $\varphi_n(u)$ with coefficients $f_n(u)$:

$$\Phi(x, y) = \sum \int f_n(u) \varphi_n(u; x, y) du, \quad (6)$$

and the problem comes down to obtaining and solving the equation for the envelope $f_n(u)$. The sought-for eigenfunction of the total Hamiltonian $\hat{H}_0 + U(x, y)$, where U — potential of the impurity center, satisfies the equation

$$(\hat{H}_0 + U)\Phi_n = \varepsilon_n \Phi_n, \quad (7)$$

where ε_n — the energy of the state localized on the impurity.

After substituting expansion (6) into equation (7), multiplying both sides by $\varphi_m^*(w)$ and integrating over $dxdy$ we obtain

$$\langle \varphi_m^*(w) \hat{H}_0 \Phi \rangle = \int f_m(u) E_m(u - w) du,$$

which after introducing the shift operator on u' in the form $\exp(u'\partial/\partial w)$ gives

$$\langle \varphi_m^*(w) \hat{H}_0 \Phi \rangle = E_m(-i\partial/\partial w) f_m(w) \quad (8)$$

Thus, for the envelope $f_m(w)$ we obtain the equation

$$E_m(-i\partial/\partial w) f_m(w) + \sum_n \int \varphi_m^*(w) f_n(u) \varphi_n(u) U(x, y) dx dy = \varepsilon f_m(w).$$

3. Impurity states

Next, we introduce the assumptions usual in the Vanier technique, they relate the nature of the impurity potential. The function $U(x, y)$ will be assumed smooth, and the magnetic field is strong enough, so the characteristic size of the potential a (in the case of a Coulomb center the effective Bohr radius a_B^*) is much larger than the magnetic length: $a \ll l$. The strong field also means that the potential amplitude U_0 (Rydberg energy in the Coulomb case) is much less than the Landau quantum: $U_0 = \omega_c$. Recall that the characteristic size $\Psi_{np}(x)$ by x, as well as the size $\varphi_n(u)$ by u is about l, t.e. the functions under the integral in the second term in (9) have narrow maxima compared to the size $U(x, y)$. For example, for an infinite plane at the zero Landau level we have

$$\Psi_{0p}: \exp\left[ipy - (x - X)^2/2l^2\right],$$

$$\varphi_0(u): \exp\left[(y - u)^2/2l^2 + ix(y - u)/l^2\right].$$

Therefore, the maximum contribution from the matrix element U_{mn} occurs at $n = m$, $y \approx u \approx w$, $x \approx 0$ (more precisely, we are talking about the areas $|y - w|: l$, $|x(y - w)|: l^2$; outside these areas the exponentials decay quickly or oscillate rapidly).

It follows that in (9) we shall substitute $U(x = 0, y = w)$ and remove this value from the integral. The point $x = 0$ is determined by writing the wave function in the problem without admixture. For a band with identical (zero) boundary conditions at the edges this point is the middle of the band. If the maximum (minimum) of the impurity potential is located at $x = s$, $y = 0$ (y can always be counted from the impurity), then the value removed from the integral is $U(x = s, y = w)$. Thus, the problem was reduced to a one-dimensional one, but with an arbitrary law of electron dispersion

$$E_n(-i\partial/\partial w) f_n(w) + U(s, w) f_n(w) = \varepsilon_n f_n(w). \quad (9)$$

Localized (decreasing at $w \to \pm\infty$) solutions of equation (9) determine the energy values of the impurity state ε_n associated with the n-th Landau subband. If the impurity potential is axially symmetric, i.e. $U = U(\rho)$, $\rho^2 = x^2 + y^2$, then in (9):

$$U(s, w) = U(\sqrt{s^2 + w^2}).$$

Next, we carry out the same calculations as in [1], §45. Inside the potential well $U(\rho)$we neglect ε, considering the level ε shallow compared to the depth of the well ($\varepsilon = |U|$) and assume $f_n = 1$, and outside the potential radius, when $|w| \ll a$, we look for the solution in the form $f_n(w)$: $e^{-\gamma_n|w|}$. Inside the well we integrate over w:

$$\int \hat{E}_n(-i\partial/\partial w) f_n(w) dw = -\int_{-\infty}^{\infty} U(w) dw \equiv -\lambda \quad (10)$$

The operator $\hat{E}_n(-i\partial/\partial w)$, acting on $e^{-\gamma_n w}$ gives $E_n(i\gamma)$. Expanding $\hat{E}_n(-i\partial/\partial w)$ into a power series $(-i\partial/\partial w)$, we see that integration over w reduces the power of each term in the series by one. Summing the series again after this, we get

$$\int \hat{E}_n(-i\partial/\partial w) e^{-\gamma w} dw = -E(i\gamma)/\gamma.$$

Due to the parity of $e^{-\gamma_n|w|}$, the equation for ε_n takes the form $\varepsilon = E(i\gamma_n)$, where γ_n is the root of the equation

$$\frac{2E_n(i\gamma_n)}{\gamma_n} = \int_{-\infty}^{\infty} U(w) dw, \quad (11)$$

i. e. $\varepsilon_n = \lambda\gamma_n/2$.

Equation (11), together with the definition $\varepsilon_n = E(i\gamma_n)$ generalizes the well-known formula for the shallow level in one-dimensional potential well ([1], §45) to the case of an arbitrary electron dispersion law.

For the standard dispersion law $E = p^2/2m$ from (11) we obtain the well-known result [1]: $\varepsilon_n = -m\lambda^2/2$, i. e. the binding energy of the particle on the impurity is quadratically small compared to the depth of the potential well.

4. Numerical modeling of the magnetic subband case

Landau's subband dispersion law $E_n(p)$ cannot be expressed in elementary or known special functions. It is specified as an implicit parameter function $X/l = pl$, which is the subscript q in equation (2). Graphs $E_n(p)$ for the two lower subbands are shown in Figure 1, *a*. Their form is quite understandable and was repeatedly cited in the literature (e. g. [2,3,4]). The form of these functions for a purely imaginary argument, appearing in equation (11) for the energy of the impurity state, turned out to be quite unexpected — see Figure 1, *b*. It can be seen that for γl over a certain threshold value, there are no real roots of the dispersion equation (2). We checked that the left side of equation (2) as a function q crosses the abscis axis many times. The minimum lying between adjacent intersection points rises with parameter γl increasing, two intersection points merge into one tangent point, which corresponds to the merger of the solid and dotted curves in Figure 1, *b*. With further γl increasing the minimum becomes a positive

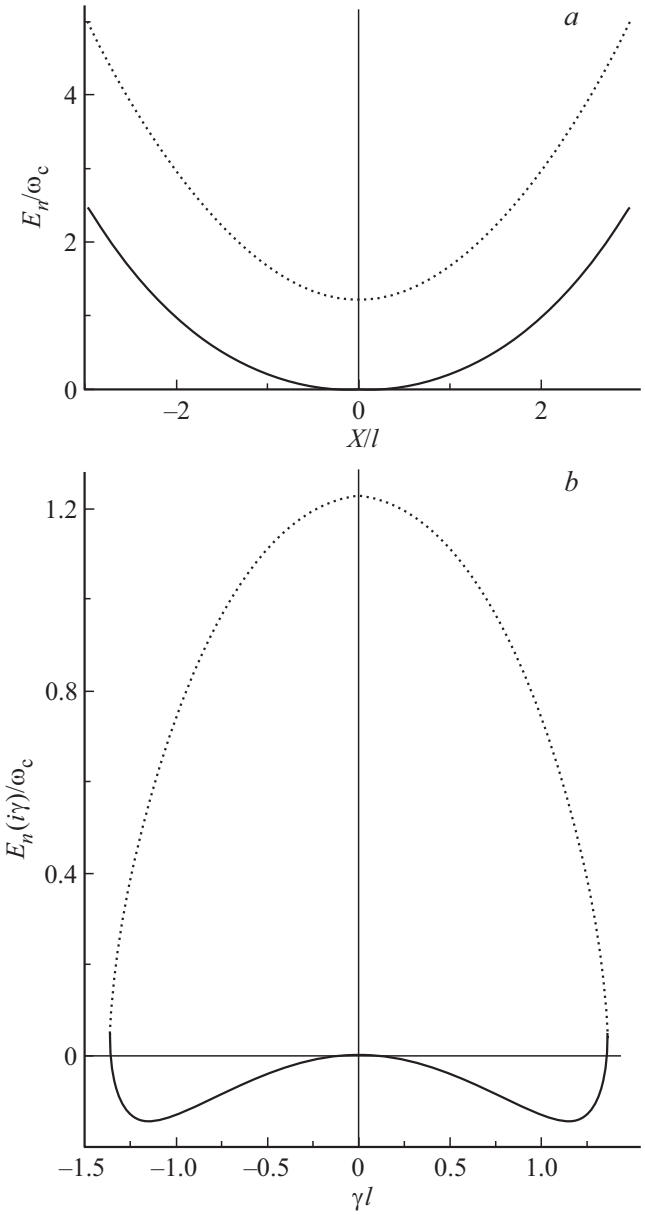

Figure 1. *a*) Two lower Landau levels (solid line for $n = 0$, dots for $n = 1$) in band $L = 4l$ wide. Energy is counted from $E_0(X = 0)$. *b*) The same functions with an imaginary argument.

value, and this pair of real roots of eq. (2) disappears. The following roots lie at significantly higher values q and correspond to higher subbands.

The minimum for positive gamma on the solid curve in Figure 1, *b* means that equation (11) has two roots. The results of their numerical calculation are shown in Figure 2. At some value of the dimensionless parameter $ml\lambda$ the roots merge in accordance with what was said above about the behavior of the laws of subband dispersion for imaginary argument. Consequently, there are two localized states on a short-range impurity associated with the zero subband.

In the case of Coulomb center at the point $x = s$, $y = 0$, the potential U is equal to $-e^2/\sqrt{s^2 + w^2}$. The integral

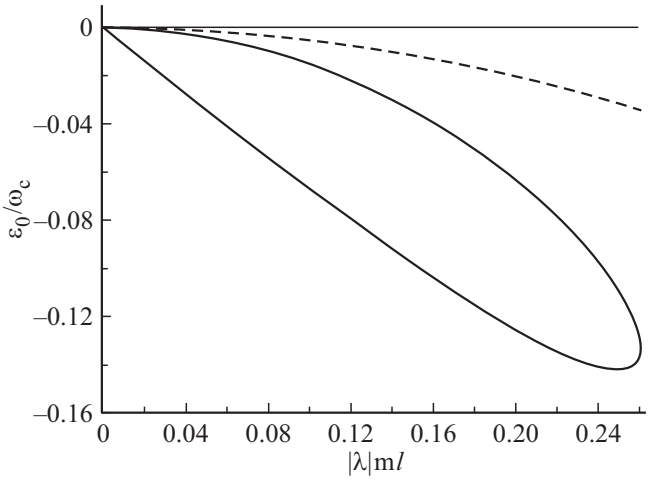

Figure 2. Solid lines show the bond energies of two localized states. The dotted line corresponds to the quadratic dispersion law: $\varepsilon = -m\lambda^2/2$.

in (10) diverges and is „cut off" at the top at $w: a_B$, and at the bottom at w exceeding the larger of the quantities s and l. Then with logarithmic precision

$$\lambda = 2\ln\left[\frac{a_B + \sqrt{a_B^2 + s^2}}{\max(s, l)}\right],$$

and at $s = l\lambda$ depends on the magnetic field.

So, the paper shows that the energy of impurity levels associated with magnetic edge states in 2D electron gas is determined by the behavior of the dispersion law of magnetic subbands at imaginary values of momentum. The energies of impurity states belonging to the zero subband were found numerically.

Conflict of interest

The authors declare that they have no conflict of interest.

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