Quantum Limit in a Parallel Magnetic Field in Layered Conductors

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We show that electron wave functions in a quasi-two-dimensional conductor in a parallel magnetic field are always localized on conducting layers. In particular, wave functions and the electron spectrum in a quantum limit, where the sizes of quasiclassical electron orbits are of the order of nanoscale distances between the layers, are determined. ac infrared measurements to investigate Fermi surfaces and to test Fermi-liquid theory in quasi-two-dimensional organic and high-T_c materials in high magnetic fields, $H \simeq$ 10–45 T, are suggested.

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Layered quasi-one-dimensional and quasi-two-dimensional (Q2D) organic conductors exhibit unique magnetic properties [1–6]. Recently [4], it has been understood that most of them can be explained in terms of effective space dimensionality crossovers for electron wave functions in a magnetic field. In their simplest forms, 3D → 2D dimensional crossovers were suggested to explain field-induced spin-density-wave phases [1,5–7] and to predict reentrant superconductivity (RS) phenomenon [8–10].

In particular, in a Q2D conductor with electron spectrum

$$\epsilon(\mathbf{p}) = \epsilon_{\parallel}(p_x, p_y) + 2t_{\perp}\cos(p_z d), \qquad t_{\perp} \ll \epsilon_{\parallel}(p_x, p_y) \sim \epsilon_F, \tag{1}$$

in a parallel magnetic field

$$\mathbf{H} = (0, H, 0), \qquad \mathbf{A} = (-Hz, 0, 0), \tag{2}$$

quasiclassical electron trajectories, determined by the equations of motion,

$$dp_z/dt = ev_x(p_x, p_y)H/c, \qquad v_x(p_x, p_y) = d\epsilon_{\parallel}(p_x, p_y)/dp_x, \tag{3}$$

become periodic and restricted along the $\mathbf{z}$ axis:

$$z(t, p_x, p_y, H) = -l_{\perp}(p_x, p_y, H)\cos[\omega_c(p_x, p_y, H)t], \quad l_{\perp}(p_x, p_y, H) = 2dt_{\perp}/\omega_c(p_x, p_y, H), \quad \omega_c(p_x, p_y, H) = ev_x(p_x, p_y)Hd/c. \tag{4}$$

Periodic along the $\mathbf{z}$ axis, electron trajectories (4) correspond to "two-dimensionalization" of electron wave functions [9]. It is important that quasiclassical (QC) 3D → 2D dimensional crossovers happen at weak magnetic fields [5,9], where the "sizes" of electron orbits (4) are much larger than the interplane distances, $l_{\perp}(p_x, p_y, H) \gg d$. For instance, these QC crossovers are responsible for a novel type of cyclotron resonance (CR) on open orbits [11–15]. In particular, Kovalev *et al.* [15] have suggested a new method to investigate Q2D Fermi surfaces (FS) by means of CR [11–14] and studied FS in organic conductor κ-(ET)$_2$I$_3$. For theoretical justification of the method, they used a QC kinetic equation, which is appropriate under experimental conditions [15], where $l_{\perp}(p_x, p_y, H) \geq d$ at $H \simeq$ 1–5 T.

Meanwhile, in high experimental fields, $H \simeq$ 10–45 T, typical sizes of electron orbits (4) become of the order of or less than interlayer distances [8,9],

$$l_{\perp}(p_x, p_y, H) \leq d \simeq 10\text{–}30A, \tag{5}$$

in a number of Q2D organic and high-T_c materials. Under condition (5) [which we call the quantum limit (QL)], theoretical methods used so far [5–15] are not justified. On the other hand, it is known that existence or not of Q2D Fermi surfaces is one of the main problems in the area of high-T_c and organic materials [16]. In this context, it is important to suggest a quantum mechanical variant of the Kovalev *et al.* method [15] to investigate Q2D FS in high fields [i.e., in the QL case (5)], where the method is less sensitive to impurities existing in doped high-T_c materials.

The main goal of our Letter is to determine the electron spectrum and wave functions in a Q2D conductor (1) in a parallel magnetic field (2). We show that, in contrast to the extended Bloch waves [17,18], all wave functions are localized on conducting planes and are characterized by some quantum number N at $H \neq 0$. Quantization law, obtained in this Letter, is qualitatively different from well-known Landau levels quantization [17,18] in a perpendicular magnetic field. As a result, ac infrared properties are shown to be unusual. As an example, we use our common results to extend the QC method [15] to study the Q2D FS to QL case (5). We hope that this allows us to test the existence of FS in numerous Q2D organic and high-T_c compounds.

To determine electron wave functions in a Q2D conductor (1) in a parallel magnetic field (2), we make use of the QC description of electron motion within conducting $(\mathbf{x}, \mathbf{y})$ planes and solve the fully quantum mechanical problem for electron motion between the planes. After QC Peierls substitutions for in-plane momenta, $p_x \to p_x - (\frac{e}{c})A_x$, $p_x \to -i(\frac{d}{dx})$, $p_y \to -i(\frac{d}{dy})$ [17], one can represent the electron Hamiltonian in the form:

$$\hat{H} = \epsilon_{\|}\left(-i\frac{d}{dx} + \frac{eHz}{c}, -i\frac{d}{dy}\right) + \frac{1}{2m}\left(-i\frac{d}{dz}\right)^2 - \frac{V}{m}\sum_{n=-\infty}^{\infty}\delta(z - dn), \qquad (6)$$

where the last term introduces the potential energy of a crystalline lattice along the **z** axis, $V > 0$; $\delta(\ldots)$ is the Dirac delta function. Note that Hamiltonian (6) is the exact one for an isotropic Q2D case. As it follows from general theory [17], the suggested method disregards only corrections of the order of $\omega_c^2(p_x, p_y, H)/\epsilon_F$ to electron energy for arbitrary function $\epsilon_{\|}(p_x, p_y)$. As is seen from Eqs. (4) and (5), the QL condition corresponds to $t_\perp \sim \omega_c(p_x, p_y, H)$, and, thus, the above mentioned corrections are of the order of $t_\perp^2/\epsilon_F \ll \omega_c(p_x, p_y, H)$ under quantum limit condition (5), where $\omega_c(p_x, p_y, H)$ is a characteristic energy scale in a magnetic field. Therefore, Hamiltonian (6) allows one to study both QC and QL (5) dimensional crossovers.

Arbitrary solution of the Schrödinger equation for Hamiltonian (6) can be written as

$$\Psi_\epsilon(x, y, z) = \exp(ip_x x)\exp(ip_y y)\Psi_\epsilon(p_x, p_y; z), \qquad (7)$$

which corresponds to free electron motion within $(\mathbf{x}, \mathbf{y})$ planes. After substitution of Eq. (7) into Hamiltonian (6), it can be rewritten as follows:

$$\hat{H} = \epsilon_{\|}\left(p_x + \frac{eHz}{c}, p_y\right) - \left(\frac{1}{2m}\right)\frac{d^2}{dz^2} - \frac{V}{m}\sum_{n=-\infty}^{\infty}\delta(z - dn). \qquad (8)$$

By expanding in-plane energy in powers of H, it is easy to make sure that the Schrödinger equation for Hamiltonian (8) with the same accuracy can be expressed as:

$$\left[-\left(\frac{1}{2m}\right)\frac{d^2}{dz^2} + \omega_c(p_x, p_y, H)\left(\frac{z}{d}\right) - \frac{V}{m}\sum_{n=-\infty}^{\infty}\delta(z - dn)\right]\Psi_\epsilon(p_x, p_y; z) = [\epsilon - \epsilon_{\|}(p_x, p_y)]\Psi_\epsilon(p_x, p_y; z). \qquad (9)$$

It is possible to prove [19] that, if one uses tight binding approximation for solutions of Eq. (9),

$$\Psi_{\epsilon_N}(p_x, p_y; z) = \sum_{m=-\infty}^{\infty} A_{m-N}(p_x, p_y)\Phi_{\epsilon_0}(z - dm), \qquad (10)$$

[where $\Phi_{\epsilon_0}(z - dm)$ is the wave function of the individual mth layer at $H = 0$, corresponding to energy $\epsilon_0 < 0$, $|\epsilon_0| \sim \epsilon_F$], then one disregards only corrections of the order of $\omega_c^2(p_x, p_y, H)/[\epsilon_{\|}(p_x, p_y), \epsilon_0] \sim t_\perp^2/\epsilon_F$ to electron energy.

Therefore, the equation

$$[\epsilon - \epsilon_0 - \epsilon_{\|}(p_x, p_y) - m\omega_c(p_x, p_y, H)]A_m(p_x, p_y) = -A_{m+1}(p_x, p_y)t_\perp - A_{m-1}(p_x, p_y)t_\perp, \qquad (11)$$

[where $t_\perp = (V^2/m)\exp(-Vd)$], which can be derived after substitution of wave functions (10) into Hamiltonian (9) by means of tight binding approximation for the nearest neighbors, has the same accuracy as Hamiltonian (6) and, thus, can be used to describe 3D → 2D QL dimensional crossovers (5). At given in-plane momenta p_x and p_y, Eq. (11) is mathematically equivalent to the so-called Stark-Wannier ladder equation in the electric field [20]. Using Ref. [20], one can express wave functions and energy levels in the following way:

$$\Psi_{\epsilon_N}(p_x, p_y; z) = \sum_{m=-\infty}^{\infty} J_{m-N}[2t_\perp/\omega_c(p_x, p_y, H)] \times \Phi_{\epsilon_0}(z - dm),$$
$$\epsilon_N(p_x, p_y) = \epsilon_0 + \epsilon_{\|}(p_x, p_y) + N\omega_c(p_x, p_y, H), \qquad (12)$$

where $J_N(\ldots)$ is the Bessel function of Nth order [21]. [An important difference between wave functions and energy spectrum (12) and that in Ref. [20] is that the envelope functions $J_{N-m}(\ldots)$ and energy levels $\epsilon_N(\ldots)$ in Eq. (12) depend on p_x, p_y, and magnetic field H.]

Equation (12) represents the main result of our Letter. In contrast to textbook extended Bloch waves with complex envelope $\exp(ikz)$ [17], the envelope functions in Eq. (12) are real functions localized on the Nth conducting layer [see Figs. 1(a) and 1(b)]. Therefore, one concludes that, in a parallel magnetic field, all wave functions are localized on layers with the energy gap between two neighboring wave functions being $\omega_c(p_x, p_y, H)$. Equation (12) is valid in both QC and QL cases. As is seen from Fig. 1(b), in the QL case (5), wave function (12) is essentially localized on a single conducting layer with probability to jump on the neighboring layers being small. In contrast, in the QC case, the localization length of wave function (12) is approximately equal to the corresponding "size" of the QC electron orbit [see Fig. 1(a) and Eq. (4)].

Below, we show that quantization law (12) leads to unusual ac infrared properties and suggest a method to investigate Q2D FS. For these purposes, we calculate the ac conductivity component, perpendicular to conducting layers, $\sigma_\perp(H, \omega)$, using known wave functions and energy spectrum (12). Let us first find matrix elements of the momentum operator, $\hat{p}_z = -i\frac{d}{dz}$, responsible for interactions between electrons and the electric field, $\mathbf{E} \parallel \mathbf{z}$. It is possible to make sure that the matrix elements are nonzero only for wave functions with the same in-plane momenta, p_x and p_y, and energies $\epsilon_1 - \epsilon_2 = \pm\omega_c(p_x, p_y, H)$:

$$p_z^{N,N+1} = \int \Psi_N^*(z)\left(-i\frac{d}{dz}\right)\Psi_{N+1}(z)dz = -p_z^{N+1,N} = -imdt_\perp. \qquad (13)$$

[In other words, only optical transitions between electrons, localized on neighboring conducting layers and having the same in-plane momenta, are allowed.]

To calculate $\sigma_\perp(H, \omega)$, we make use of the following extension [22] of the Kubo formalism:

$$\sigma_\perp(H, \omega) = -i\frac{2e^2}{m^2V}\sum_{N_1,N_2}\frac{|p_z^{N_1,N_2}|^2}{(E_{N_1} - E_{N_2})}\frac{[n(E_{N_2}) - n(E_{N_1})]}{(E_{N_2} - E_{N_1} - \omega - i\nu)}, \qquad \nu \to 0, \qquad (14)$$

where $n(E)$ is the Fermi-Dirac distribution function, and V is a volume. After substituting matrix elements (13) and energy spectrum (12) in Eq. (14) and straightforward calculations, one obtains:

$$\sigma_\perp(H, \omega) \sim i\int\frac{dp}{|\mathbf{v}_F(p_x, p_y)|}\left[\frac{1}{\omega_c(p_x, p_y, H) - \omega - i\nu} + \frac{1}{-\omega_c(p_x, p_y, H) - \omega - i\nu}\right], \qquad \nu \to 0. \qquad (15)$$

[Note that in the exact Eq. (15) we omit only some coefficient which is not significant for further consideration. Integration in Eq. (15) is made along 2D contour $\epsilon_\|(p_x, p_y) = \epsilon_F$; $\mathbf{v}_F(p_x, p_y) = d\epsilon_\|(p_x, p_y)/d\mathbf{p}$; we use the approximation $n(E_{N_2}) - n(E_{N_1}) = (E_{N_2} - E_{N_1}) \times [dn(E)/dE]$ since $|E_{N_2} - E_{N_1}| = \omega_c(p_x, p_y, H) \ll \epsilon_F$.]

It is convenient to write explicitly real and imaginary parts of conductivity (15):

$$\Re\sigma_\perp(H, \omega) \sim \int\frac{dp}{|\mathbf{v}_F(p_x, p_y)|} \times \delta[\omega_c(p_x, p_y, H) - \omega] = \begin{cases} \neq 0, & \omega < \omega_c^{\max}(H) \\ 0, & \omega > \omega_c^{\max}(H) \end{cases}, \qquad (16)$$

$$\Im\sigma_\perp(H, \omega) \sim \int\frac{dp}{|\mathbf{v}_F(p_x, p_y)|}\left[\frac{1}{\omega_c(p_x, p_y, H) - \omega} - \frac{1}{\omega_c(p_x, p_y, H) + \omega}\right], \qquad (17)$$

where $\omega_c^{\max}(H)$ is the maximum value of the energy gap, $\omega_c(p_x, p_y, H)$, corresponding to the maximum value of velocity, $v_x = \max|v_x(p_x, p_y)|$, on the contour of integration [see Fig. 2 and Eq. (4)]; the integral in Eq. (17) is determined as its principal value.

The main difference between Eqs. (16) and (17) and the results of Ref. [15] is that Eqs. (16) and (17) are valid in both QC and QL (5) cases, whereas the results of [15] are essentially QC. Another difference is that Eqs. (16) and (17) describe "optical" conductivity (i.e., conductivity in the absence of impurities), in contrast to kinetic equation results [15]. From Eqs. (16) and (17), it follows that ac properties in a parallel magnetic field are unusual. Indeed, integration of the δ function in Eq. (16) results in a nonzero value of the real part of conductivity for ac frequencies at $0 < \omega < \omega_c^{\max}(H)$ (see Fig. 2). Therefore, electrons absorb electromagnetic waves at $0 < \omega < \omega_c^{\max}(H)$ (in the absence of impurities), in contrast to textbook properties of metals [18].

Let us demonstrate that the real part of conductivity (16) diverges at a resonant frequency,

$$\omega = \omega_c^{\max}(H) = ev^{\max}Hd/c. \qquad (18)$$

Indeed, in the vicinity of its maximum $\omega_c(p_x, p_y, H) \simeq \omega_c^{\max}(H) - A(H)|\mathbf{p}|^2$, with $\mathbf{p}$ being the momentum component perpendicular to $\mathbf{v}_F(p_x, p_y)$ at the point where $|v_x(p_x, p_y)|$ takes its maximum (see Fig. 2). In this case, integral (16) can be estimated as

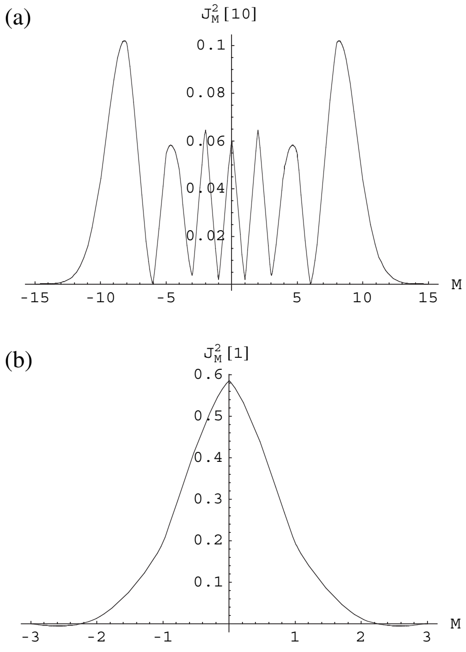

FIG. 1. Probability of an electron with a wave function, centered on conducting layer $M = 0$, to exist on conducting layer M, $J_M^2[2t_\perp/\omega_c(p_x, p_y, H)]$, is calculated for integer values of M [see Eq. (12)], where solid lines are interpolation curves. (a) The QC wave function with $l_\perp(p_x, p_y, H)/d = 2t_\perp/\omega_c(p_x, p_y, H) = 10 \gg 1$ [see Eqs. (4) and (12)] is characterized by a localization length approximately equal to the size of the corresponding QC orbit, $l_\perp(p_x, p_y, H) = 10d$. (b) The QL wave function with $l_\perp(p_x, p_y, H)/d = 2t_\perp/\omega_c(p_x, p_y, H) = 1$ [see Eqs. (4) and (12)] is localized on a single conducting layer $M = 0$, where the probability to jump on neighboring layers is less than 0.5.

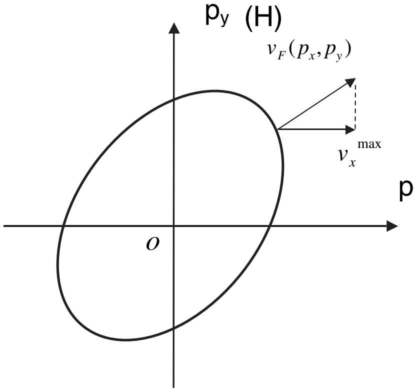

FIG. 2. Resonant frequency $\omega_c^{\max}(H)$ corresponds to the maximum value of $|v_x(p_x, p_y)|$, $v_x^{\max}$, on a 2D Fermi surface, $\epsilon_{\|}(p_x, p_y) = \epsilon_F$, as follows from Eq. (4).

$$\Re\sigma_{\perp}(H,\omega) \sim \frac{1}{\sqrt{\omega_c^{\max}(H)-\omega}}, \quad \omega_c^{\max}(H)-\omega \ll \omega_c^{\max}(H). \tag{19}$$

Therefore, by measuring $\omega_c^{\max}(H)$ at different directions of the field, one can determine the angular dependence of $v_x^{\max}$ (see Ref. [15] and Fig. 2). We stress, however, that the physical meaning of resonant frequency (18) at high magnetic fields (5), where electrons are almost completely localized on conducting layers (see Fig. 1), is completely different from its kinetic equation interpretation [15,23].

To summarize, wave functions and electron spectrum of a Q2D conductor in a parallel magnetic field are determined. A method to test the Fermi-liquid picture in Q2D organic and high-T_c materials is suggested. We hope that this method is a useful experimental tool to study Fermi-liquid versus non-Fermi-liquid behavior in low-dimensional compounds, especially as there have been some inconsistencies claimed [24] between angular resolved photoemission methods [16] and magneto-optical measurements in a perpendicular magnetic field [24]. We also think that 3D → 2D QL dimensional crossover and quantization law (12), suggested in the Letter, will be useful for studies of RS superconductivity [8–10] and for explanations of unusual phenomena observed in high parallel magnetic fields (see, for example, Refs. [25,26]).

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[1] T. Ishiguro, K. Yamaji, and G. Saito, *Organic Superconductors* (Springer-Verlag, Heidelberg, 1998), 2nd ed.

[2] See review articles in J. Phys. I (France) **6** (1996), and references therein.

[3] See review by S. E. Brown, M. J. Naughton, I. J. Lee, E. I. Chashechkina, and P. M. Chaikin, in *More is Different (Fifty Years of Condensed Matter Physics)*, edited by N. P. Ong and R. N. Bhatt, Princeton Series in Physics (Princeton University, Princeton, NJ, 2001), and references therein.

[4] See recent Letters: A. G. Lebed and M. J. Naughton, Phys. Rev. Lett. **91**, 187003 (2003); A. G. Lebed, N. N. Bagmet, and M. J. Naughton, Phys. Rev. Lett. **93**, 157006 (2004), and references therein.

[5] L. P. Gor'kov and A. G. Lebed, J. Phys. (Paris), Lett. **45**, L433 (1984); A. G. Lebed, Phys. Rev. Lett. **88**, 177001 (2002).

[6] P. M. Chaikin, Phys. Rev. B **31**, 4770 (1985).

[7] M. Heritier, G. Montambaux, and P. Lederer, J. Phys. (Paris), Lett. **45**, L943 (1984).

[8] A. G. Lebed, Pis'ma Zh. Eksp. Teor. Fiz. **44**, 89 (1986) [JETP Lett. **44**, 114 (1986)].

[9] A. G. Lebed and K. Yamaji, Phys. Rev. Lett. **80**, 2697 (1998).

[10] N. Dupuis, G. Montambaux, and C. A. R. Sa de Melo, Phys. Rev. Lett. **70**, 2613 (1993).

[11] T. Osada, S. Kagoshima, and N. Miura, Phys. Rev. B **46**, 1812 (1992).

[12] L. P. Gor'kov and A. G. Lebed, Phys. Rev. Lett. **71**, 3874 (1993).

[13] A. Ardavan, J. M. Schrama, S. J. Blundell, J. Singleton, W. Hayes, M. Kurmoo, P. Day, and P. Goy, Phys. Rev. Lett. **81**, 713 (1998).

[14] A. Ardavan, S. J. Blundell, and J. Singleton, Phys. Rev. B **60**, 15 500 (1999).

[15] A. E. Kovalev, S. Hill, K. Kawano, M. Tamura, T. Naito, and H. Kobayashi, Phys. Rev. Lett. **91**, 216402 (2003).

[16] See, for example, H. Ding, M. R. Norman, T. Yokoya, T. Takeuchi, M. Randeira, J. C. Campuzano, T. Takahashi, T. Mochiku, and K. Kadowaki, Phys. Rev. Lett. **78**, 2628 (1997).

[17] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics*, Part 2 (Butterworth-Heinemann, New York, 1980).

[18] A. A. Abrikosov, *Fundamentals of Theory of Metals* (Elsevier Science Publisher B. V., Amsterdam, 1988).

[19] A. G. Lebed (to be published).

[20] E. E. Mendez and G. Bastard, Phys. Today **46**, No. 6, 34 (1993).

[21] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, London, 1994) 5th ed.

[22] G. Grosso and G. P. Parravicini, *Solid State Physics* (Academic, New York, 2000); the same expression for conductivity in the case of isotropic impurities scattering can be derived by means of a Green functions technique [see, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1963)].

[23] A. G. Lebed and N. N. Bagmet, Phys. Rev. B **55**, R8654 (1997).

[24] L. B. Rigal, D. C. Schmadel, H. D. Drew, B. Maiorov, E. Osquiguil, J. S. Preston, R. Hughes, and G. D. Gu, Phys. Rev. Lett. **93**, 137002 (2004).

[25] N. E. Hussey, M. Kibune, H. Nakagawa, N. Miura, Y. Iye, H. Takagi, S. Adachi, and K. Tanabe, Phys. Rev. Lett. **80**, 2909 (1998).

[26] N. E. Hussey, M. N. McBrien, L. Balikas, J. S. Brooks, S. Horii, and H. Ikuta, Phys. Rev. Lett. **89**, 086601 (2002).