Weakly bound electrons in external magnetic field

I.V. Mamsurov\textsuperscript{1} and F. Kh. Chibirova\textsuperscript{2}
\textsuperscript{1}Faculty of Physics, Moscow State University, 119899, Moscow, Russia
\textsuperscript{2}Karpov Institute of Physical Chemistry, 103064, Moscow, Russia

The effect of the uniform magnetic field on the electron in the spherically symmetric square-well potential is studied. A transcendental equation that determines the electron energy spectrum is derived. The approximate value of the lowest (bound) energy state is found. The approximate wave function and probability current density of this state are constructed.

I. INTRODUCTION

Quantum nonrelativistic systems in external electromagnetic field have attracted permanent interest due to possible application of their models in many phenomena of quantum mechanics. Particularly it concerns so-called bound electron states. For example, it is well known that the integer quantum Hall effect is correlated with the presence of weakly bound electron states in corresponding samples. Nonrelativistic electrons in an external magnetic field are also responsible for such remarkable macroscopic quantum phenomena as, for example, high-temperature superconductivity. \cite{1}. Magnetic fields are also likely to effect on weakly bound electrons into singular potentials of defects in defect films \cite{2, 3}. The effect of magnetic fields on loosely bound electron in two dimensions models was studied in \cite{4}. To this problem are also related such phenomena as parity violation, the Aharonov-Bohm effect \cite{5}, and others. The behavior of an electron in a constant uniform magnetic field and single attractive $\delta$ potential in three spatial dimensions was studied in \cite{6}, in which it was also obtained non trivial result for probability current density of the loosely bound electron state. This current resembles “pancake vortices” in the high-temperature superconductors.

In this paper is studied a more general case of the electron behavior in external uniform magnetic field in the presence of spherically symmetric square-well potential of finite radius. The calculations are made supposing small size of this radius compared to the magnetic length $a = \sqrt{\hbar/m\omega}$. In the first approximation in the small parameter $\xi = R^2/2a^2 \ll 1$ is derived transcendental equation for the electron energy spectrum, and also approximate value of the bound energy state. Accordingly in zero approximation a wave function of the bound state is obtained, and the value of probability current for this state is calculated. This current, as also in \cite{6}, appears to have non zero circulation around the axis parallel to the external magnetic field and to be mostly confined within the perpendicular plane.

II. SCHRODINGER-PAULI EQUATION

Let us consider an electron in a spherically symmetric square-well potential of the form:

$$U(r) = \begin{cases} 
- U_0, & r < R \\
0, & r > R 
\end{cases}$$

in the presence of uniform magnetic field $H$, which is directed along the axis $z$. Vector potential is specified in a cylindrically symmetric gauge:

$$A_\phi = \frac{H \rho}{2}, A_\rho = A_z = 0.$$  \hspace{1cm} (2)

Let us write the Schrödinger-Pauli equation for this electron:

$$i\hbar \frac{\partial}{\partial t} \psi(t, \mathbf{r}) = \hat{H} \psi(t, \mathbf{r}),$$

where Hamiltonian in cylindrical coordinates has the form:

$$\hat{H} = \frac{\hbar^2}{2m} \left[ \frac{\partial}{\rho \partial \rho} \left( \frac{\partial}{\partial \rho} \right) + \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\rho^2 \partial \phi^2} \right] - \frac{i\hbar \omega}{2} \frac{\partial}{\partial \phi} + \frac{m\omega^2}{8} \rho^2 + U(\sqrt{\rho^2 + z^2}) + \mu \sigma_3 H,$$  \hspace{1cm} (4)

where:

$$\omega = \frac{|e|m}{\hbar c}, \mu = \frac{|e|\hbar}{2mc}, \sigma_3 = \begin{pmatrix} 1 & 0 \\
0 & 1 \end{pmatrix}.$$  \hspace{1cm} (5)
We are interested in a stationary solution of the equation (3):

$$\psi(t, r) = e^{-i\frac{\hbar}{m}t} \psi_E(r).$$  

(6)

It is reasonable to seek the spatial part of the wave function in the form:

$$\psi_E(r) = \int_{-\infty}^{+\infty} dp_z \sum_{n_p = 0}^{+\infty} C_{E_n, l^2} \psi_{n_p, l^2}(r).$$  

(7)

Wave functions on the right side of this equation (7) are eigenfunctions of Hamiltonian (4) in the absence of spherically symmetric potential (see, for example, (7)).

$$\psi_{n_p, l^2}(r) = \frac{1}{\sqrt{(n_p + |l|)! n_p!}} e^{-\frac{z^2}{2a^2}} l^{(l)} Q_n^{(l)}(x)$$  

(8)

Where \(s = \pm 1\) is a constant quantum spin number of an electron, \(a = \sqrt{\hbar/m\omega}\), and Laguerre functions:

$$I_{n,l}(x) = \frac{1}{\sqrt{(n_p + |l|)! n_p!}} e^{-x/2} x^{\frac{|l|}{2}} Q_n^{(l)}(x)$$  

(9)

are expressed through corresponding polynomials. Multiplying the both sides of (7) by \(\psi_{N_p, l^2}\), transferring to the right side the term containing the potential \(U(r)\), and to the left side all other terms, and integrating over all spatial coordinates, we obtain:

$$C_{E_{N_p, l^2}} \left( \hbar \omega \left( N_p + \frac{|L| + L + 1 + s}{2} \right) + \frac{P_z^2}{2m} - E \right) =$$

$$= \frac{U_0}{\pi} \int_{-\infty}^{+\infty} dp_z \sum_{n_p = 0}^{+\infty} C_{E_n, l^2} \frac{1}{P_z - p_z}$$

$$\frac{1}{a^2} \int_{0}^{R} \rho dp I_{n_p, l} \left( \rho^2/2a^2 \right) I_{N_p, l} \left( \rho^2/2a^2 \right) \sin \left( \frac{P_z - p_z}{\hbar} \sqrt{R^2 - \rho^2} \right).$$  

(10)

Taking into account a small radius of the potential well compared with magnetic length: \(R^2/a^2 << 1\), we expand the product of Laguerre functions on the right side of (10) in a power series of parameter \(\rho^2/2a^2\), up to the terms of the first order. We also suppose that in reality the integral over \(p_z\) on the right side of (10) has the finite limits. Accordingly we put: \(\sqrt{R^2 - \rho^2} (P_z - p_z)/\hbar << 1\) and substitute the sinus on the right side of (10) by its argument. Then integrating over \(\rho\) and using designation: \(U_0R^3 = \lambda\), we obtain the following result:

$$C_{E_{N_p, 0^2}} \left( \hbar \omega \left( N_p + \frac{1 + s}{2} \right) + \frac{P_z^2}{2m} - E \right) =$$

$$= \frac{\lambda}{\pi \hbar a^2} \int_{-\infty}^{+\infty} dp_z \sum_{n_p = 0}^{+\infty} C_{E_{N_p, 0^2}} \left[ \frac{1}{3} - \frac{2}{15} \xi (1 + n_p + N_p) \right], L = 0. $$  

(11)

$$C_{E_{N_p, l^2}} \left( \hbar \omega \left( N_p + \frac{|L| + L + 1 + s}{2} \right) + \frac{P_z^2}{2m} - E \right) =$$

$$= \frac{\lambda}{\pi \hbar a^2} \int_{-\infty}^{+\infty} dp_z \sum_{n_p = 0}^{+\infty} C_{E_{N_p, l^2}} \left[ \frac{2}{15} \xi (n_p + 1)(N_p + 1) \right], L = \pm 1.$$  

(12)

Where \(\xi = m\omega R^2/2\hbar\). In case of all other values of \(L\) the right side of (12) in the first approximation equals to zero. It means that corresponding coefficients \(C_{E_{N_p, l^2}}\) also equal to zero when \(L \neq 0, \pm 1\).
III. ENERGY SPECTRUM

Because we are interested in the lowest energy state, we consider only the case \(L = 0\). We seek coefficients \(C_{E n,0 p_z}\) in the form:

\[
C_{E n,0 p_z} = C_E \frac{1 - \frac{2}{5} \xi (1/2 + n_\rho)}{\hbar \omega \left(n_\rho + \frac{1 + s}{2}\right) + \frac{p_z^2}{2m} - E}.
\]  

(13)

Inserting (13) in (11) and neglecting the term proportional to \(\xi^2\), we obtain the equation for energy spectrum:

\[
1 = \lambda \frac{\lambda}{3 \pi \hbar a^2} \int_{-\infty}^{+\infty} dp_z \sum_{n_\rho=0}^{\infty} \frac{1 - \frac{4}{5} \xi (1/2 + n_\rho) \sqrt{n_\rho + \frac{1 + s}{2}}}{\hbar \omega \left(n_\rho + \frac{1 + s}{2}\right) - E}.
\]

(14)

Integrating over \(p_z\) we finally have:

\[
1 = \sqrt{\frac{2m}{3 \hbar a^2}} \sum_{n_\rho=0}^{\infty} \frac{1 - \frac{4}{5} \xi (1/2 + n_\rho)}{\sqrt{n_\rho + \frac{1 + s}{2}} - E}.
\]

(15)

This equation may be solved graphically. In order to find the approximate value of lowest (bound) state, we put in (15): \(n_\rho = 0\), \(s = -1\). Then we obtain the following result:

\[
E_{\text{min}} = - \frac{2 m \lambda^2}{9 \hbar^2 a^4} \left(1 - \frac{2}{5} \xi\right).
\]

(16)

IV. WAVE FUNCTION AND PROBABILITY CURRENT

Let us find in zero approximation of \(\xi\) the wave function \(\psi_E(r)\) for lowest energy state. In this case in expansion of the product of Laguerre functions in (10) we consider only one term, which does not contain \(\xi\). Then the right side of (10) does not equal to zero only when \(L = 0\). In the formula for coefficients \(C_{n_\rho,0 p_z}\) (13) we must neglect the member proportional to \(\xi\). We find coefficient \(C_E\) from the normalizing equation:

\[
\int_{-\infty}^{+\infty} dp_z \sum_{l=-\infty}^{+\infty} \sum_{n_\rho=0}^{\infty} \left|C_{E n,lp_z}\right|^2 = 1.
\]

(17)

Taking into account that in the summation over \(l\) only one term of zero order is present, after integration over \(p_z\) we have:

\[
C_E = \frac{1}{m \sqrt{2\pi}} \left[\sum_{n_\rho=0}^{\infty} \frac{1}{(\hbar \omega n_\rho - E)^{3/2}}\right]^{-1/2}.
\]

(18)

Inserting (18) in (13), and (13) in (7), and again taking into account that in the summation over \(l\) only term of zero order is rest, we obtain the following formula:

\[
\psi_{E,s=-1} = \frac{1}{2 \pi a \sqrt{\hbar}} C_E \sum_{n_\rho=0}^{\infty} \int_{-\infty}^{+\infty} dp_z \frac{1}{\hbar \omega n_\rho + \frac{p_z^2}{2m} - E} e^{\frac{ip_z z}{\hbar}} I_{\rho^2/2a^2}.
\]

(19)

Because we are interested in the lowest (bound) state, we consider only term with \(n_\rho = 0\). Then integrating over \(p_z\) we finally obtain:

\[
\psi_{E,s=-1} = \frac{1}{2 \pi a \sqrt{2m \hbar E}} C_E \exp \left(-\sqrt{2m|E|} \frac{\theta(z) z}{\hbar}\right) \exp \left(-\frac{m \omega^2 \rho^2}{4 \hbar}\right).
\]

(20)
Where $\theta(z) = 1(-1)$ when $z > 0(<0)$. Using well known expression for the density of probability current:

$$j = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) - \frac{e}{me} A \psi^* \psi,$$

we obtain the following result:

$$j_\phi = -\frac{eH\rho}{16\pi^2a^2m^2c\hbar|E|} C_E^2 \exp\left(-2\sqrt{2m|E|/\hbar}\theta(z)z\right) \exp\left(-\frac{m\omega\rho^2}{2\hbar}\right), j_\rho = j_z = 0. \quad (22)$$

V. DISCUSSION

So it is established that the presence of external magnetic field and potential well of finite depth produces an interesting bound energy state of an electron. Its probability current has nonzero circulation along the field axis. This fact attracts significant interest for it contributes to explanation of many quantum mechanics phenomena, in the first place such as high-temperature superconductivity.

Acknowledgments

This paper was supported by a Joint Research Project of the Taiwan National Science Council (NSC-RFBR No. 95WF040022, Republic of China) and the Russian Foundation for Basic Research (No. NSC-a-89500.2006.2) under contract No. RP06N04-1, by the U.S. Department of Energy’s Initiative for Proliferation Prevention (IPP) Program through Contract No. 94138 with the Brookhaven National Laboratory, and, in part, by the Program for Leading Russian Scientific Schools (Grant No. NSH-5332.2006.2)(I.V. M.).

The authors are grateful to V. R. Khalilov for fruitful discussions.

[1] F. Wilczek, Fractional and Anyon Superconductivity (World Scientific, Singapore, 1990).
[2] F. Kh. Chibirova, Mod. Phys. Lett. B19, No 23, 1119 (2005).
[3] F. Kh. Chibirova, 43(7) 1239 (2001).
[4] F. Kh. Chibirova and V. R. Khalilov, Mod. Phys. Lett. A20, No 9, 663 (2005).
[5] Y. Aharonov and D. Bohm, Phys. Rev. 115, 485 (1959).
[6] V. R. Khalilov and F. Kh. Chibirova, Int. Journ. Mod. Phys. A21, No 15, 3171, (2006).
[7] L.D. Landay, E.M. Lifshitz, Quantum Mechanics, 2nd ed. (Pergamon, New York, 1978).