Bound states of an electron at a small-radius center in a magnetic field

S. P. Andreev and A. V. Koshelkin
Moscow Engineering Physics Institute

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The spectrum of bound and quasibound states is derived for an electron with an arbitrary angular momentum at a center of arbitrary depth in a magnetic field in an arbitrary Landau band N. The effective range of the attractive potential is assumed small in comparison with the magnetic length.

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1. The spectrum of an electron in the field of a center having a small radius $a \ll l$ [$l=(c\hbar/|e|H)^{1/2}$ is the magnetic length] in a magnetic field was studied in Refs. 1–4. Demkov and Drukarev[2] used the method of a zero-radius potential to study a weakly bound state of an electron with a zero projection ($m=0$) of its orbital angular momentum (L) on the direction of the magnetic field **H** in the $N=0$ band. They used a single phenomenological parameter: the amplitude for scattering of the electron by the center at $H=0$. Andreev[3] studied the spectrum of bound and quasibound states of an electron in the field of a small center $U \ll \hbar^2/m^*a^2$ in an arbitrary Landau band for the case of a slight mixing of Landau levels by the center. In Ref. 4, Demkov and Drukarev studied weakly bound states with $L \neq 0$ by using two phenomenological parameters: the binding energy at $H=0$ and the effective radius of the center, $a(H=0)$. For weakly bound states, the Landau levels are extensively mixed by the center, so that the problem becomes three-dimensional, and the question of boundary conditions must be dealt with. The boundary condition of a continuous logarithmic derivative is extremely sensitive to the distance ΔU of the potential from resonance, and at $L \neq 0$ it is also extremely sensitive to the energy of the particle, $E(H)$. Demkov and Drukarev[4] replaced this boundary condition by a boundary condition (averaged over angles) on the wave function on the surface of the sphere $a(H=0)$, but they ignored the change in the normalization coefficient of the wave function at $H \neq 0$, which is just as sensitive to ΔU and E. The boundary condition of Ref. 4 is valid for $\Delta U \lesssim \hbar\omega_H$ if $\Delta U > 0$ ($\omega_H = eH/m^*c$ is the cyclotron frequency), but it requires some refinement if $\Delta U < 0$. Furthermore, the question of the boundary conditions for a spectrum in an arbitrary Landau band $N \neq 0$ remains open.

In this letter we will derive the spectrum of bound and quasibound states of an electron at a center of arbitrary depth in an arbitrary Landau band N, with an arbitrary value of m, in a uniform magnetic field $\mathbf{H} \parallel z$, adopting only the one assumption $a \ll l$. We assume that the system of solutions of the Schrödinger equation for the electron in the field $U(r)$ at $H = 0$ is known.

2. The wave function of an electron with a given projection (m) of its orbital angular momentum on the magnetic field direction satisfies the integral equation

$$\psi_m(\rho; z) = -\frac{m^*}{2\pi\hbar^2}\int d^3r'\, \psi_m(\rho'; z')U(r')\, C_m(\mathbf{r}; \mathbf{r}'; E; H). \tag{1}$$

Here $C_m(\mathbf{r}; \mathbf{r}'; E; H)$ is the Green's function of the electron in the magnetic field. It can be seen from (1) that the solution $\psi_m(\rho'; z')$ in the "interior" region $r \lesssim a$ determines the wave function throughout the space. In the case of a center of small radius $\ll l$ we may ignore the effect of the oscillatory potential of the magnetic field, $\sim m^*\omega_H^2\rho^2 \propto \hbar\omega_H a^2/l^2$, on the electron in the effective range of the potential $U(r)$ if $\hbar\omega_H a^2/l^2 \ll \max(\Delta U; E)$. In this case the solution of the Schrödinger equation in the interior region describes the electron in the field $U(r)$ at $H = 0$ (with a replacement of the energy, $E \to E - m/2\,\hbar\omega_H$). In other words, since the radius of the center is small, the wave function ψ_m in the interior region depends on H only through the parameter E (which is to be found), and the Schrödinger equation can be solved for small $r \lesssim a$ without knowledge of the Green's function of the electron, $C_m(E;H)$. This circumstance radically simplifies the solution of the problem.

Furthermore, the Green's function $C_m(\mathbf{r}; \mathbf{r}'; E; H)$ in (1) also depends on the energy of the electron as a parameter, and it depends in a complicated way on the magnetic field. If E is known, then Eq. (1) should become an identity in the interior region. The system of solutions of the Schrödinger equation in the interior region is the product of radial and spherical wave functions[5]:

$$\psi_{Lm}(\rho; z) = R_{Lm}(E; r)\Theta_{Lm}(\theta), \tag{2}$$

where the function R_{Lm} satisfies the usual boundary condition at the origin, $R_{Lm}(r \to 0) = 0$. Since L is not a good quantum number at $H = 0$, the wave function in (1) in the interior region is a superposition of (2) with arbitrary coefficients $C_{L \geqslant |m|}$. It is easy to show that the energy of a state with a given value of m in a magnetic field is determined by the state with $L = |m|$, and the incorporation of states with $L > |m|$ gives rise to small corrections on the order of $\min\{a^2 l^{-2}; |1/2 - E/\hbar\omega_H|\}^{L-|m|}$. As ψ_m in the interior region, we accordingly adopt (2) with $L = |m|$. Even in this case, however, the structure of $G_m(\mathbf{r}; \mathbf{r}'; E, H)$ in the magnetic field is such that for an arbitrary value of E and for a finite value of r it is not possible to separate the angular and radial variables in the Green's function. A third circumstance, which contributes to the solution of this problem, is that the angular and radial variables separate in G_m in the limit $r \to 0$. Here,

$$G_m(r \to 0) \propto \rho^{|m|} \propto r^{|m|}\sin^{|m|}\theta \propto r^{|m|}\Theta_{mm}(\theta). \tag{3}$$

If $U(r \to 0)$ increases more slowly than r^{-2}, then

$$R_L(r \to 0) = A^{(L)} r^L. \tag{4}$$

Substituting (2) with $L = |m|$ in (1), taking the limit $r \to 0$, using (3) and (4), and separating the angular and radial variables in G_m, we find an equation which determines the energy spectrum of an electron in a state with an arbitrary value of m, in the field of an attractive center which has a small radius but an arbitrary depth, and in a uniform magnetic field. For the $N = 0$ Landau band, this equation can be written as ($|m| \to m$)

$$A^{(m)} a^m = -\frac{\Delta^{2m}}{(2m+1)!!} \int_0^\infty f_m(x) dx \left\{ \sum_{n=0}^{m} B_n^{(m+1)} \frac{1}{n!} \left(-\frac{d}{\Delta^2 x dx} \right)^{m-n} \frac{e^{-\sqrt{2\eta}\Delta x}}{x} \right.$$

$$\left. - \sqrt{\frac{2}{\pi}} \Delta \int_0^\infty dt\, e^{-\eta t^2} \left[(1 - \exp(-t^2))^{-m-1} - \sum_{n=0}^{m-1} B_n^{(m+1)} \frac{(t^2)^{n-m}}{n!} \right] \right\}, \tag{5}$$

$$\Delta \equiv a l^{-1};\ \eta = \frac{1}{2} - E/\hbar\omega_H;\ f_m(x) = x^{m+2} R_{mm}(x) v(x),\ v(x) = \frac{U(x)}{\hbar^2/m^* a^2};\ x = r/a .$$

Here $B_n^{(m)}$ are the Bernoulli numbers of index m (Ref. 6). In the derivation of (5) we made use of the circumstance that the Green's function in (1) can be summed over all the Landau bands.[6] Equations analogous to (5) can be derived for the spectrum in an arbitrary Landau band $N \neq 0$.

3. From Eq. (5) we can draw several general conclusions about the electron energy spectrum. The most interesting case is that of a well near resonance, in which the depth U is such that there is a virtual or real weakly bound state in the well in the absence of a magnetic field. The energy of the electron is small in this case, $\sqrt{2\eta}\,\Delta \ll 1$, and the exponential functions in (5) can be expanded. For $m = 0$, the nonvanishing term of this expansion containing η is proportional to $\sqrt{\eta}$, while for $m \neq 0$ it is proportional to η itself.

If the depth of the well is such that it contains no shallow bound states with $E \ll \hbar^2/m^* a^2$ in the absence of a magnetic field, then the application of a magnetic field will lead to the appearance of levels which lie below the bottom of the Landau band and which are sensitive to the magnetic field.[2-4] In the limit $H \to 0$, such states correspond to $\eta \ll 1$; the typical range of the integration over t in (5) is large in comparison with unity; and the integral can be replaced by its asymptotic value $\propto 1/\sqrt{\eta}$. The electron energy can be ignored in the constant $A^{(m)}$ and in the function f_m in (5). As a result, we find for the magnetic states

$$\frac{\hbar\omega_H}{2} - E = \frac{\alpha_m^2}{2}\Delta^{4m+2}\hbar\omega_H \quad . \tag{6}$$

It can be shown that the constant α_m is proportional to $(\hbar^2/m^*a^2)E_m^{-1}$, where E_m is the energy of the virtual level with given m at $H=0$. In the particular case $m=1$, Eq. (6) becomes the same as the equation derived in Ref. 4.

If there is a real bound state in the well, and the magnetic field acts on this state as a perturbation, i.e., if $|E| \gg \hbar\omega_H$ or $\eta \gg 1$, then the range of the integration over t in (5) is typically small in comparison with unity. Expanding the arguments of the exponential functions in (5), and retaining terms up to those $\propto t^4$, we find on the right side a sum of terms $\propto [-\eta+(m+1)/2] \propto E+(1/2)m\hbar\omega_H$. The energy appears in the same combination in the constant for the interior region, A^m. The equation found from (5) in this case does not contain a different dependence on H, and we arrive at an expression for the energy levels of the electron with paramagnetic corrections:

$$E = E_m - \frac{1}{2}m\hbar\omega_H \, .$$

By taking into account small terms of higher order in t in (5), we can derive diamagnetic corrections to the electron energy spectrum.

Furthermore, in the particular case with $m=0$ and $\sqrt{\eta}\,\Delta \ll 1$, the equation found from (5) is the same as the equation found for the spectrum in Ref. 2.

4. In contrast with the spectrum in the lower Landau band, the states in the $N>0$ bands with $m<N$ are approximately stationary. The quasibound state with $m=0$ in the $N=1$ Landau band at $U \ll \hbar^2/m^*a^2$ lies a distance $\mathrm{Re}E \propto \hbar\omega_H\Delta^2 U^2$ below the bottom of band 1 and has a width $\mathrm{Im}E \propto \hbar\omega_H\Delta^3 U^3$, in accordance with Ref. 3. As U is increased, the level goes deeper, but its depth initially increases much more rapidly than its width, so that at $\mathrm{Re}E \cong 0{,}5\hbar\omega_H$ we have $\mathrm{Im}E/\mathrm{Re}E = 0, 1$. Later, beginning at $\mathrm{Re}E \approx 0, 5\hbar\omega_H$, the width of the level increases rapidly in comparison with its depth.

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