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Magnetic breakdown in an array of overlapping Fermi surfaces

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ABSTRACT

We develop a theoretical framework for a magnetic breakdown in an array of circular two-dimensional bands with a finite overlap of neighboring Fermi surfaces due to the presence of a presumably weak periodic potential, and apply the obtained results to the electron bands in carbon honeycomb structures of doped graphene and intercalated graphite compounds. In contrast to the standard treatment, inaugurated more than fifty years ago by Slutskin and Kadigrobov, with electron semiclassical trajectories encircling significantly overlapping Fermi surfaces, we examine a configuration in which bands are related in a way that the Fermi surfaces only slightly overlap, forming internal band pockets with areas of the size comparable to the area of the quantum magnetic flux for a given external magnetic field. Such band configuration has to be treated quantum mechanically. The calculation leads to the results for magnetic breakdown coefficients comprising an additional large factor with respect to the standard results, proportional to the ratio of the Fermi energy and the cyclotron energy. Also, these coefficients show oscillating dependence on energy, as well as on the wave number of periodic potential. Both mentioned elements enable the adjustment of the preferred wave vector of possible magnetic breakdown induced density wave instability at the highest possible critical temperature.

1. Introduction

Since its discovery in sixties, magnetic breakdown (MB) theory [1] has been an important tool in understanding the influence of magnetic field on the electronic properties of conductors and semiconductors with rather small gaps at the Fermi surface. In the series of earlier works we have analyzed the MB mechanisms for electron bands of reduced dimensionality, more specifically the possibility of the stabilization of density wave (DW) ordering in the external magnetic field through the gain of band energy induced by MB. This kind of DW is possible already in the so-called anti-nesting regime in quasi-one-dimensional materials [2], in which MB takes place between equivalent pockets much larger than the characteristic surface for a quantum of magnetic flux, $\sigma \equiv \hbar eH/c$ [3]. Here H is the strength of magnetic field, and $\hbar$, e, and c are Planck constant, electron charge and velocity of light respectively. Even more favorable appears to be the ordering with touching Fermi sheets and largest possible pockets, having a more subtle mechanism of tunneling due to the internal structure of the MB barrier [4]. In this work we use previously developed formalism to investigate the MB properties of two-dimensional isotropic band dispersions with circular Fermi surfaces. Assuming the presence of uniaxial periodic potential which induces the formation of an array of slightly overlapping Fermi surfaces, we calculate the MB scattering matrix and ensuing electron spectrum, and apply the general results to the Dirac type of band dispersion characterizing honeycomb structures in the graphene and intercalated graphite compounds.

2. Model

The problem will be here illustrated by a simplified model of two-dimensional conducting band with a set of circular electronic orbits encircling the Fermi surface with a radius p_F (see Fig. 1(a)). The extensions to more general band dispersions do not alter the main conclusions of present analysis. Further on, we assume the presence of a weak periodic potential with the uniaxial periodicity, $V(\mathbf{r}) = V(x)$, defined by the wave vector $\mathbf{Q} = (Q, 0)$. Here we are interested in the range of values of the wave number Q of the lattice periodic modulation for which there is a presumably slight overlap between closed Fermi surfaces from neighboring new Brillouin zones, leading to the formation of the continuous chain of overlapping electron orbits in the momentum space [5], as shown in Fig. 1(a). Simultaneously, the periodic potential lifts the degeneracy at the crossing points of this chain, by opening gaps, so that the initial chain is converted into a set of small closed trajectories at the connection points, enwraped between two large

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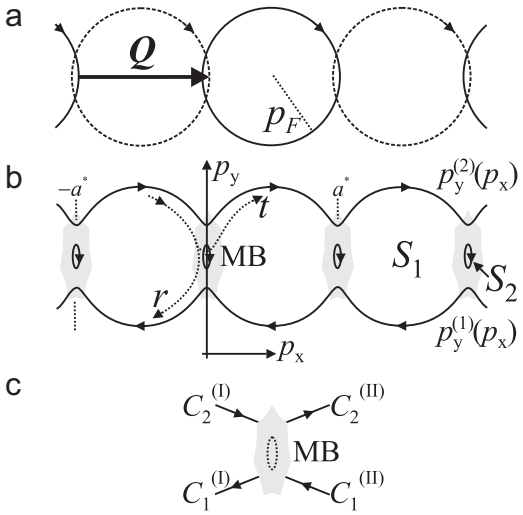

Fig. 1. (a) Closed electron trajectories in momentum space, encircling Fermi surfaces characterized by p_F, are related by perturbation wave vector **Q** in the way to slightly overlap, thus forming a connected chain. (b) The perturbation potential lifts the degeneracy and opens gaps at crossing points, so that the structure attains the form of periodic set of large surfaces S_1 (approximately equal to surface of starting trajectory) enwrapped between two closed trajectories $p_y^{(1,2)}(p_x)$, with much smaller closed trajectories S_2 at connection points between them. At these points (shaded areas in (b)), one has the magnetic breakdown in perpendicular magnetic field, with probability amplitude r for electron to get reflected, and t to pass through the MB region. (c) Magnetic breakdown scattering process: $C_i^{(J)}$ are constants in electron wave functions for incoming and outgoing electrons (arrows depict direction of motion), index $i=1, 2$ corresponds to trajectory $p_y^{(1,2)}(p_x)$, while $J = I, II$ marks regions on the "left" and "right" side of the chosen MB area.

open trajectories, as shown in Fig. 1(b). Note that, due to the slight overlap of initial Fermi surfaces, the surface of small trajectory in momentum space S_2 is much smaller than the surface of main constituent of periodic structure S_1, which is in turn approximately equal to the surface of starting trajectory πp_F^2.

With a finite magnetic field H directed perpendicularly to the plane of electron delocalization, one has the orbital motion of electrons indicated by arrows in Fig. 1(b). However, in the regions where trajectories $p_y^{(1)}(p_x)$ and $p_y^{(2)}(p_x)$ get close to each other in momentum space the magnetic field also causes the tunneling of electrons between the lower (1) and upper (2) Fermi surfaces. Assuming that this MB takes place only in the narrow regions of connection points designated by shaded areas in Fig. 1(b), the further analysis can be performed by treating semiclassically the parts of trajectories outside these ranges, and by calculating fully quantum mechanically the wave functions in the MB regions, aiming to determine the effective MB scattering matrix characterizing the present situation. Such configuration of orbits differs significantly from the standard situation examined in Ref. [6] in which the surfaces S_1 and S_2 are of comparable sizes and much larger than σ, so that both can be treated in the semiclassical manner, while the MB regions between them have much simpler structure.

The present approach is inevitable for magnetic fields satisfying the condition $S_2 < \sigma \ll S_1$, where $\sigma \equiv e\hbar H/c$ is, we remind again, the characteristic surface for a quantum of magnetic flux. We also assume that the Larmor radius $R_L = cp_F/eH$ is much smaller than the electron mean free path l_0.

3. Semiclassical trajectories

In order to solve the problem of semiclassical trajectories we start from the standard Onsager–Lifshitz Hamiltonian [7]

$$E\left(P_x, P_{y0} - i\sigma\frac{d}{dP_x}\right)G(P_x, P_{y0}) = \varepsilon G(P_x, P_{y0}), \tag{1}$$

for electron wave functions $G(P_x, P_{y0})$ in the ranges between the MB regions. Here we use the Landau gauge of the vector potential, $\mathbf{A} = (0, Hx, 0)$, as the most convenient one for the geometry of Fig. 1. Then the y-component of the generalized momentum **P** is conserved, $P_y = P_{y0}$. The diagonal matrix elements of the periodic potential $V(x)$, which introduce simple energy shift into the spectrum of Eq. (1), will be included into the calculations later in matching of the present semiclassical solutions with the asymptotic parts of wave functions from the MB regions in Fig. 1(b).

The solution of Eq. (1) must also satisfy the periodic boundary condition $G(P_x, P_{y0}) = G(P_x + a_*, P_{y0})$, where $a_* = Q$ is the period of the chained structure in the P_x – direction. It reads

$$G_i^{(J)} = \frac{C_i^{(J)}}{\sqrt{|v_i|}}\exp\left[-\frac{i}{\sigma}\int_0^{P_x}\left(p_y^{(i)}(P_x') - P_{y0}\right)dP_x'\right], \tag{2}$$

where $v_i = \partial E/\partial p_y$ at $p_y = p_y^{(i)}(P_x)$, with indices $i=1,2$ denoting lower and upper trajectories. Indices $J = I, II$ denote semiclassical region, along which the integration over P_x is taken, that is left and right with respect to the MB region respectively. At a given energy ε, the dependence $p_y^{(i)}(P_x)$ is determined by the equation $E(P_x, p_y) = \varepsilon$, where $E(P_x, p_y)$ is the two-dimensional electron dispersion in the absence of magnetic field. Note that it is negligibly affected by the periodic potential $V(\mathbf{r})$ in the semiclassical ranges of the momentum space.

Constants $C_i^{(J)}$ in regions I and II are generally matched via the MB scattering matrix (see Fig. 1(c)), relating the incoming and outgoing waves, i.e.

$$\begin{pmatrix} C_1^{(I)} \\ C_2^{(II)} \end{pmatrix} = e^{i\Theta}\begin{pmatrix} t & r \\ -r^* & t^* \end{pmatrix}\begin{pmatrix} C_1^{(II)} \\ C_2^{(I)} \end{pmatrix}, \tag{3}$$

where $|r|^2$ and $|t|^2$ are probabilities that electron gets reflected or pass through the MB region, satisfying condition $|r|^2 + |t|^2 = 1$. Corresponding amplitudes r and t, together with the phase factor Θ, bear sufficient physical information about the MB process, taking into account the internal details of the MB barrier in a given situation. In what follows we calculate them for the MB configuration that we have already described and presented as shadow areas in Fig. 1(b).

4. Quantum mechanical treatment of the MB regions

The wave function $\Psi_{\mathbf{p}}(\mathbf{r})$ for the electron in the shaded area of Fig. 1(b) can be written as a linear combination $\Psi_{\mathbf{p}}(\mathbf{r}) = \beta_1(\mathbf{p})\varphi_{1,\mathbf{p}}(\mathbf{r}) + \beta_2(\mathbf{p})\varphi_{2,\mathbf{p}}(\mathbf{r})$, where $\varphi_{s,\mathbf{p}}(\mathbf{r}) = w_{s,\mathbf{p}}(\mathbf{r})\exp(i\mathbf{pr})$ ($s=1,2$) represent states from two bands brought into touch by the wave number Q, which also determines period of periodic functions $w_{s,\mathbf{p}}(\mathbf{r})$. The Schrodinger equation

$$[\mathcal{H}_0 + V(x)]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{4}$$

then reduces to the system of equations for the coefficients $\beta_{1,2}(\mathbf{p})$

$$\begin{aligned} &\left[\varepsilon_1(\mathbf{p}) + V_{11} - E\right]\beta_1 + V_{12}\beta_2 = 0 \\ &V_{12}^*\beta_1 + \left[\varepsilon_2(\mathbf{p}) + V_{22} - E\right]\beta_2 = 0, \end{aligned} \tag{5}$$

where $V_{ss'} \equiv \langle\varphi_s|V(x)|\varphi_{s'}\rangle$, $s=1,2$ are matrix elements of the periodic potential $V(x)$. The diagonalized band dispersion for general initial bands $\varepsilon_{1,2}(\mathbf{p})$ follows from Eq. (5). Here we shall follow for illustration the case of honeycomb graphene layer with the initial