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Physics

Electron in Magnetic Field under Restricted Geometry

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ABSTRACT. Eigenvalue problem related to planar electron subject to homogeneous orthogonal magnetic field is considered on a stripe. It is discussed how the dispersion relation becomes affected by boundary conditions supplied. Comparison is carried out between Dirichlet and Neumann boundary conditions and essential differences leading to distinct physical outcomes are pointed out. *© 2016 Bull. Georg. Natl. Acad. Sci.*

Key words: Schrödinger equation, magnetic field, boundary conditions

Quantum mechanical problem of an electron in magnetic field is the fundamental building block for many physical constructions. The problem acquired further applications after the discovery of such low-dimensional phenomena as the quantum Hall effect [1]. Interesting applications emerge in connection with topological insulators [2], edge states [3,4] and the developing field of spintronics. The later aims in generating, manipulating and detecting the spin current [5] representing directional flow of electron spin. Most of the interest is attracted by the so-called pure spin currents – the flow of electron spin without flow of electric charge. Therefore, the physical constructions generating the flow of electrons with vanishing electric current are of special interest. In the given paper we present the scheme where electric currents in many-particle states vanish due to special boundary conditions. Namely, we consider the problem of electrons on a strip where the eigenvalue problem is supplied by boundary condition. We show that the Neumann boundary conditions generate special type of edge states consisting of two counter-directional flow of electrons which exactly cancel out each other. Provided the net electric currents are absent, such scenario is an appropriate start point for further development of spin effects.

Planar Electron in Homogeneous Orthogonal Magnetic Field

We consider quantum mechanical problem of an electron in the presence of orthogonal magnetic field. The corresponding Hamiltonian is given by [6]

$$H = \frac{1}{2m}(i\partial_x + eA_x)^2 + \frac{1}{2m}(i\partial_y + eA_y)^2, \quad (1)$$

where m is an electron mass, and $A_{x,y}$ are the vector potentials describing homogeneous magnetic field orthogonal to the plane $B = \partial_x A_y - \partial_y A_x = const$.

Geometry of the problem corresponds to the stripe of the finite width d and infinitely extended in the y-direction $-d/2 \le x \le +d/2$, $-\infty < y < +\infty$. The eigenvalue problem $H\psi(x,y) = E\psi(x,y)$ must be supplemented by the boundary conditions (BC) imposed on the wave function ψ. Physical interpretation of the later is that $|\psi(x,y)|^2$ measures the density of probability that electron is found at a point (x,y). The chosen BC must confine electron to move inside of the finite width strip, without leakage away across the edges. The flow of probability is related to the density current

$$J_n = \frac{1}{2im}\left[\psi^*(\partial_n\psi - ieA_n\psi) - (\partial_n\psi - ieA_n\psi)^*\psi\right], \tag{2}$$

which satisfies the continuity equation

$$\partial_t |\psi(x,y)|^2 + \partial_x J_x + \partial_y J_y = 0. \tag{3}$$

Provided the system is located between $x_L \equiv -d/2$ and $x_R \equiv +d/2$ the BC on $\psi(x,y)$ must guarantee the x-component of (2) vanishes at boundaries

$$J_x(x_L, y) = J_x(x_R, y) = 0 \tag{4}$$

This may be realized in different ways. In what follows we consider two options

- Dirichlet boundary conditions

$$\psi(x_L, y) = \psi(x_R, y) = 0, \tag{5}$$

- Neumann boundary conditions

$$\partial_x\psi(x_L, y) = \psi(x_R, y) = 0 \tag{6}$$

Both alternatives reproduce equation (4) but lead to different dispersion relations and as a result give different physical outcomes.

Natural choice of gauge for the vector potential is given by $(A_x, A_y) = (0, Bx)$ known as Landau gauge. In that case the Hamiltonian (1) is translational invariant in y-direction and the momentum $k = k_y$ is a good quantum number and the solution to the eigenvalue problem $H\psi = E\psi$ can be searched in the factorized form

$$\psi(x,y) = e^{+iky}\varphi_k(\xi) \tag{7}$$

where

$$\xi \equiv \ell^{-1}x - k\ell \tag{8}$$

with ℓ being the magnetic length set by ($eB > 0$ is assumed)

$$\frac{1}{\ell^2} = eB. \tag{9}$$

Then the eigenvalue problem is reduced to $h\varphi_k(\xi) = E(k)\varphi_k(\xi)$, where

$$h = \omega_c\left(-\frac{1}{2}\partial_\xi^2 + \frac{1}{2}\xi^2\right) \tag{10}$$

with $\omega_c \equiv (m\ell^2)^{-1}$ the cyclotron frequency.

It is convenient to parameterize the energy by the variable ν as

$$E = \omega_c\left(\nu + \frac{1}{2}\right). \tag{11}$$

Then the general solution to $h\varphi_k(\xi) = E(k)\varphi_k(\xi)$ appears as

$$\varphi_k(\xi) = e^{-\xi^2/2}\left[c_1 M\left(-\frac{1}{2}\nu, \frac{1}{2}, \xi^2\right) + c_2 M\left(\frac{1}{2} - \frac{1}{2}\nu, \frac{3}{2}, \xi^2\right)\right], \tag{12}$$

where $M(a,b,z)$ is the Kummer function [7], and $c_{1,2}$ are the constants to be adjusted so that BC are satisfied.

Dirichlet boundary conditions imply $\varphi_k(\xi_L) = \varphi_k(\xi_R) = 0$, where

$$\begin{aligned} \xi_L &\equiv -\frac{1}{2}\ell^{-1}d - k\ell \\ \xi_R &\equiv +\frac{1}{2}\ell^{-1}d + k\ell \end{aligned} \tag{13}$$

Taking into account (12) we rewrite the Dirichlet BC as

$$\begin{aligned} c_1 M\left(-\frac{1}{2}\nu, \frac{1}{2}, \xi_L^2\right) + c_2 M\left(\frac{1}{2} - \frac{1}{2}\nu, \frac{3}{2}, \xi_L^2\right) &= 0, \\ c_1 M\left(-\frac{1}{2}\nu, \frac{1}{2}, \xi_R^2\right) + c_2 M\left(\frac{1}{2} - \frac{1}{2}\nu, \frac{3}{2}, \xi_R^2\right) &= 0. \end{aligned} \tag{14}$$

Nontrivial solution for c_1 and c_2 exists only if the corresponding determinant vanishes. Employing the Kummer transformation $M(a,b,z)=e^zM(b-a,b,-z)$ this condition appears as

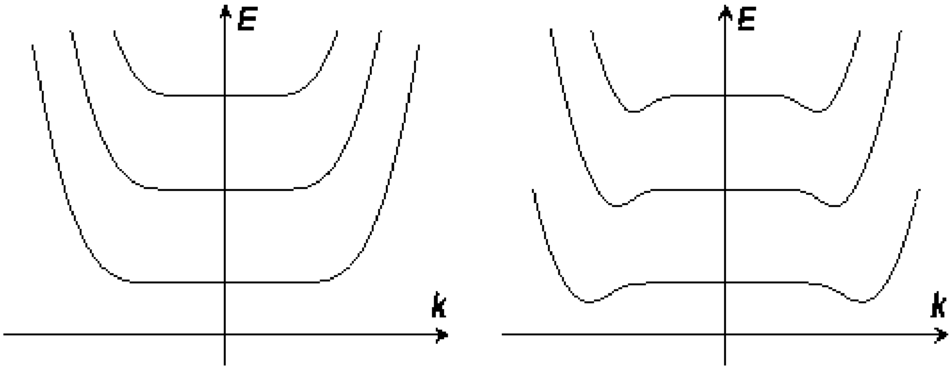

Fig. 1. Dispersion relations $E(k)$ for Dirichlet (left) and Neumann (right) boundary conditions.

$$f_D(\xi_L) = f_D(\xi_R) \tag{15}$$

where

$$f_D(\xi) \equiv \frac{M(\frac{1}{2}+\frac{1}{2}\nu,\frac{1}{2},-\xi^2)}{\xi M(1+\frac{1}{2}\nu,\frac{3}{2},-\xi^2)}. \tag{16}$$

For a given value of the momentum k, the equation (15) generates infinite number of solutions for the parameter ν . Hence, one obtains an infinite amount of functions $\nu(k)$, and the corresponding energies $E(k) = \omega_c\left[\nu(k)+\frac{1}{2}\right]$. Fig. 1a shows the lowest three bands $E_{0,1,2}(k)$ obtained by numeric calculations.

Neumann BC imply $\varphi'(\xi_L) = \varphi'(\xi_R) = 0$ and lead to

$$f_N(\xi_L) = f_N(\xi_R), \tag{17}$$

where

$$f_N(\xi) \equiv \left[\xi M(\frac{1}{2}+\frac{1}{2}\nu,\frac{1}{2},-\xi^2)+2\nu\xi M(\frac{1}{2}+\frac{1}{2}\nu,\frac{3}{2},-\xi^2)\right]\Big/ \left[(1-\xi^2)M(1+\frac{1}{2}\nu,\frac{3}{2},-\xi^2)+\frac{2}{3}(1-\nu)\xi^2 M(1+\frac{1}{2}\nu,\frac{5}{2},-\xi^2)\right]. \tag{18}$$

Fig. 1b demonstrates the corresponding dispersion law.

Remark that the employed BC both produce the similar flat segments in $E(k)$ having origin in the Landau level structure. Differences occur in the regions of non-zero dispersion $dE/dk \neq 0$.

Certain comments are in order here. Increasing the width of the strip ($d \to \infty$), the flat segments become wider, while the depth and the width of wells remain unaffected. In order to verify this observation, consider the right well $(k > 0)$ in the case of Neumann BC. Introduce the quantity $\kappa \equiv k\ell - \frac{1}{2}d/\ell^2$, which measures the deviation of k from the value of $\frac{1}{2}d/\ell^2$. Then the Neumann BC (17) appears as

$$f_N(\kappa) = f_N(\kappa + d/\ell) \tag{19}$$

In the vicinity of $k = \frac{1}{2}d/\ell^2$ with $d/\ell >> 1$, the value of κ is regarded finite. Then the right hand side of (19) can be replaced by the value corresponding to $d \to \infty$ and we come to

$$\left[\kappa M(\frac{1}{2}+\frac{1}{2}\nu,\frac{1}{2},-\kappa^2)+2\nu\kappa M(\frac{1}{2}+\frac{1}{2}\nu,\frac{3}{2},-\kappa^2)\right]\Big/ \left[(1-\kappa^2)M(1+\frac{1}{2}\nu,\frac{3}{2},-\kappa^2)+\frac{2}{3}(1-\nu)\kappa^2 M(1+\frac{1}{2}\nu,\frac{5}{2},-\kappa^2)\right] = -\frac{\Gamma(\frac{1}{2}-\frac{1}{2}\nu)}{\frac{1}{2}\Gamma(-\frac{1}{2}\nu)}. \tag{20}$$

This relation generates infinite number of solutions for $\nu(\kappa)$ which for finite κ are independent of d.

Note, that when the value of k belongs to the area where $dE/dk = 0$ the quanity $|\varphi_k(\xi)|^2$ is finite only for $\xi_L \le \xi \le \xi_R$, i.e. represents the bulk state. At the same time, $|\varphi_k(\xi)|^2$ with $k \sim \pm\frac{1}{2}d/\ell^2$ are localized at $\xi \sim \xi_{L,R}$ thus representing the edge states.

Matter Current

Due to the translational invariance the eigenfunctions take the form (7) and the eigenvalue problem becomes one-dimensional set up on the segment $\xi_L \le \xi \le \xi_R$. As a result, the scalar product of two wave functions is defined as

$$\langle \varphi | \phi \rangle = \int_{\xi_L}^{\xi_R} \varphi^*(\xi)\phi(\xi)d\xi \,. \qquad (21)$$

Within the class of wave functions set by Dirichlet or Neumann BC the Hamiltonian (10) is hermitian with respect to the scalar product (21). Provided $\varphi_k(\xi)$ is the normalized wave function, we have $E(k) = \langle \varphi_k | H\varphi_k \rangle$ where from we obtain

$$\frac{dE}{dk} = \int_{\xi_L}^{\xi_R} \varphi_k^* \frac{dH}{dk} \varphi_k d\xi +$$

$$\int_{\xi_L}^{\xi_R} \frac{d\varphi_k^*}{dk} H\varphi_k d\xi + \int_{\xi_L}^{\xi_R} \varphi_k^* H \frac{d\varphi_k}{dk} d\xi \,. \qquad (22)$$

Due to $\langle \varphi | H\phi \rangle = \langle H\varphi | \phi \rangle$ and $H\varphi_k = E(k)\varphi_k$ the last two terms cancel out each other. Comparing the resulted relation to J_y set by (2) we obtain

$$J_y(k) \equiv \int_{x_L}^{x_R} J_y dx = \frac{dE}{dk}, \qquad (23)$$

where the left hand side is the matter current in y-direction carried by the quantum state with momentum *k*.

As a matter of the relation (23), any quantum state with momentum from the flat segment carries no current due to $E'(k) = 0$. The current carrying states are those with $E'(k) \ne 0$, i.e. the ones with $k \sim \pm\frac{1}{2} d / \ell^2$. However, certain difference occurs between the cases of Dirichlet and Neumann BC. In the first case the momenta with $k \sim +\frac{1}{2} d / \ell^2$ are localized at the right edge $(x \sim x_R)$ and carry positive current due to $E'(k) > 0$, while those with $k \sim -\frac{1}{2} d / \ell^2$ are localized at the left edge $(x \sim x_L)$ and carry negative current due to $E'(k) < 0$. Thus, the Dirichlet BC generate current carrying edge states.

Consider now the states in the right well in the case of Neumann BC (same is true for the left well). These states are all localized at the right edge $(x \sim x_R)$ and correspond to $k \sim +\frac{1}{2} d / \ell^2$. Assume the system is filled by electrons up to the Fermi level E_F as shown in Fi. 2.Then the occupied one-particle states are those with $k_1 \le k \le k_2$. The total current carried by this many-particle state can be calculated by integrating over the occupied one-particle states. Taking into account the relation (23) together with $E_F = E(k_1) = E(k_2)$ we find

$$J_y^{tot}(k) = \int_{k_1}^{k_2} J_y(k)dk =$$

$$\int_{k_1}^{k_2} \frac{dE}{dk} dk = E(k_1) = E(k_2) = 0 \qquad (24)$$

i.e. the total current is precisely zero. The same is true for the left edge $(x \sim x_L)$.

Summarizing, in the many-particle quantum state shown in Fig. 2 all electrons are localized at boundaries and the total electric current flowing along the boundary vanishes precisely. Roughly speaking, each boundary comprises two opposite flows of electrons, which cancel out each other thus producing vanish-

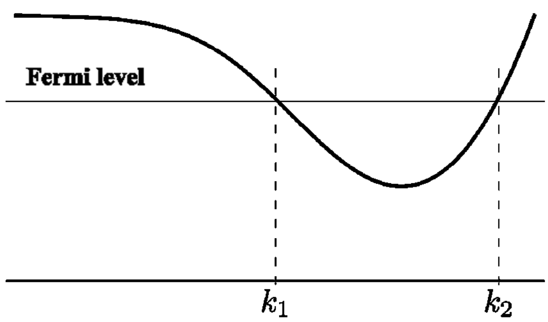

Fig. 2. Inset of the well in the case of Neumann boundary conditions. The system is filled with electrons up to the Fermi level thus occupying one-particle states with $k_1 \le k \le k_2$.

ing edge currents. The precise vanishing of electric current is a good start point for developing the spin effects. In particular, assume the electrons are supplied with the spin degree of freedom subject to spin-orbit interaction, which supports the spin to point up, if electron moves in certain direction, and to point down if it moves in opposite direction. In that case the electrons traveling in positive direction will carry the spin-up, while the ones traveling in negative direction will carry the spin-down, what results in spin transport with no charge transport. This is what is usually referred to as pure spin current. Such scenario of generating pure spin currents will be investigated in a separate article.

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