Manifestation of Berry's Phase in Metal Physics

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It is shown that in crystals the semiclassical quantization condition for energy levels of electrons in the magnetic field depends on Berry's phase. When the electron orbit links to the band-contact line of the metal (i.e., surrounds it), Berry's phase is nonzero and the quantization condition differs from that commonly used. This result is closely analogous to the Aharonov-Bohm's effect provided the band-contact line plays the role of the infinitely thin "solenoid" with the fixed "magnetic flux." The predicted effect must manifest itself in oscillation phenomena for a number of metals. [S0031-9007(99)08623-8]

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In 1984 Berry [1] discovered the important result which aroused considerable interest in many fields of physics (see, e.g., [2,3]). According to Berry, if a Hamiltonian of a quantum system depends on parameters and the parameters undergo adiabatic changes so that they eventually return to the original values, then the wave function of the system can acquire the so-called geometrical phase in addition to the familiar dynamical one. This additional phase is completely determined by a closed trajectory of the system in the parameter space and does not depend on details of the temporal evolution. The manifestations of Berry's phase were found in molecular physics [4], optics [5], resonance phenomena in nuclear quadrupole systems [6], etc. As for solid state physics, Zak [7] argued that Berry's results are applicable to an electron moving in a crystal, with the Brillouin zone playing the role of the parameter space. In this paper, we consider an electron of a metal in the external magnetic field $\mathbf{H}$ and show that Berry's phase appears in the semiclassical quantization condition for its energy levels. Interestingly, when the phase is nonzero, the condition turns out to be different from that commonly used [8,9]. Since the semiclassical energy levels of electrons provide the basis for the analysis of oscillation phenomena in metals [8,10], the Berry's phase must manifest itself in a number of the well-known physical effects (e.g., the de Haas–van Alphen effect, the Shubnikov–de Haas effect, etc.) and, hence, can be detected through their experimental investigation. In our subsequent analysis, we shall assume that the crystal under study has a center of inversion (most metals fall into this class of solids). Besides, to elucidate the heart of the matter, we completely neglect the spin-orbit interaction and spin of the electron [11].

It is well known (see, e.g., Refs. [9,12]) that the correspondence between a semiclassical electron trajectory in a crystal (i.e., in the coordinate space) and the orbit in the space of wave vectors $\mathbf{k}$ (i.e., in the Brillouin zone) exists. The latter orbit is the intersection of the constant-energy surface, $\varepsilon(\mathbf{k}) = \text{const}$, with the plane, $k_z = \text{const}$, where z is the direction of the magnetic field $\mathbf{H}$. In the case of the closed orbit, the quantization condition for energy levels of the electron looks like [13,14]

$$S(\varepsilon, k_z) = \left(\frac{2\pi|e|H}{\hbar c}\right)(n + \gamma), \tag{1}$$

where S is the cross-sectional area of the orbit in $\mathbf{k}$ space, n is the large integer ($n > 0$), γ is the constant ($0 \le \gamma < 1$), and e is the electron charge. In what follows we shall consider only those orbits for which probabilities of intraband and interband magnetic breakdowns are negligible. In other words, the orbit under study does not come close to any other trajectory with the same k_z, and its shape differs noticeably from an intersecting one. In this case, according to Zilberman [15] (see also Ref. [9]), γ always has the value

$$\gamma = \frac{1}{2}. \tag{2}$$

It is this value that is commonly used in describing oscillation phenomena in metals [8]. If a magnetic breakdown occurs, γ essentially depends on ε and k_z [16] but, as noted above, we shall not consider this situation.

Now we express the quantity γ in terms of the Berry's phase. Denote the Bloch wave function of the electron in the band with index l by $\psi_{\mathbf{k}l}(\mathbf{r})$:

$$\psi_{\mathbf{k}l}(\mathbf{r}) = \exp(\imath\mathbf{k}\mathbf{r})u_{\mathbf{k}l}(\mathbf{r}),$$

where $u_{\mathbf{k}l}(\mathbf{r})$ is the periodic function of $\mathbf{r}$. Let the closed semiclassical orbit in $\mathbf{k}$ space, Γ, correspond to some band with $l = 0$, i.e., it is intersection of the surface $\varepsilon_0(\mathbf{k}) = \text{const}$ with the plane $k_z = \text{const}$. Then γ is determined by the formula that follows from Eqs. (42) and (43) of Ref. [17]:

$$\gamma - \frac{1}{2} = -\frac{1}{2\pi}\oint_\Gamma \frac{M_0(\mathbf{k})}{v_\perp(\mathbf{k})}\, d\kappa, \tag{3}$$

where $v_\perp$ is the absolute value of the projection of the electron velocity $\mathbf{v} = \hbar^{-1}\nabla_{\mathbf{k}}\varepsilon_0$ on the plane of the orbit; $d\kappa$ is the length of an infinitesimal element of Γ; M_0 is

the matrix element,

$$M_0 = \frac{1}{2}\langle \mathbf{k}0|\left[\left(\frac{\hat{\mathbf{p}}}{m} + \mathbf{v}\right) \times \hat{\mathbf{r}}\right]_z |\mathbf{k}0\rangle,$$

calculated with the use of the Bloch function $\psi_{\mathbf{k}0}(\mathbf{r})$. Here, m is the electron mass, $\hat{\mathbf{p}}$ is the momentum operator whose diagonal part is $m\mathbf{v}$, and $\hat{\mathbf{r}}$ is the periodic (in $\mathbf{k}$) part of the coordinate operator $\hat{\mathbf{R}}$ in the Crystal Momentum Representation [9,18], $\hat{\mathbf{R}} = \imath\nabla_{\mathbf{k}} + \hat{\mathbf{r}}$. It is well known [9,18] that the contribution of interband matrix elements of $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ in M_0 is equal to zero in crystals with the inversion symmetry. This follows from the fact that electron states $|\mathbf{k}l\rangle$ are invariant under the transformation $U = KI$, where K and I are the operators of complex conjugation and inversion, respectively. Hence,

$$M_0 = [\mathbf{v} \times \mathbf{\Omega}]_z,$$

where $\mathbf{\Omega}$ is the intraband matrix element of $\hat{\mathbf{r}}$ which has the form [see Eq. (44) in Ref. [17]]

$$\mathbf{\Omega}(\mathbf{k}) = \imath \int d\mathbf{r}\, u^*_{\mathbf{k}0}(\mathbf{r})\nabla_k u_{\mathbf{k}0}(\mathbf{r}).$$

Here the integration is carried out over a unit cell of the crystal. Substitution of M_0 in Eq. (3) gives

$$\gamma - \frac{1}{2} = -\frac{1}{2\pi}\oint_\Gamma \mathbf{\Omega}\, d\mathbf{k}, \tag{4}$$

where $d\mathbf{k} \equiv d\kappa[\mathbf{i}_z \times \mathbf{v}]/v_\perp$, and $\mathbf{i}_z$ is the unit vector parallel to $\mathbf{H}$ ($d\mathbf{k}$ is aligned with the tangent to Γ and $|d\mathbf{k}| = d\kappa$). The integral in the right-hand side of Eq. (4) is just the Berry's phase for the orbit Γ [7]. When this phase is equal to zero, we arrive at Eq. (2).

The difference of Berry's phase from zero is usually due to degeneracy of electron states [1,19]. In this connection, let us list the various possible types of degeneracy of the electron energy bands in crystals with a center of inversion. It is common knowledge that the contact of the bands in a metal can occur *at symmetry points* and *along symmetry axis* of its Brillouin zone. Besides, as was shown by Herring [20], there are *lines of an accidental contact* between the bands in crystals. The term "accidental" means that the degeneracy of electron states is not caused by their symmetry. Such band-contact lines must exist in many metals. This statement is easily understood when one takes into account Herring's result: If there is a point of an intersection of two energy bands in an axis of symmetry of the Brillouin zone, and the interband matrix element of the velocity operator is nonzero at this point, then a band-contact line has to pass through the point. Intersection of bands at points in axes are known to occur in many metals [21]. As for the matrix element of the velocity operator, the necessary information on it follows from the irreducible representations of the appropriate bands. The simple analysis of literature data shows that the lines of the accidental contact must exist, for example, in Be, Mg, Zn, Cd, Al, and other metals (see Figs. 1a and 1b).

As early as 1962, Blount [22] established properties of the integral in the right-hand side of Eq. (4). He found that, if the contour Γ surrounds a line of the contact between the band under study and some other one, and the energies of the bands separate linearly in $\mathbf{k}$ in the vicinity of the line, then

$$\int_\Gamma \mathbf{\Omega}\, d\mathbf{k} = \pm\pi, \tag{5}$$

where the sign in the right-hand side of Eq. (5) is determined by a direction of the integration [23]. If in the vicinity of the band-contact line the energy splitting of electron states is quadratic in the distance of the point $\mathbf{k}$ from the line, then

$$\int_\Gamma \mathbf{\Omega}\, d\mathbf{k} = 0. \tag{6}$$

It should be emphasized that the integrals in Eqs. (5) and (6) do not depend on the shape and the size of the contour Γ. This is not surprising, since the equation

$$\nabla_k \times \mathbf{\Omega}(\mathbf{k}) = 0 \tag{7}$$

holds everywhere outside the band-contact line [22] (but in the line $u_{\mathbf{k}0}$ is the nonanalytical function of $\mathbf{k}$, and $\mathbf{\Omega}$ is undefined).

Now we are able to find γ for any semiclassical electron orbit Γ. The above-mentioned condition of the linear separation of the energy bands is fulfilled in the vicinity of any line of the accidental contact [20] and also near a threefold symmetry axis when the degeneracy of

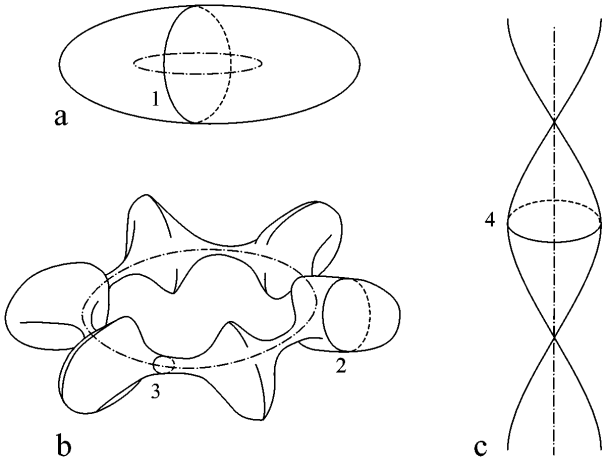

FIG. 1. The schematic sketch of Fermi surfaces for several metals with band-contact lines: the third-band electron "lens" of Zn and Cd (a); the second-band hole "coronet" ("monster") of Be and Mg (b); the self-intersecting Fermi surface of graphite (c). The band-contact lines are shown as the dash-dotted lines. The semiclassical orbits 3 and 4 link to the band-contact lines while the orbits 1 and 2 do not.

states occurs in it. If Γ links to such a line or an axis (see, e.g., the orbits 3 and 4 in Fig. 1), it follows from Eqs. (4) and (5) that

$$\gamma = 0 \tag{8}$$

($\gamma = 1$ and $\gamma = 0$ are equivalent). If the linking is absent (the orbits 1 and 2 in Fig. 1), a surface with boundary Γ necessary exists which does not intersect the band-contact line [for the surface in the case of the orbit 1 (or 2) we can take a part of the constant-energy one shown in Fig. 1]. Transforming the right-hand side of Eq. (4) into the integral over this surface with the use of Stokes' theorem and taking into account Eq. (7), we arrive at formula (2). Interestingly, Eq. (2) is also obtained when Γ links to an even number of band-contact lines (such a situation takes place, e.g., for any central cross section of the second-band Fermi surface of Al). In the case of a symmetry axis different from a threefold one, the separation of the bands is quadratic in a distance of $\mathbf{k}$ from the axis and one always has Eq. (2). The same result is true for symmetry points in the Brillouin zone. This follows from the same considerations that have been used in the case of the absence of the linking.

The obtained result for γ is closely analogous to the Aharonov-Bohm's effect [24]. As pointed out by Blount [18], the quantity $\mathbf{\Omega}$ is similar to a vector potential for a magnetic field. Indeed, the phase transformation,

$$u_{\mathbf{k}0} \rightarrow u'_{\mathbf{k}0} = u_{\mathbf{k}0} \exp[\imath\varphi(\mathbf{k})], \tag{9}$$

where $\varphi(\mathbf{k})$ is some regular function of $\mathbf{k}$, results in the change of $\mathbf{\Omega}$:

$$\mathbf{\Omega} \rightarrow \mathbf{\Omega}' = \mathbf{\Omega} - \nabla_{\mathbf{k}}\varphi, \tag{10}$$

which is characteristic of a vector potential. Taking into account Eqs. (5) and (7), we can treat a band-contact line as an infinitely thin "solenoid" which carries the fixed flux of the "field" $[\nabla_k \times \mathbf{\Omega}]$. With this in mind, the above-mentioned analogy becomes apparent. Although the semiclassical electron moving round the band-contact line does not reach the region in which the "field" is nonzero, it experiences the vector potential $\mathbf{\Omega}$ that cannot be made to vanish along the whole length of the orbit linking to the solenoid. The semiclassical electron state with the energy determined by Eq. (1) is the standing wave. If the electron orbit surrounds the band-contact line (i.e., the solenoid), the interference picture corresponding to this wave is shifted as compared to the case when the line is absent. This Aharonov-Bohm's shift manifests itself as the change in γ.

Berry [1] analyzed the geometrical phase of a quantum system when the orbit of this system in the parameter space is located near the point of degeneracy of its states. The Hamiltonian of the system was assumed to be a Hermitian matrix which is linear in deviations of the parameters from the point. Berry presented his results in the pictorial form. He found that such a point can be considered as the "monopole" in the parameter space when the geometrical phase is calculated. In other words, the point "generates" the field which coincides in the form with that of the monopole, and the flux of this field through the contour Γ gives the geometrical phase of the system. In crystals with the inversion symmetry, the Berry's phase of electrons has the specific features which are due to the fact that electron states are invariant under the transformation U (for the definition of U, see above). First, in any point of the Brillouin zone the Hermitian Hamiltonian can be transformed into the real one. As a consequence, the character of the energy-band splitting near the point of the degeneracy is changed as compared with the general case considered by Berry (now the splitting does not occur along some direction), and the monopole in $\mathbf{k}$ space disappears. Second, the field of Berry $[\nabla \times \mathbf{\Omega}]$ satisfies Eqs. (5) and (7), and Berry's phase does not depend on the shape and the *size* of the electron orbit but is specified by its topological characteristics (there is a linking or it is absent). Thus, it is valid to say that, instead of the monopoles, the solenoids associated with band-contact lines appear in metals.

The value γ can be experimentally determined through the investigation of oscillation effects in metals [8]. Since the measurement of γ is easiest to make for semiclassical orbits corresponding to small extremal cross sections of a Fermi surface, we point out that such orbits exist, e.g., in beryllium, magnesium, and graphite, and in these metals they link to the band-contact lines (see Fig. 1). In Be and Mg, the accidental contact between the second and third bands occurs in the basal plane of the crystals. If $\mathbf{H}$ lies, e.g., in this plane also, Eq. (8) must be valid for the orbits on the "necks" of the second-band hole coronet (or monster). It should be noted that in Zn and Cd which are akin, in many respects, to Be and Mg the same band-contact line is located in the third-band electron lens and does not link to the semiclassical orbits (therefore, in this case $\gamma = 1/2$). In graphite the degeneracy of two bands takes place along the vertical edge *HKH* of the Brillouin zone (i.e., along the threefold symmetry axis). Thus Eq. (8) is expected to be true for the extremal orbit surrounding the point *K* (see orbit 4 in Fig. 1).

In summary, we have shown that in quantization condition (1) γ is equal to zero when in $\mathbf{k}$ space the closed electron orbit associated with a certain energy band $\varepsilon_0(\mathbf{k})$ surrounds the line of degeneracy of this band with some other one. This result depends neither on the form of $\varepsilon_0(\mathbf{k})$ in the neighborhood of the orbit nor on the shape and the size of the electron trajectory and is topological in nature. It is due to the fact that the electron orbit *links* to the band-contact line which is the line of singularities for the Bloch wave functions. If the linking is absent, the conventional result, $\gamma = 1/2$, holds. Measurements of γ can provide a possibility of detecting band-contact lines in metals (beryllium, magnesium, and graphite appear to have considerable promise on this point).

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