Magnetic oscillations in organic superconductors (theory)

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A theory is proposed for the oscillatory behavior of spin-density waves in $(TMTSF)_2X$ organic superconductors in strong magnetic fields.

Organic conductors with the chemical formula $(TMTSF)_2X$ have attracted considerable interest in recent years (see the reviews by Jerome and Schulz[1] and Gor'kov.[2] In these materials, a superconductivity competes with a spin-density wave. In addition to the "ordinary" spin-density wave, which is commensurate with the crystal structure, an "extraordinary" spin-density wave forms in a strong magnetic field after the destruction of superconductivity. In this event, oscillations are observed in the resistance and, apparently, the phase-transition temperature. We have recently proposed a theory[3] according to which the existence of superconductivity in these compounds stems from the formation of a certain crystalline superstructure which causes neighboring conducting chains to become nonequivalent. In the present letter we show that the presence of a structure of this sort also explains the behavior in strong magnetic fields.

We consider a layer of chains spaces at a distance b. We assume that there is a crystal field which oscillates along the b axis with a period of $2b$ [this is the structure of $(TMTSF)_2ClO_4$ in the superconducting R phase). If the integral representing hopping between chains, t, is far smaller than the potential difference between neighboring chains, κ, the Fermi momentum of the electrons will depend on the chain index n: $k_F^{(n)} = k_F + (-1)^n\kappa/2\hbar v_F$, where v_F is the Fermi velocity. Beats between the different $k_F^{(n)}$ create a large period $l = 2\pi\hbar v_F/\kappa$ along the chains in the system. Let us assume that a magnetic field H is imposed in the direction perpendicular to the layer. We would expect that when the magnetic flux through the natural cell $l \times b$ is comparable to the quantum of flux, ϕ_0 there will be distinctive features in the behavior of the system. In the present letter we show that the temperature at which a spin-density wave forms rises in a magnetic field which satisfies the condition

$$Hbl = 2\phi_0/M, \quad M = 2m + 1, \tag{1}$$

where M is an odd number.

We set $\hbar = v_F = \pi/k_F = 1$. We introduce the operators $\psi_{n,\alpha}(x)$, which annihilate electrons with momenta near αk_F, $\alpha = \pm$, at the point x in chain n. For simplicity, we will omit the spin indices, since our theory describes spin- and charge-density waves equally well. In the presence of a magnetic field and a crystalline superstructure, it is convenient to introduce the gauge transformation

$$\psi_{n,\alpha}(x) = \tilde{\psi}_{n,\alpha}(x) \exp\left[\alpha i k_F^{(n)} x + inb\frac{e}{c}Hx\right]. \tag{2}$$

The Hamiltonian of the system then becomes

$$\hat{H} = \sum_{n;\,\alpha=\pm 1} \hat{H}_0(\tilde{\psi}^+_{n,\alpha};\ \tilde{\psi}_{n,\alpha}) + \sum_{\alpha=\pm 1,\,p=\pm 1} \int dx\,[t_{n,p,\alpha}(x)\,\tilde{\psi}^+_{n+p,\,\alpha}(x)\,\tilde{\psi}_{n,\alpha}(x) + \text{H.a.}]; \tag{3}$$

$$t_{n,p,\alpha}(x) = t\exp[-ipqx + i\alpha(-1)^n \kappa x], \quad q = \frac{e}{c} bH. \tag{4}$$

Here $\hat{H}_0$ is the Hamiltonian of the one-dimensional interacting electrons.[4] We wish to call attention to the fact that the influence of the magnetic field and the crystalline superstructure is seen only in the oscillatory nature of hopping integrals (4). The interactions in $\hat{H}_0$ are assumed to be of such a nature that there are no gaps in the spin and charge channels. In this case, according to the results found in solutions of one-dimensional models,[4] the correlation function for two electrons calculated with the help of $\hat{H}_0$ is (within logarithmic dependences)

$$K_0(z_1, z_2, z_3, z_4) = \langle \tilde{\psi}_{n_1+}(z_1)\,\tilde{\psi}_{n,-}(z_2)\,\tilde{\psi}^+_{n,+}(z_3)\,\tilde{\psi}^+_{n,-}(z_4)\rangle_0$$

$$= \frac{\text{const}}{s(z_1 - z_3)\,s^*(z_2 - z_4)\,|s(z_1 - z_3)\,s(z_2 - z_4)|^{\eta_F - 1}} \times \left| \frac{s(z_1 - z_4)\,s(z_2 - z_3)}{s(z_1 - z_2)\,s(z_3 - z_4)} \right|^{\nu}; \tag{5}$$

$$s(z) = \operatorname{sh}(\pi T z)/\pi T, \quad z = x + i\tau,$$

where T is the temperature, and τ is the Matsubara time. The indices ν and η_F can be regarded as phenomenological constants. In the case of a weak interaction of the type g_2 we would have $\nu = -g_2/2\pi$, $\eta_F = 1 + (g_2/2\pi)^2$ (Ref. 4). Working from the experimental data, we consider the case $\nu > 0$, which corresponds to superconducting ordering in the absence of a magnetic field.[3]

We consider a spin-density wave characterized by an anomalous Green's function $O_p(z_1 - z_2) = \langle \tilde{\psi}_{n,+}(z_1) \times \tilde{\psi}^+_{n+p,-}(z_2)\rangle$, $p = \pm 1$, which describes the pairing of particles in adjacent chains. The transition temperature T_c is determined by the divergence of the corresponding correlation function. We will calculate this function, treating the hopping amplitude t in Hamiltonian (3) as a perturbation, and using the ladder approximation in t (Ref. 3). Figure 1 shows a typical diagram of the series. The squares with diagonals represent correlation functions (5) for electrons in chains n, $n+1$; each line represents a factor from (5), which depends on the corresponding difference in coordinates; the isolated lines at the ends of the diagram correspond to single-particle Green's functions; the dashed lines represent the hopping integral t; and the wavy and broken lines represent, in accordance with (4), the incoming and outgo-

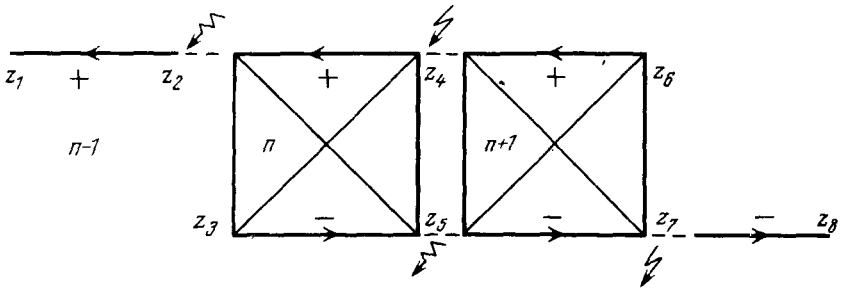

FIG. 1.

ing momenta $q-\kappa$ and $q+\kappa$. The results are determined primarily by those regions of the integration variables in which the large momenta $\sim\kappa$, $q \gg T$ cross a minimum number of lines of the diagram, while the integrals over loops converge at small momenta. In the coordinate representation, this behavior means that the points of the diagram between which the momenta $\sim q$, κ pass can be effectively contracted to a single point because of the rapid convergence of integrals of the product of an oscillating function and a decreasing function. The subsequent integration contains no oscillatory functions and is cut off at distances $\sim T^{-1}$. In the case $\nu > 0$, the following pairs of points in Fig. 2 contract: (z_2, z_5) and (z_4, z_7). Momenta $q \pm \kappa$ pass between them. Evaluating the integrals, we find that the series diverges at the temperature

$$T_c^{(0)}(q) \sim \left[\frac{t^4}{|\kappa^2 - q^2|^{2-\nu}}\right]^{1/\beta}, \quad \beta \equiv 2 - 2\eta_F + \nu > 0, \quad 2 - \nu > 0. \tag{6}$$

To find the transition temperature $T_c^{(1)}$ for $q = \kappa$, it is sufficient to cut off the increase in $T_c^{(0)}(q)$ in (6) at $|q-\kappa| \sim T_c^{(0)}(q)$:

$$T_0^{(1)} \sim \left[\frac{t^4}{(2\kappa)^{2-\nu}}\right]^{\frac{1}{\beta + 2\beta_F}}$$

$$\sim T_c^{(0)}(q=0)\left(\frac{\kappa}{T_{3d}}\right)^{\frac{2\beta_F(2-\nu)}{\beta(\beta+2\beta_F)}}, \quad \beta_F = 2 - \eta_F, \tag{7}$$

where $T_{3d} \sim (t)^{1/\beta_F}$ is the effective transverse width of the one-electron band.

An analogous study of higher-order diagrams shows that, in addition to the main resonance at $q = \kappa$, there are narrow peaks $T_c^{(m)}$ against the background of (6) at $q = \kappa/(2m+1)$: $T_c^{(m)}/T_c^{(1)} \sim (T_{3d}/\kappa)^a$, where $a = 4\beta_F m/(\beta + 2\beta_F)$.

A theory of magnetic oscillations in $(TMTSF)_2X$ compounds was first offered in Refs. 5 and 2. The effect with which we are concerned here differs in physical nature.

The case $\kappa = 0$ was studied in Refs. 5 and 2; the effect is based on a semiclassical description of the magnetic field and is determined by the Fermi surface (by the absence of nesting). Our model, in contrast, assumes a strong nonequivalence ($\kappa \gg T_{3d}$) of neighboring chains, describes quantum commensurability effects in strong magnetic fields, and predicts $l \sim \kappa^{-1}$. If we apply the theory of Refs. 5 and 2 to our model, we find $l \sim (T_{3d}^*)^{-1}$, where T_{3d}^*, the transverse width of the single-particle band, is equal to $T_{3d}^* = T_{3d}^2/\kappa$ in the given model.[3] Methodologically, the Gor'kov-Lebed' theory and the theory set forth in this paper have additional regions of applicability in the magnetic field: $q \lesssim T_{3d}^*$ and $q > T_{3d}^*$. We suggest that these two mechanisms describe respectively the "slow" (with a frequency $H_0 = 23$ T) and "fast" (275 T) oscillations which have been observed[6] in the R phase of $(TMTSF)_2ClO_4$.

Comparing (1) with experimental data,[6,7] we find that for oscillations of the magnetoresistance in $(TMTSF)_2PF_6$ under pressure we have $l = 344$ Å, while for the "fast" oscillations in $(TMTSF)_2ClO_4$ we have $l = 98$ Å. Using the simple band formula $v_F = t_a a/\sqrt{2}\hbar$, $t_a = 0.25$ eV, and $l = 3.7$ Å for an estimate, we find $\kappa = 12$ meV and $\kappa = 40$ meV, respectively.

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