Spin density waves and the quantum Hall effect in organic superconductors

A. G. Lebed'

L. D. Landau Institute for Theoretical Physics, USSR Academy of Sciences

Equations for the order parameter of spin density waves (SDW) induced by a magnetic field in (TMTSF)$_2$X superconductors are derived. The solutions of these equations for $T = 0$ correspond to the coexistence of several plane spin density waves.

The main feature of the phase diagram of the family of (TMTSF)$_2$X-compounds (X = ClO$_4$, PF$_6$, etc.) is a cascade of transitions in a magnetic field to states with spin density waves (SDW),[1,2] in which an analog of the two-dimensional quantum Hall effect is observed.[3,4]

The conventional explanation of the induction of SDW by a magnetic field is based on the effect of "one-dimensionalization" of the electron spectrum suggested for the first time in Ref. 5. In this effect the electron motion in a field **H** parallel to the z-axis along the open portions of the Fermi surface of a quasi-two-dimensional electron spectrum

$$\varepsilon (\mathbf{p}) = \pm v_F(p_x \mp p_F) + t(p_y, p_z),$$

$$t(p_y, p_z) = 2t_b \cos (p_y b) + 2t_b' \cos (2p_y b) + 2t_c \cos (p_z c),$$

$$t_b \gg t_b', \ t_c, \tag{1}$$

corresponds, in real space, to a periodic bounded motion across the chains

$$y = y_0 + \frac{2ct_b}{eHv_F} \sin \left(\frac{eHv_F b}{c} \tau\right). \tag{2}$$

(Here p_F and v_F are the "Fermi" momentum and velocity, respectively, t_b, t_b', and t_c are overlap integrals of the electron wave functions across the chains; a, b, and c are the crystal lattice constants.) In this situation the electron motion is infinite only in the direction of the chains, and the latter acquire some properties of a one-dimensional electron gas. Such a gas, as is well known, is unstable with respect to the "Peierls pairing." In the case concerned this gives rise to instability in the spin channel and SDW formation.

The resulting spin density waves, due to the periodic electron motion (2), are characterized by the quantum values of the longitudinal wave vector[6-8]

$$Q = (2p_F + 2n\omega_c/v_F, \ \pi/b, \ \pi/c), \tag{3}$$

where ω_c is the cyclotron frequency of the electron motion on the Fermi surface (1).

The electron spectrum of such states with SDW was found in Ref. 9 and consists of wide Landau bands separated by narrow gaps (with the largest gap at the Fermi level). The problem of the "Hall conductivity" of such a dielectric spectrum can be solved by means of the Streda formula,[10] and for the phase (3) with the quantum number n we have[11]

$$\sigma_{xy} = \frac{2ne^2}{h}. \tag{4}$$

The main drawback of these and other treatments is, to our mind, the description of SDW by a single value of n in the formula for the wave vector (3). In Ref. 12 it has been shown in the Landau approximation for the free energy expansion

that this description contradicts the real symmetry of the lattice, i.e., the existence of one electron per unit cell. Below we study the case $T = 0$ which is of interest for experimental applications and suggest a means of finding the Hall conductivity σ_{xy} when the order parameter is a periodic function of position and is expanded in a series of the plane waves (3).

We work, as usual, the quantum limit $\omega_c \gg T, \Delta$, where Δ is the amplitude of the SDW order parameter

$$\Phi (\mathbf{r}) = \Delta (x) \exp (2ip_F x + i\pi y/b + i\pi z/c) + \text{c.c.} \tag{5}$$

In this case the Green's functions in the self-consistent equations for the order parameter in the magnetic field,[5]

$$G^{\pm\pm}(i\omega_n, p_y, p_z; x, x') = \pm \frac{\text{sign } \omega_n}{i v_F}$$

$$\times \exp\left\{\frac{i}{v_F} \int_{x'}^{x} t\left(p_y - \frac{eHu}{c}, p_z\right) du\right.$$

$$\left. - \frac{\omega_n}{v_F}(x - x')\right\},$$

can be averaged over the rapid electronic oscillations,[7] and the resulting perturbation series can be reduced to the following expression for the free energy (see Fig. 1):

$$\mathscr{F} = \int dx \left\{ g\Delta\Delta^* + \frac{g_3}{2}[(\Delta^*)^2 + \Delta^2] - [(g^2\Delta\Delta^* + g_3^2\Delta\Delta^*) \right.$$

$$\left. + gg_3((\Delta^*)^2 + \Delta^2)] \ln\left(\frac{\Omega}{t'}\right) - \frac{1}{4\pi}\int_0^{2\pi} dp |\delta_p|^2 \left[\ln\left(\frac{\omega_c^2}{|\delta_p|^2}\right) + 1\right]\right\}, \tag{6}$$

$$\delta_p = \frac{1}{2\pi}\int_0^{2\pi} du (g\Delta + g_3\Delta^*)\exp[2i\lambda \sin(p - u)], \tag{6'}$$

where Ω is the "cutoff energy," g_3 is the constant of electron interactions connected with Umklapp processes, g is the usual electron-electron interaction constant, and $\lambda = 8t_b'/\omega_c$.

The most interesting term in (6) is the third one. It gives the lowering of the electron energy due to the gap in the spectrum. It is not trivial that in this case the energy depends
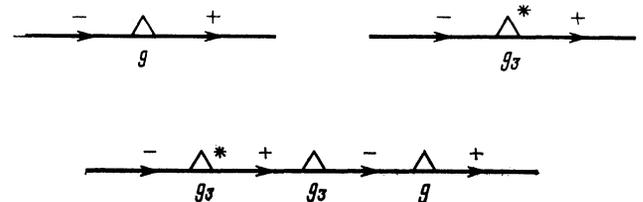

FIG. 1. Examples of first- and third-order diagrams in the self-consistent equation for $\Delta(x)$ (the lines with arrows denote Green's functions).
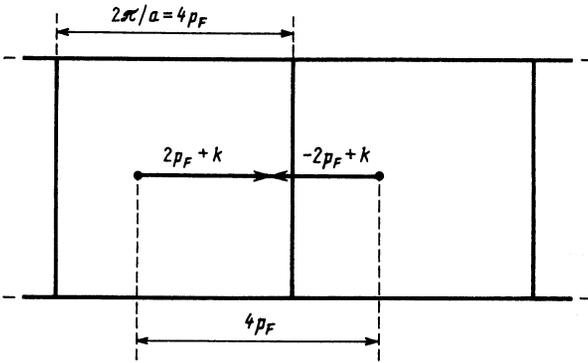
FIG. 2. Equivalence of the wave vectors $(2p_F + k_0 n)$ and $(-2p_F + k_0 n)$, $k_0 = 2\omega_c/v_F$, the sum of which is equal to the reciprocal lattice vector $|\mathbf{q}| = 2\pi/a$ $(2\pi/a = 4p_F)$ in the case of two-fold commensurability.

on the transverse momentum p and, in principal, can vanish at some momentum $p = p_0$. In general, this dependence is a sharp function of δ_p, which may qualitatively explain the small experimental value of the activation gap.

The solution corresponding to the minimum of the expression (6) is sought in the small-coupling-constant approximation. For a given value of the magnetic field we choose those harmonics in the series (3), for which the effective value of the coupling constant is maximum. As seen from a simple construction in the extended Brillouin zone (see Fig. 2), in the case of one electron per unit cell the wave vectors with $n = n_0$ and $n = -n_0$ in (3) are equivalent. This makes it necessary to consider a two-wave approximation for the solutions of the functional (6):

$$g\Delta + g_3 \Delta^* = \delta_n \exp\left(i \frac{eHx}{c} n\right) + \delta_{-n} \exp\left(-i \frac{eHx}{c} n\right). \quad (7)$$

Though the initial free energy is invariant with respect to the substitution $\delta_n \to \delta_{-n}$, when we minimize it, as often happens, a spontaneous symmetry-breaking occurs, and the solution is given by an asymmetrical linear combination

$$\delta_n = \delta_{-n} \left\{ \left[1 + \frac{(g^2 - g_3^2)J_n^2(\lambda)}{16g_3^2}\right]^{1/2} - \frac{(g^2 - g_3^2)J_n^2(\lambda)}{4g_3} \right\}.$$

(Here $J_n(\lambda)$ is the Bessel function of order n.) Note that the constant g_3 enters in the combination $g_3/g^2 J_n^2(\lambda)$, so a small Umklapp constant is sufficient to change drastically the properties of the system.

Thus, in the weak-coupling approximation, the whole range of existence of SDW can be divided into intervals where there are different vector order parameters (7).

However, the question of the coexistence of these vector order parameters near a phase boundary arises. The answer to this question can be obtained analytically: the vector subphases coexist in narrow intervals near their boundary. The expression for the range of coexistence of the harmonics (7) with $n = 0$ and $n = \pm 1$ has the form

$$\frac{1}{2}(\ln 2 - 1) + \frac{g \ln (t'/t_0')}{J_0^2(\lambda)}$$

$$< \frac{g \ln (t'/t_0')}{J_1^2(\lambda)} < \frac{g \ln (t'/t_0')}{J_0^2(\lambda)} + \frac{1}{2},$$

where

$$t_0' = \Omega \exp(-1/2g), \qquad g = g_3.$$

Thus, the whole range of existence of SDW in the weak-coupling approximation is divided into intervals where there are plane waves either with two different values of the quantum number n from (3), or with four. This conclusion differs radically from the results of earlier treatments[5-8] and is confirmed, in the opinion of the authors of Ref. 13, by the results of their experiments.

The calculations of the Hall conductivity[11] [see (4)] cannot be directly extended to the present case, and the experimental quantization of σ_{xy} is to be considered as a consequence of the more general Thouless-Halperin theorem.[14,15]

Note in conclusion that the minimum of the free energy (6) has been found here only approximately. The exact solution corresponds to a periodic arbitrary function $\Delta(x)$, which can be expanded in plane waves (3), and can be found numerically. We believe that in this way we can also explain the existence of the fine structure of subphases in the compound $(TMTSF)_2ClO_4$.

The author is grateful to L. P. Gor'kov and V. M. Yakovenko for helpful discussions.

[1] M. Ribault, D. Jerome et al., J. Phys. Lett. 44, 953 (1983).
[2] P. M. Chaikin et al., Phys. Rev. Lett. 51, 2333 (1983).
[3] J. R. Cooper et al., Phys. Rev. Lett. 63, 1984 (1989).
[4] S. T. Hannahs et al., Phys. Rev. Lett. 63, 1988 (1989).
[5] L. P. Gor'kov and A. G. Lebed, J. Phys. Lett. 45, 433 (1984).
[6] M. Heritier, G. Montambaux, and P. Lederer, J. Phys. Lett. 45, 943 (1984).
[7] A. G. Lebed, Zh. Eksp. Teor. Fiz. 89, 1034 (1985) [Sov. Phys. JETP 62, 595 (1985)].
[8] K. Maki and A. Virosztek, Phys. Rev. B 37, 7564 (1988).
[9] M. Ya. Azbel et al., Phys. Rev. Lett. 59, 926 (1987).
[10] P. Streda, J. Phys. C 15, 717 (1982).
[11] D. Poilblanc et al., Phys. Rev. Lett. 58, 2701 (1987).
[12] A. G. Lebed, Pis'ma Zh. Eksp. Teor. Fiz. 51, 583 (1990) [JETP Lett. 51, 663 (1990)].
[13] F. Tsobnang et al., Preprint, 1990.
[14] D. J. Thouless et al., Phys. Rev. Lett. 49, 504 (1982).
[15] B. I. Halperin, Japan J. Appl. Phys. Suppl. 3 26, 1913 (1987).

Translated by E. Khmelnitski