Peierls structural phase transition in 2*D* systems due to magnetic breakdown

V. M. Gvozdikov and É. A. Kaner
Institute of Radio Engineering and Electronics, Academy of Sciences of the USSR

(Submitted 20 March 1986)
Pis'ma Zh. Eksp. Teor. Fiz. **43**, No. 8, 393–395 (25 April 1986)

A Peierls superstructure may arise on chains of magnetobreakdown trajectories in 2*D* conductors. In the case of a well-developed magnetic breakdown, this superstructure will take the form of a sequence of structural phase transitions which are periodic in the reciprocal of the magnetic field. The critical temperature is calculated as a function of the field. Experimental data which qualitatively reproduce the features of this effect are discussed.

The reason for the unusual low-temperature properties of organic conductors is known to be the quasi-1*D* of their electron spectrum. Systems with a 1*D* electron spectrum can be produced in materials other than organic conductors. Another possibility results from the fact that a magnetic field effectively reduces the dimensionality of an electron system. For this reason, certain 1*D* effects, e.g., a Peierls structural phase transition, can be induced by a weak magnetic field in 2*D* systems under conditions of a coherent magnetic breakdown. In the present letter we offer the first analysis of this phenomenon. We show that a magnetic breakdown can indeed give rise to a series of structural phase transitions which are periodic in the reciprocal of the magnetic field.

We consider a 2*D* metal in a magnetic field perpendicular to the plane of the metal. In this case the semiclassical trajectories determined by the cross section of the

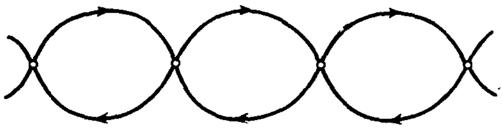

FIG. 1.

Fermi surface are chains of closed orbits (Fig. 1). We know that in strong fields $H > H_0$, where H_0 is the breakdown field, a magnetic breakdown can occur in such systems, with the result that the electrons are coherently displaced along the chain. The Landau levels expand into magnetic bands, and the energy spectrum becomes dependent on not only the index of the magnetic breakdown but also the quasimomentum $\hbar k$. In the case of circular orbits, the spectrum can be found explicitly:

$$E_n(k) = \hbar\Omega (n + {}^1/_2) + (-1)^n \epsilon_\rho(k),$$
$$\epsilon_\rho(k) = \frac{\hbar\Omega}{\pi} \arcsin(\rho \cos kL) . \tag{1}$$

Here Ω is the cyclotron frequency, $\rho = \exp(-H_0/H)$ is the probability for magnetic breakdown, and L is the spatial period of the magnetic-breakdown chain. At a fixed value of n, the spectrum becomes effectively one-dimensional and satisfies the condition

$$\epsilon_\rho(k + Q) = - \epsilon_\rho(k) \tag{2}$$

with a wave vector $Q = \pi/L$. When the magnetic bands are half-filled, in complete analogy with organic quasi-1D systems, condition (2) leads to a Kohn anomaly in the polarization operator $\pi(q, \omega, H)$ at $\omega = 0$ and $q = Q$, which is responsible for a doubling of the period of the chain. Making use of the explicit expression[2] for the operator π along with relations (1) and (2), we write the equation determining the period-doubling condition in the form

$$g = \int_0^{\pi/2} dy \frac{\tanh(pz)}{z} \frac{1 - \tanh^2(\pi p \Delta)}{1 - \tanh^2(\pi p \Delta)\tanh^2(pz)} \tag{3}$$

Here $g = \pi N \hbar^2 / M m S_*^2$, N is the 2D electron density, m is the electron mass, M is the ion mass, S_* is the ion contribution to the sound velocity, $p = \hbar\Omega/2\pi T$, T is the temperature, $z = \arcsin(\rho \cos y)$, and the function $\Delta(1/H)$, which is periodic in $1/H$, is defined as the fractional part of the quantity $E_F/\hbar\Omega - 1/2$.

As H is varied, the magnetic bands periodically cross the Fermi level E_F, so that the critical temperature (T_c) of the phase transitions with a period doubling turns out to be a function which is periodic in $1/H$ with a period $\delta(1/H) = \hbar e/mcE_F$, as in the de Haas-van Alphen effect. The functional dependence $T_c(H)$ is a sequence of "pulses," whose shape, found numerically from (3), is shown in Fig. 2. It can be seen from this figure that as the field is increased, the height of these pulses and their width increase. At $H_0 \sim 10^4$–10^5 Oe, the width of a pulse can reach $\sim 10^2$ Oe, and its height can reach $\sim$1–20 K. The maximum of T_c is reached at $\Delta = 0$. An estimate of $T_c^{\max}$

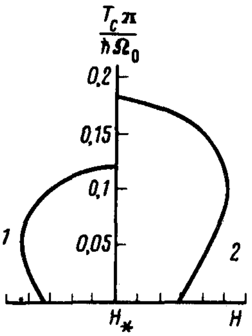

FIG. 2. The functional dependence $T_c(H)$ found numerically from (3) with $E_F = 10^3\ \hbar\Omega$ and $g = 5$. It takes the form of "pulses" which are periodic in the reciprocal of the field. Curve 1 shows a pulse which is centered at the field value $H_* = H_0$, while curve 2 shows a pulse centered at $H_* = 10H_0$. The division along the H scale for curve 1 is $10^{-5}H_0$, while that for curve 2 is $10^{-4}H_0$. For clarity, only half of each of the symmetric pulses is shown.

from (3), with logarithmic accuracy yields

$$T_c^{\max} \simeq \frac{\hbar\Omega}{\pi^2}\,\gamma \arcsin\rho \exp(-g\rho), \tag{4}$$

where $\ln\gamma = C \approx 0.577...$ is the Euler constant. At $\rho \ll 1$ we find from (4)

$$T_c^{\max} \simeq 0.18\hbar\Omega \exp(-H_0/H). \tag{5}$$

As the center of the magnetic band is shifted with respect to the Fermi level, the quantity Δ increases, while T_c falls off sharply, as can be seen from Fig. 2. At the same time, the nature of the filling of the magnetic band intersecting E_F is also a function which is periodic in $1/H$, so that, in addition to the well-developed magnetic breakdown, it is necessary that the upper band be half-filled. If the field intervals, in which the filling is approximately half, are equal to $H^{(i)} - H^{(i+1)}$, this phase transition unfolds in the following way as the field is varied: In weak fields ($H < H_0$), there is no effect. The effect first arises against the background of a well-developed magnetic breakdown, when a threshold is reached, $H^{(1)} > H_0$. As H is increased further, we see a series of structural phase transitions ["pulses" of $T_c(H)$] with a period $\delta(1/H)$; this series cuts off at $H^{(2)}$ and then reappears in intervals $H^{(i)} - H^{(i+1)}$, but with a higher $T_c(H)$ pulse.

The features of the structural transition described above correspond qualitatively to those observed experimentally in the compounds[3,4] [$(TMTSF)_2ClO_4$], since the same type of Kohn anomaly is responsible for the phase transition of the spin-density-wave type. In these compounds, a trajector of the sort shown in Fig. 1 arises because of the formation of "electron pockets," which results from the spin-density wave along conducting filaments. In other words, this effect may supplement the Gor'kov mechanism.[3]

Iye and Dresselhaus[5] have observed the formation of a superstructure induced by a strong magnetic field in a layered crystal. Their empirical dependence $T_c(H)$ agrees in shape with expression (5), with $H_0 \simeq 1047$ kOe, and with ≈ 69 K as the coefficient of the exponential function.

The conditions for the realization of a coherent magnetic breakdown in $2D$ systems are less stringent than in $3D$ systems. In particular, a coherent magnetic breakdown is not disrupted when the field is rotated around the axis of the magnetic-breakdown chain. The $3D$ nature of the spectrum also disrupts the "nesting"[2] and suppresses the structural phase transition under discussion here. The transformation from circular orbits to orbits of arbitrary shape reduces to the replacement $E_F/\hbar\Omega_0 \rightarrow cS/2\pi e\hbar H_0$, where S is the area of the orbit. For the common case in which the magnetic-breakdown chain consists of an alternation of large and small orbits, whose areas differ greatly and satisfy the inequalities $S_1 \gg S_2 \gg e\hbar H/c$, the effective probability for magnetic breakdown through a small orbit is[1]

$$\rho_{\rm eff} = \rho^2[\rho^4 + 4(1-\rho^2)\cos^2\varphi_2]^{-1/2},$$

where $\varphi_2 = cS_2(E_F)/2e\hbar H$. After the replacement $\rho \rightarrow \rho_{\rm eff}$, Eqs. (1)–(4) remain in force, so that the oscillations of $T_c(H)$ described above will be modulated periodically by oscillations of the phase of the small orbit.

[1]M. I. Kaganov and A. A. Slutskin, in: Elektrony provodimosti (Conduction Electrons), Nauka, Moscow, 1985, p. 416.
[2]É. A. Kaner and L. V. Chebotarev, Zh. Eksp. Teor. Fiz. **73**, 1813 (1977) [Sov. Phys. JETP **46**, 953 (1977)].
[3]L. P. Gor'kov, Usp. Fiz. Nauk **144**, 381 (1984) [Sov. Phys. Ups. **27**, 809 (1984)].
[4]P. Pesty, P. Garoshe, and K. Bechgaard, Phys. Rev. Lett. **55**, 2495 (1985).
[5]Y. Iye and G. Dresselhaus, Phys. Rev. Lett. **54**, 1182 (1985).

Translated by Dave Parsons