Ideally Conducting Phases in Quasi Two-Dimensional Conductors

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The possibility of the existence of ideal conductivity at finite temperatures in *clean* quasi *two-dimensional* conductors under conditions similar to the quantized Hall effect is discussed. It is found that for metallic electron densities and realistic values of the magnetic field the electronic system should break into two coexisting diamagnetic phases, for which the chemical potential is pinned in the middle of a magnetic energy gap, and the system is *nondissipative*. The experimental feasibility of the proposed mechanism is briefly discussed.

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Recently Azbel[1] discussed the possibility of the existence of ideal conductivity at relatively high temperatures in *bulk* anisotropic materials under conditions similar to the quantized Hall effect[2,3] (QHE). In order to achieve such an ideal conductivity three conditions should be met: (1) The material under consideration should have a highly two-dimensional (2D) electronic band structure. (2) A magnetic field applied along the hard axis of the sample should be strong enough to yield a cyclotron frequency ω_c significantly larger than $k_B T/\hbar$ (k_B is the Boltzmann constant and T is the temperature). (3) The chemical potential μ should be located sufficiently far (on the scale of $k_B T$) from any Landau level to assure that the level just below μ is completely filled while that above μ is completely empty. Under these circumstances dissipation is extremely small (i.e., the relaxation time is extremely long[1]); both longitudinal resistivity and conductivity vanish while the Hall conductivity is finite.

In a clean highly 2D conductor, however, the chemical potential is known to be pinned to the highest occupied Landau level at almost all values of the magnetic induction B, except for certain discrete values of B, around which the chemical potential varies rapidly between adjacent Landau levels. This makes the validity of the above idea crucially dependent on the existence of an *extrinsic* mechanism for the pinning of the chemical potential within a magnetic energy gap, such as, for example, pinning to localized impurity states, which may be present within the magnetic gaps.[3]

Our aim in this note is to show that, under certain reasonable conditions, it is not necessary to invoke such an extrinsic mechanism, since there is an *intrinsic* mechanism for the pinning of the chemical potential in the middle of a magnetic gap. We find that, for metallic electron densities and realistic values of the magnetic field, the pinning of the chemical potential to a Landau level corresponds to a thermodynamically unstable situation, so that thermodynamic stability imposes creation of coexisting diamagnetic phases, for which the chemical potential is located in the *middle* of a magnetic gap. Creation of magnetic domains in 3D metals under conditions of the de Haas–van Alphen effect have been previously discussed by a number of authors.[4-8] This effect should be much more important, however, in quasi 2D conductors since in these systems the energy bands are separated by large magnetic gaps.[9] As we shall show below, this should lead to the establishment of an ideal conductivity in the interior of each diamagnetic phase.

To show this we consider a simple model for a quasi 2D conductor[10]; the model consists of an anisotropic electron gas having two equivalent easy axes (x and y) and a perpendicular hard axis (z). A static magnetic field H is applied along the z axis so that the single-electron energies are given by

$$\epsilon(n, k_z) = (n + \tfrac{1}{2})\hbar\omega_c + \Delta_z[1 - \cos(k_z d)], \qquad (1)$$

where ω_c is the cyclotron frequency, d is the lattice constant in the z direction, and $n = 0, 1, 2, \ldots$. For highly 2D cyclotron orbits the maximum value of the longitudinal kinetic energy Δ_z is much smaller than $\hbar\omega_c$. Note that the electron spin is ignored in Eq. (1). The inclusion of spin would introduce some difficulties into our analysis.[11] A preliminary study of this problem indicates, however, that the inclusion of spin would not alter our results in any essential way.

We thus proceed by considering the thermodynamic potential

$$\Omega = -k_B T \sum_{k_z} \sum_{k_y} \sum_{n=0}^{\infty} \ln(1 + \exp\{[\mu - \epsilon(n, k_z)]/k_B T\}). \qquad (2)$$

As we have already mentioned the condition $\Delta_z \ll \hbar\omega_c$ guarantees the two dimensionality of the cyclotron orbits. Under these circumstances we may neglect the longitudinal kinetic energy term in the single-electron energy [Eq. (1)] so that the summands in Eq. (2) are independent of both k_y and k_z. The double sum over k_z and k_y thus yields a degeneracy factor $g = VB/\varphi_0 d$, where V is the volume of the sample and $\varphi_0 = 2\pi\hbar c/e$ is the magnetic flux quantum. A closed analytical expression for Ω can thus be obtained once the chemical potential μ is known. The chemical potential is determined by the equation

$$g\sum_{n=1}^{\infty}\{1+\exp[x(n)-\alpha]\}^{-1}=N, \tag{3}$$

where $x(n)=(n\hbar\omega_c-\mu)/k_BT$, $\alpha \equiv \hbar\omega_c/2k_BT$. Note that the only effect of the interplane coupling in this approximation is to introduce a cutoff ($k_z = \pi/d$) along the z axis in phase space. Let us denote by n_F the value of n in Eq. (3) corresponding to the highest occupied level, $\hbar\omega_c(n_F-\frac{1}{2})$. Now $(n_F+\frac{1}{2})\hbar\omega_c > \mu$ and $(n_F-\frac{1}{2})\hbar\omega_c < \mu$ and since $\hbar\omega_c \gg k_BT$ (i.e., $\alpha \gg 1$) we may replace the value of each term in Eq. (3) up to $n = n_F - 1$ by unity. To take into account correctly, however, the depinning of the chemical potential from the level $(n_F+\frac{1}{2})\hbar\omega_c$ and the pinning to the level $(n_F-\frac{1}{2})\hbar\omega_c$ we should retain the exact expression for both the n_Fth and the (n_F+1)th terms.

Using this approximation in Eq. (3) we obtain the equation

$$\sinh(x_F)/[\cosh(x_F)+\cosh\alpha]=A(B), \tag{4}$$

where $x_F \equiv x(n_F)$ and $A \equiv n_F - N/g$. Solving Eq. (4) we obtain

$$\mu=\hbar\omega_c n_F - k_BT\ln\{[A\cosh\alpha+(1+A^2\sinh^2\alpha)^{1/2}]/(1-A)\}. \tag{5}$$

The corresponding result for the magnetization is given by

$$M(B)=-V^{-1}(\partial\Omega/\partial B)_{T,V,\mu}=(\varphi_0 d)^{-1}\{n_F\mu(B)+\hbar\omega_c A[n_F+\sinh\alpha/2\sinh(x_F)] \\ -\hbar\omega_c(n_F{}^2+1)+k_BT\ln[2\cosh(x_F)+2\cosh\alpha]\}. \tag{6}$$

As can be readily seen from Eq. (5), around the value $B^* \equiv (N/V)\varphi_0{}^d/n_F$ of the magnetic induction B, where $A \approx 0$, the chemical potential moves rapidly from the close vicinity of the upper Landau level $\hbar\omega_c(n_F+\frac{1}{2})$, to the close vicinity of the lower level $\hbar\omega_c(n_F-\frac{1}{2})$, as B moves from slightly below B^* to slightly above B^* [see Fig. 2(a)]. For values of B sufficiently far from B^* the magnetization $M(B)$ exhibits essentially a linear dependence on B [see Figs. 1(b) and 2(b)] with a slope

$$\chi_0=\hbar e n_F{}^2/m_c c\varphi_0 d = n_F{}^2e^2/2\pi d m_c c^2, \tag{7}$$

which is identical to the value of the de Haas–van Alphen susceptibility obtained by Azbel[1] (see also Peierls[9] and Halperin.[12])

The corresponding H vs B diagram is shown in Fig. 1(c). In the high-field portion of the diagram, where the slope $\chi_0(n_F)$ of the $M(B)$ curve is smaller than $1/4\pi$, the slope of the $H(B)$ curve is positive and for each value of the external field H in this region there is only one value of B on the $H(B)$ curve. Since the chemical potential is almost everywhere pinned to a Landau level, ideal conductivity is practically impossible in this region. If the field H is sufficiently low, however, such that $\chi_0(n_F) > 1/4\pi$ the slopes of the linear portions of the $H(B)$ curve are always negative and for each value of H there are at least three different values of B on the $H(B)$ curve. The value of $B^*(n_F)$ for which this phenomenon starts to occur is given by

$$B_c{}^{\mathrm{I}}=[4\pi(N/V)\hbar e/m_c c]n_F. \tag{8}$$

It can be readily shown that for all values of B^* between $B_c{}^{\mathrm{I}}$ and $B_c{}^{\mathrm{II}} \equiv B_c{}^{\mathrm{I}}/\sqrt{2}$ there are no more than three values of B ($B_<$, B_0, and $B_>$ in Fig. 1) on the $H(B)$ curve for each value of H. Let us for the sake of simplicity assume that this is our case. The slope of the $H(B)$ curve near $B_<$ and $B_>$ is positive so that they correspond to thermodynamically stable situations. B_0, however, is located in the linear portion of the $H(B)$ curve and since the slope $(\partial H/\partial B)$ there is negative it corresponds to an unstable situation. Thus thermodynamic stability imposes the breaking of the originally homogeneous system into two diamagnetic phases, one having magnetic induction $B = B_<$ and the other $B = B_>$. Thus the cyclotron frequency for an electron in the first phase is $\omega_c{}^> \equiv eB^>/m_c c$ while that for an electron in the second phase is $\omega_c{}^< \equiv eB^</m_c c$.

Applying the Maxwell construction[7] to determine the equilibrium condition for coexistence between the two phases, one finds that the chemical potential for the entire system is located

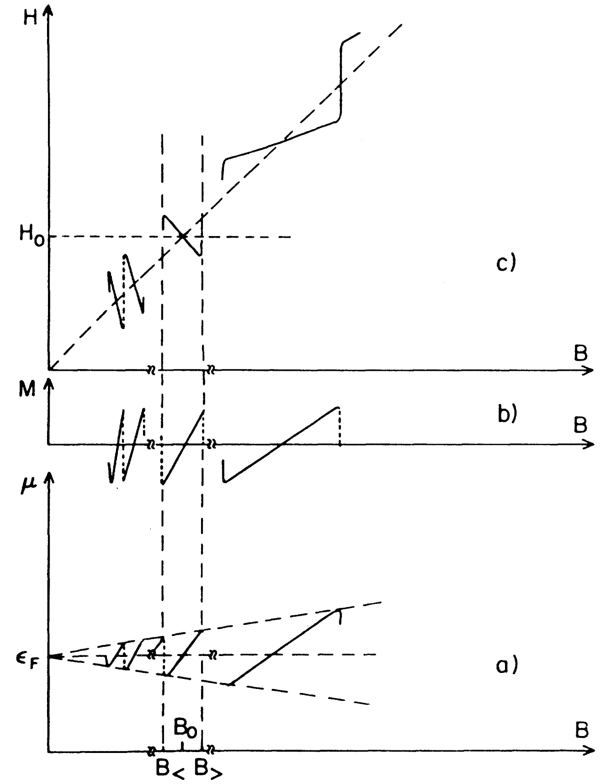

FIG. 1. Schematic illustrations of (a) the chemical potential μ, (b) the magnetization M, and (c) the magnetic field H as functions of the magnetic induction B at zero temperature. $B_<$, $B_>$, and B_0 are defined in the text and ϵ_F is the value of the chemical potential at zero magnetic field.

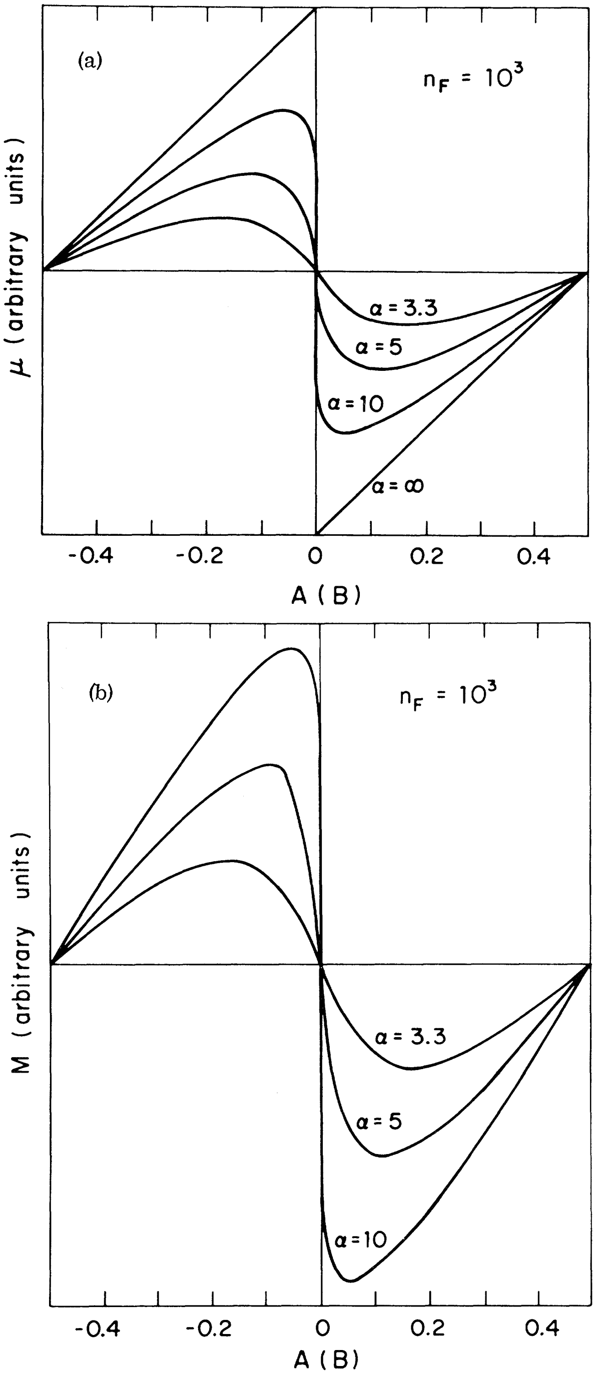

FIG. 2. The variation of (a) the chemical potential μ and (b) the magnetization M as functions of $A(B) = n_F - N\varphi_0 d/VB$ around $A(B) = 0$ (i.e., $B = B^*$) for various values of the parameter $\alpha \equiv \hbar\omega_c^*/2k_BT$, $\omega_c^* \equiv eB^*/m_cC$.

exactly at

$$\mu = \hbar\omega_c{}^{>} n_F = \hbar\omega_c{}^{<}(n_F + 1) = (N/V)2\pi\hbar^2 d/m_c\,.$$

In other words, for each phase the chemical potential is located exactly in the middle of the gap separating the highest occupied level from the level just above it. Thus in both phases the highest occupied level is completely filled so that ideal conductivity is expected to occur in the interior of each phase. Significant deviations from ideal conductivity may occur in the transition zones separating different phases but the overall effect on the conductivity of the whole sample should be small because of the small size of the transition zones.[7,8]

As we have already mentioned, several conditions should be met in order that the proposed mechanism for ideal conductivity would be operative: (1) The cyclotron frequency ω_c should be much larger than both $\Delta_z/\hbar$ and $k_BT/\hbar$. This implies that one should look for a material with a small in-plane cyclotron mass m_c such as, for example, the linear-chain mercury compound $Hg_{3-x}AsF_6$, which exhibits a number of large cyclotron frequencies in de Haas–van Alphen experiments[13] (the largest ω_c observed corresponds to $m_c \sim m_e/50$, where m_e is the free electron mass). (2) The de Haas–van Alphen susceptibility $\chi_0(n_F)$ [Eq. (7)] should be larger than $1/4\pi$ for the diamagnetic instability to appear. The meaning of this condition is that the applied magnetic field H should be smaller than $(2m_c/d)^{1/2}E_F/\hbar$, where E_F is the chemical potential at zero magnetic field. Taking for E_F a typical value of 1 eV and assuming $m_c = 0.1m_e$ (see later) we obtain for a typical value of the interplane distance d (e.g., $d < 10$ Å) that $H < 3$ T. A single bistable situation can thus be obtained for magnetic fields satisfying $B_c^{\mathrm{I}}/\sqrt{2} < B < B_c^{\mathrm{I}}$. This is a sufficiently large range for B_c^{I} of the order to several tesla.

Note that since condition (1) requires a large magnetic field while condition (2) requires a sufficiently small one it might be difficult to satisfy them simultaneously. To check how restrictive these conditions really are we assume that H satisfies condition (2) and then determine the values of E_F, m_c, d, Δ_z, and T for which condition (1) can be satisfied. The result is $\Delta_z, k_BT < [(2e^2/m_cC^2)/d]^{1/2}E_F$. Thus for our typical values (i.e., $E_F = 1$ eV, $d = 10$ Å, $m_c = 0.1m_e$) we find that (Δ_z/k_B), $T < 30$ K.

Our conclusion is therefore that the effect may be observed experimentally under realistic magnetic fields and at reasonably low temperatures in the family of the intercalated graphite compounds since in this family the in-plane effective mass is small (for clean graphite the in-plane effective mass is about $0.1m_e$ [14]) and the interplane distance may be controlled experimentally. The effect may also appear in the linear-chain mercury compound $Hg_{3-x}AsF_6$, since it exhibits a highly two-dimensional dynamics of the conduction electrons in de Haas–van Alphen experiments[13] and large in-plane cyclotron frequencies.

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