Magnetic-field influence on the collective properties of charge- and spin-density waves

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Taking account of a quasi-one-dimensional electron band with an imperfect nesting, we consider the orbital effects of a transverse magnetic field on systems with a charge- or spin-density-wave ground state. Assuming that the cyclotron frequency is small with respect to the critical temperature, we analyze the effects of magnetic field on the quasiparticle Green's function, the equilibrium value of the order parameter, and the density of collective carriers (i.e., the condensate density). It is shown that the order parameter decreases, while the condensate density increases in the magnetic field at low temperatures.

I. INTRODUCTION

The transport properties of quasi-one-dimensional charge-density-wave systems like $NbSe_3$ are well described within mean-field theory starting from the Fröhlich Hamiltonian as used by Lee, Rice, and Anderson[1] with one exception. The quasiparticle spectrum has a transverse dispersion. Such a model was first considered by Gor'kov and Lebed[2] in their analysis of the field-induced spin-density waves in a Bechgaard salt tetramethyl-tetraselenafulvalene perchlorate, $(TMTSF)_2ClO_4$, and it can be deduced from a two-dimensional tight-binding model as first done by Yamaji.[3]

One of the anomalous properties, which are not well understood, is the strong magnetic-field dependence of the second charge-density wave (CDW) below $T_c=59$ K in $NbSe_3$. Although the CDW transition temperature is hardly affected by magnetic field, the electric resistance is enormously increased.[4,5] Also, the condensate density which characterizes the extra electric current associated with the sliding CDW appears to be increased by magnetic field.[6,7]

The object of the present paper is to study the effect of a transverse magnetic field on some of the parameters which characterize the CDW transport. The method used here is a generalization of the one introduced by Montambaux[8] in his analysis of the effects of a magnetic field on spin-density waves in Bechgaard salts like $(TMTSF)_2PF_6$. Although we are interested principally in the CDW, our results for the order parameter and condensate density applies to the spin-density wave (SDW) as well, since we neglect the effect of Zeeman splitting completely. The Zeeman energy is practically negligible in SDW, while it is not negligible in general in CDW except in the weak-field limit ($\omega_c/\Delta_0 \ll 1$, where $\omega_c = veBb$ is the cyclotron frequency in the CDW, Δ_0 is the CDW order parameter at $T=0$, and v and b are the Fermi velocity and lattice constant, respectively).

We find that at low temperatures the condensate density in both the static and dynamic limits increases with increasing magnetic field, while the order parameter decreases with magnetic field. However, our results appear to be too small to describe the observed field dependence of the condensate density.

II. FORMULATION

We shall consider the Fröhlich Hamiltonian given by

$$H=\sum_{p,\alpha}\epsilon(p)c^\dagger_{p\alpha}c_{p\alpha}+\sum_q \omega(q)b^\dagger_q b_q + ig\sum_{p,q,\alpha}\sqrt{\omega(q)/2}(b^\dagger_q+b_{-q})c^\dagger_{p\alpha}c_{p+q\alpha}\ , \quad (1)$$

with

$$\epsilon(p)=v(p_1-p_F)-2t_b\cos(bp_2)-\epsilon_0\cos(2bp_2)\ . \quad (2)$$

Here $c^\dagger_{p\alpha}$, $c_{p\alpha}$, $b^\dagger_q$, and b_q are the creation and annihilation operators for electrons with momentum $\mathbf{p}$ and spin α, and phonons with momentum $\mathbf{q}$, respectively. We neglect the third direction for simplicity. As already mentioned, the quasiparticle spectrum (2) has been introduced by Gor'kov and Lebed.[2] Within a mean-field approximation, the quasiparticle Green's function in a spinor representation is given by

$$G^{-1}(\mathbf{p},\omega_n)=i\omega_n-\epsilon_0\cos(2bp_2)-\xi\rho_3-\Delta\rho_1\ , \quad (3)$$

where ρ_1 and ρ_3 are Pauli spin matrices operating on the spinor space formed by the right- and left-going electrons, ω_n is the Matsubara frequency, and

$$\xi\equiv v(p_1-p_F)-2t_b\cos(bp_2)\ . \quad (4)$$

The order parameter Δ is determined from

$$\Delta=g^2T\sum_n\int\frac{d^3p}{(2\pi)^3}\mathrm{Tr}[\rho_1 G(\mathbf{p},\omega_n)]\ . \quad (5)$$

All the results in the following apply also for a SDW as long as $\omega_c/\Delta_0\ll 1$.

For later purposes we consider the quasiparticle Green's function with a space-time-dependent order parameter

$$\Delta(x,t)=\exp(-i\dot{\phi}t+i\phi' x)\Delta \ , \quad (6)$$

where $\phi'=\partial\phi/\partial x$ and $\dot{\phi}=\partial\phi/\partial t$. It is given by

$$G_0^{-1}(\mathbf{p},\omega_n)=i\omega_n-\tfrac{1}{2}v\phi'+\epsilon_0\cos(2p_2b) -(\xi-\tfrac{1}{2}\dot{\phi})\rho_3-\Delta\rho_1 \ . \quad (7)$$

Finally, the effect of a magnetic field B perpendicular to the x-y plane is incorporated in Eqs. (3) and (7) by replacing p_2 by p_2-eBx. We note that this transformation does not affect ξ, since we always integrate over ξ from $-\infty$ to ∞. Then the Green's function in the presence of a magnetic field satisfies

$$G_0^{-1}(\mathbf{p},\omega_n)G(\mathbf{p},\omega_n)=1-\frac{\epsilon_0}{2}[e^{2ibp_2}G(p_1+2q,p_2,\omega_n) +e^{-2ibp_2}G(p_1-2q,p_2,\omega_n) -2\cos(2bp_2)G(p_1,p_2,\omega_n)], \quad (8)$$

with $q=eBb$ and $G_0(\mathbf{p},\omega_n)$ as already given in Eq. (7). Especially for $\omega_c/\Delta_0\ll 1$, which is valid for CDW's in $NbSe_3$, we can expand $G(\mathbf{p},\omega)$ in powers of ω_c, and to the lowest-order terms in q we obtain

$$G(\mathbf{p},\omega_n)=G_0+G_1+G_2+\cdots \ , \quad (9)$$

where

$$G_1=2i\epsilon_0\omega_c\sin(2bp_2)G_0G_0' -2\omega_c^2\epsilon_0\cos(2bp_2)G_0G_0''+O(\omega_c^3) \ , \quad (10)$$

and

$$G_2=-4\omega_c^2\epsilon_0^2\sin^2(2bp_2)G_0(G_0'G_0)'+O(\omega_c^3) \ , \quad (11)$$

where

$$G_0'=\partial G_0(\mathbf{p},\omega_n)/\partial\xi \ . \quad (12)$$

The terms G_n with $n\geq 3$ comprise only the contributions of the third and higher orders in ω_c.

III. ORDER PARAMETER AND CONDENSATE DENSITY

A. Order parameter

The field-dependent order parameter is determined from Eq. (5). Substituting Eq. (9) into Eq. (5), we obtain

$$\lambda^{-1}=\frac{1}{2}\int_0^{2\pi}d\chi T\sum_n\left[1+\frac{2}{3}\epsilon_0\omega_c^2\frac{d}{d\epsilon_0}\frac{d}{dX}+(\epsilon_0\omega_c\sin\chi)^2\left[-4\frac{d^2}{dX^2}-\frac{4}{3}X\frac{d^3}{dX^3}\right]\right]d_0^{-1/2} \ , \quad (13)$$

where $X=\Delta^2$, $\chi=2bp_2$ and

$$d_0=(\omega_n-i\epsilon_0\cos\chi)^2+\Delta^2 \ . \quad (14)$$

A derivation will be given in the Appendix. The sum over the Matsubara frequency is readily done, and we obtain

$$\ln\left[\frac{\Delta(T,\omega_c)}{\Delta(T)}\right]=-\frac{1}{3}\left[\frac{\epsilon_0\omega_c}{\Delta^2}\right]^2\left[1-\frac{\Delta^3}{\epsilon_0T^2}\sum_{n=1}^{\infty}(-1)^{n+1}n^2\left[K_1+\frac{2T}{n\Delta}K_2\right]I_1\right] \ , \quad (15)$$

with

$$\ln\left[\frac{\Delta(T)}{\Delta_0}\right]=-2\sum_{n=1}^{\infty}(-1)^{n+1}K_0I_0 \ , \quad (16)$$

where K_i and I_i are modified Bessel functions, and the arguments of the nth term in the n sum are $(n\Delta/T)$ and $(n\epsilon_0/T)$ for K_i and I_i, respectively.

Equation (15) tells us that at $T=0$ the order parameter decreases when a magnetic field is applied. It is surprising that the order parameter Δ at low temperatures decreases with magnetic field, while both CDW and SDW appear to be strengthened by magnetic field. For example, this behavior is in sharp contrast to that of the transition temperature:

$$\ln\left[\frac{T_c}{T_c(\epsilon_0)}\right]=\tfrac{1}{2}(\epsilon_0\omega_c)^2\pi T\sum_{n=0}^{\infty}\left[\omega_n^2-\frac{\epsilon_0^2}{4}\right]\times(\omega_n^2+\epsilon_0^2)^{-7/2} \ , \quad (17)$$

and

$$\ln\left[\frac{T_c(\epsilon_0)}{T_{c0}}\right]=-2\pi T\sum_{n=0}^{\infty}[(\omega_n^2+\epsilon_0^2)^{-1/2}-|\omega_n|^{-1}] \ , \quad (18)$$

where T_c increases with increasing magnetic field.

The second term in Eq. (15) gradually compensates the decrease of Δ at $T=0$. At low enough temperatures $(T\ll\Delta-\epsilon_0)$, the leading terms of Eqs. (15) and (16) give

$$\ln\left[\frac{\Delta(T,\omega_c)}{\Delta_0}\right]\simeq-\frac{T}{(\Delta\epsilon_0)^{1/2}}\exp\left[-\frac{(\Delta-\epsilon_0)}{T}\right]-\frac{1}{3}\left[1-\frac{\Delta^{5/2}\exp[-(\Delta-\epsilon_0)/T]}{2T\epsilon_0^{3/2}}\right]\times\left[\frac{\epsilon_0\omega_c}{\Delta^2}\right]^2 . \quad (19)$$

The characteristic temperature above which the correction to $\Delta(T,\omega_c)$ due to the magnetic field becomes positive is thus roughly

$$T_0\simeq(\Delta-\epsilon_0)\Big/\ln\left[\frac{\Delta^{5/2}}{2(\Delta-\epsilon_0)\epsilon_0^{3/2}}\right] , \quad (20)$$

where by Δ is meant $\Delta(T_0,\omega_c=0)$. This estimation is meaningful if the expansion (19) is still valid at T_0.

B. Condensate density

The transport properties associated with sliding CDW are described in terms of the condensate density f. As noted first by Rice, Lee, and Cross,[9] the condensate density in the adiabatic limit takes two limiting values depending on whether $\omega < vp$ (static limit) or $\omega > vp$ (dynamic limit), where ω and p are the frequency and the wave vector associated with the space-time-dependent order parameter.

First, let us consider the static limit of f. In particular, the time-independent deformation of ϕ gives the extra charge associated with CDW:

$$\rho_{\rm CDW}=eQ^{-1}nf_1\phi' , \quad (21)$$

where $Q=2p_F$. Here f_1 is obtained from

$$f_1=TN_0^{-1}\sum_n\int_0^{2\pi}\frac{d\chi}{2\pi}\int d\xi\,{\rm Tr}[G(p,\omega_n)]=f_1^{(0)}+\delta f_1 , \quad (22)$$

where, again with $X=\Delta^2$,

$$f_1^{(0)}=-X\int_0^{2\pi}d\chi\,T\sum_n\frac{d}{dX}d_0^{-1/2} , \quad (23)$$

and

$$\delta f_1=\epsilon_0\omega_c^2X\int_0^{2\pi}d\chi\,T\sum_n\left[\frac{2}{3}\frac{d}{d\epsilon_0}\frac{d^2}{dX^2}+4\epsilon_0\sin^2\chi\frac{d^3}{dX^3}-\frac{4}{3}\epsilon_0X\sin^2\chi\frac{d^4}{dX^4}\right]d_0^{-1/2} . \quad (24)$$

Here we have inserted Eq. (9) into Eq. (22) and integrated over ξ (for details, see the Appendix). At low temperatures Eqs. (23) and (24) are expanded in a series involving the modified Bessel functions

$$f_1=1-2\sum_{n=0}^{\infty}(-1)^{n+1}\frac{n\Delta}{T}K_1I_0+\frac{\omega_c^2\epsilon_0}{3T^3}\sum_{n=0}^{\infty}(-1)^{n+1}n^3K_2I_1 , \quad (25)$$

with the arguments of K_i and I_i being the same as in Eqs. (15) and (16).

In contrast to Eq. (15), there is no field-dependent correction at $T=0$. At low temperatures, $T\ll\Delta-\epsilon_0$, the contribution to f_1 from the magnetic field is positive, the leading term being

$$f_1\simeq1-\exp\left[-\frac{(\Delta-\epsilon_0)}{T}\right]\left[\frac{\Delta}{\epsilon_0}\right]^{1/2}\left[1-\frac{\omega_c^2\epsilon_0}{6T^2\Delta}\right] . \quad (26)$$

Although this correction is exponentially weak, the result (26) is valid only for

$$\omega_c\langle(6\Delta/\epsilon_0)^{1/2}T , \quad (27)$$

since at still lower temperatures, f_1 would exceed unity. This is inconsistent with the requirement that the number of carriers in the condensate should not be larger than the total number of band electrons. However, we expect that the inclusion of higher-order terms in ω_c^2 will lead to an expression for f_1 which stays closer to unity at low temperatures.

Second, the dynamic limit of the condensate density is obtained from the expression for the current:

$$j=\lim_{\tau\to0+}2evT\sum_n\frac{1}{2\pi}\int_0^{2\pi}d\chi\,N_0\int_{-\infty}^{\infty}d\xi\,{\rm Tr}[\rho_3G(p,\omega_n)]e^{i\tau\omega_n} . \quad (28)$$

In the absence of magnetic field, we obtain

$$j^{(0)}=\frac{ev}{\pi}N_0\int_0^{2\pi}d\chi\int_{-\infty}^{\infty}d\xi\frac{\xi'}{E'}\tanh\left[\frac{1}{2T}(E'+\epsilon_0\cos\chi)\right] , \quad (29)$$

where

$$E'=(\xi'^2+\Delta^2),\quad \xi'=\xi-\tfrac{1}{2}\dot\phi . \quad (30)$$

The linearization of Eq. (23) in $\dot\phi$ gives

$$j^{(0)}=enQ^{-1}\dot\phi ,$$

independent of the temperature, which follows from the Galileian invariance. On the other hand, the current associated with the sliding CDW comes from the linearization of the factor (ξ'/E') in the integral (29):[10]

$$f_0^{(0)}=\frac{1}{2\pi}\int_0^{2\pi}d\chi\int_\Delta^\infty\frac{dE}{E^2\xi}\tanh\left[\frac{E+\epsilon_0\cos\chi}{2T}\right]$$
$$=1-2\sum_{n=1}^{\infty}(-1)^{n+1}\tilde{K}I_0\ , \tag{31}$$

where

$$\tilde{K}\equiv\tilde{K}\left[\frac{n\Delta}{T}\right]=\int_0^\infty dz\,\text{sech}^2 z\exp\left[-\frac{n\Delta}{T}\cosh z\right]\ , \tag{32}$$

and

$$\xi=(E^2-\Delta^2)^{1/2}\ .$$

In the presence of a magnetic field, we put G_1 and G_2 given by Eqs. (10) and (11) into Eq. (22). Similarly, as in Eq. (23), the total linearization in $\dot{\phi}$ then again leads to the result (24), while the collective CDW current follows after linearizing all factors except the Fermi distribution function $\tanh[(E'+\epsilon_0\cos\chi)/2T]$. We obtain

$$\delta f_0=\frac{1}{2\pi}\int_0^{2\pi}d\chi\int_0^\infty d\xi\left\{-2\omega_c^2\epsilon_0\frac{d}{d\epsilon_0}\left[\frac{d}{dX}\frac{X}{E^3}+\frac{1}{3}\xi^2\frac{d^2}{dX^2}\left[\frac{X}{E^3}+\frac{2}{E}\right]\right]\right.$$
$$+(2\epsilon_0\omega_c\sin\chi)^2\left[\frac{5}{2}\frac{d^2}{dX^2}\frac{X}{E^3}+\frac{10}{3}\xi^2\frac{d^3}{dX^3}\left[\frac{X}{E^3}+\frac{2}{E}\right]+\frac{2}{3}\xi^4\frac{d^4}{dX^4}\left[\frac{X}{E^3}+\frac{4}{E}\right]\right.$$
$$\left.\left.+\frac{2}{3}X\xi^2\frac{d^4}{dX^4}\left[\frac{X}{E^3}+\frac{2}{E}\right]+4X\frac{d^3}{dX^3}\frac{X}{E^3}\right]\right\}\tanh\left[\frac{E+\epsilon_0\cosh\chi}{2T}\right]\ , \tag{33}$$

where $X=\Delta^2$ and $E=(X+\xi^2)^{1/2}$. After a straightforward though rather tedious manipulation, Eq. (33) reduces to

$$\delta f_0=\frac{\omega_c^2\epsilon_0}{3T^2\Delta}\sum_{n=1}^{\infty}(-1)^{n+1}\left[n^2K_1+\frac{3nT}{\Delta}K_0+\frac{3T^2}{\Delta^2}\tilde{K}'\right]I_1\ , \tag{34}$$

where

$$\tilde{K}'=\tilde{K}\left[\frac{n\Delta}{T}\right]=\int_0^\infty dz\,\text{sech}z\exp\left[-\frac{n\Delta}{T}\cosh z\right]$$
$$=-\frac{\partial}{\partial(n\Delta/T)}\tilde{K}\left[\frac{n\Delta}{T}\right]\ , \tag{35}$$

and the arguments of K_i and I_i are the same as in Eqs. (15) and (16).

We point out that G_1 in Eq. (9) does not contribute to δf_0. Like δf_1, the correction δf_0 vanishes exponentially at low temperatures, $T\ll\Delta-\epsilon_0$. The leading term is

$$f_0\simeq1-\exp\left[-\frac{(\Delta-\epsilon_0)}{T}\right]\frac{T}{(\Delta\epsilon_0)^{1/2}}\left[1-\frac{\omega_c\epsilon_0}{6T^2\Delta}\right]\ . \tag{36}$$

The result (36), just like Eq. (26), is valid for temperatures defined by the inequality (27). Like δf_1, δf_0 is positive, i.e., the magnetic field increases both the static and dynamic densities. However, we have

$$\frac{\delta f_0}{\delta f_1}\simeq\frac{T}{\Delta}\ll1\ ; \tag{37}$$

i.e., the effect on the dynamic density is much weaker at low temperatures.

IV. CONCLUDING REMARKS

Limiting ourselves to low temperatures and small magnetic field (i.e., $\omega_c/\Delta_0\ll1$), we have studied the effects of magnetic field on the order parameter Δ and the static and dynamic condensate densities f_1 and f_0. We find that a magnetic field decreases Δ, while it increases both f_1 and f_0, though the effect is much stronger for f_1. Further, the perturbation approach used here will become invalid at low temperatures when $\omega_c\simeq(6\Delta/\epsilon_0)^{1/2}T$. Therefore, though the present result is consistent with the observed increase of the condensate density in magnetic fields in CDW II of $NbSe_3$,[4–7] we will not make a quantitative comparison with experiments here. In order to do this, we need a rather precise value of ϵ_0 for CDW II, which should be rather large ($\epsilon_0\sim0.92\Delta_0$),[11] in order to account for large $E_g/T_c\sim11$, where E_g is the quasiparticle energy gap observed by electron tunneling.[12,13] Clearly, further work on this subject is required.

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APPENDIX

In this appendix, we sketch the derivation of Eq. (15). Starting from Eq. (5), the first step is the calculation of $\text{Tr}(\rho_1 G)$, where G is given by Eqs. (7) and (9)–(12). One gets

$$\mathrm{Tr}(\rho_1 G) = -\frac{2\Delta}{d}\left\{1 - \frac{16\epsilon_0\cos\chi\,\omega_c^2(i\omega_n+\epsilon_0\cos\chi)}{d^2}\left[1-\frac{(\omega_n-i\epsilon_0\cos\chi)^2+\Delta^2}{d}\right] + \left[\frac{2\epsilon_0\omega_c\sin\chi}{d}\right]^2\left[-1+4\left[1-\frac{(\omega_n-i\epsilon_0\cos\chi)^2+\Delta^2}{d}\right]\left[1-\frac{4(\omega_n-i\epsilon_0\cos\chi)^2}{d}\right]\right]\right\}, \tag{A1}$$

where

$$d \equiv (\omega_n - i\epsilon_0\cos\chi)^2+\Delta^2+\xi^2 . \tag{A2}$$

The first, second, and third terms in Eq. (A1) originate from G_0, G_1, and G_2, respectively. The next step is the integration in terms of ξ. Generally,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\xi\, d^{-M} = 2^{-(2M-1)}\frac{(2M-2)!}{[(M-1)!]^2}d_0^{-(2M-1)/2} , \tag{A3}$$

with d_0 given by Eq. (14), and $M=1,2,3,\ldots$. Inserting these integrals into Eq. (A1), one finally arrives at the expression (13).

The calculation of f_1 proceeds in the same way, while in the calculation of f_0 the order of ξ integration and ω_n summation is reversed. In the latter case, Eq. (28), after taking the trace of $\rho_3 G$, reads as

$$j = \lim_{\tau\to 0+} 2evT\sum_n \frac{1}{2\pi}\int_0^{2\pi} d\chi \frac{1}{2\pi v}\int_{-\infty}^{\infty} d\xi\, e^{i\tau\omega_n}\left[-\frac{2\xi'}{d} - \frac{16\omega_c^2\epsilon_0\cos\chi}{d^3}(i\omega_n+\epsilon_0\cos\chi)\left[1-\frac{2\xi'^2}{d}\right] - 2(2\epsilon_0\omega_c\sin\chi)^2\frac{\xi'}{d^3}\left[5-\frac{20\xi'^2}{d}+\frac{16\xi'^2}{d^2}+\frac{16\xi'^2\Delta^2}{d^2}-\frac{8\Delta^2}{d}\right]\right], \tag{A4}$$

where ξ' is defined in Eq. (30). Replacing further the n summation by the contour integration in the ω plane and performing this integration, one arrives at

$$j = 2v\frac{1}{2\pi}\int_0^{2\pi} d\chi\frac{1}{2\pi v}\int d\xi\,\xi'\left[2-4\omega_c^2\epsilon_0\frac{d}{d\epsilon_0}\left[\frac{d}{dX}+\frac{2}{3}\xi'^2\frac{d^2}{dX^2}\right] + 2(2\epsilon_0\omega_c\sin\chi)^2\left[\frac{5}{2}\frac{d^2}{dX^2}+\frac{10}{3}\xi'^2\frac{d^3}{dX^3}+\frac{2}{3}\xi'^4\frac{d^4}{dX^4}+\frac{2}{3}\xi'^2\frac{d^4}{dX^4}+\frac{4}{3}X\frac{d^3}{dX^3}\right]\right]\frac{1}{2E'} \times\tanh\frac{(E'+\epsilon_0\cos\chi)}{2T} , \tag{A5}$$

with E' given by Eq. (30). Finally, the result (33) follows after the linearization in $\dot\phi$ of all factors except the tanh function.

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