QUASI-ONE-DIMENSIONAL CHARGE DENSITY WAVE IN THE MAGNETIC FIELD

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Abstract. *The effects of magnetic field on the charge density wave are examined within a perturbative scheme appropriate for the regime* $\hbar\omega_c \ll T_P$*, where* ω_c *and* T_P *are the cyclotron frequency and the critical temperature respectively. In particular we calculate the corrections to the order parameter and the densities of collective carriers in the static and dynamic limits, and interpret some experiments on* $NbSe_3$.

Introduction. Quasi-one-dimensional systems which show the charge (or spin) density wave C(S)DW long-range order are characterized by the high degree of nesting of two open Fermi surfaces. Yet in the real systems this nesting is never perfect. This is usually expressed through the electron spectrum

$$E_\pm(k,p) = \pm\hbar v_F k + 2t_b\cos(pb) + 2t'_b\cos(2pb) \qquad (1)$$

in which v_F is the longitudinal Fermi velocity, and for simplicity only one transverse direction with the hopping integral t_b is retained. The coefficient t'_b introduces the pockets at the Fermi surface of the ordered DW state, and even more, if strong enough, prevents the stability of this state. In the latter case the order may be induced by the magnetic field which, when applied perpendicularly to the (k,p) plane, lowers the energy of closed electronic orbits and so favors the formation of pockets. This is the well known phenomenon of field induced SDW observed in the organic Bechgaard salts.[1-3]

The series of experiments on the CDW system $NbSe_3$[4-8] indicate that orbital effects are also possible when the magnetic field is applied on the already existing DW ordered state. In the characteristic CDW systems the critical temperature T_P and the Peierls gap Δ_0 are of the order $\sim 10^2$K (T_{P2} = 59K in $NbSe_3$), while the cyclotron frequency $\hbar\omega_c \equiv eBbv_F/c$ may be up to ~10K. Thus, in contrast to the field induced SDW problem, the low temperature range is here characterized by the small parameter $\hbar\omega_c/\Delta_0 \simeq q\xi_\parallel \ll 1$, where $\xi_\parallel \simeq \hbar v_F/T_P$ is the longitudinal correlation length and $q \equiv \hbar\omega_c/v_F$ is the reciprocal magnetic length. The purpose of the present wok is to formulate the perturbation scheme appropriate for this regime, and to check its validity by discussing the integral CDW quantities like the order parameter Δ and the densities of collective carriers in the static and dynamic limit, f_1 and f_0 respectively.

Perturbative procedure. The equation of motion for the (2x2) electron propagator can be, after a convenient gauge transformation, written in the form

$$G_0^{-1}(k)\, G(k) - 1 = -t'_b\Big[\exp(2\tilde{p}bi)\, G(k+2q) + \exp(-2\tilde{p}bi)\, G(k-2q) - 2\cos(2\tilde{p}b)\, G(k)\Big] \qquad (2)$$

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where

$$\mathcal{G}(k) \equiv \mathcal{G}(k, \tilde{p}, \omega_n) = \int dx \exp(ikx)\, \mathcal{G}(x_0+x, x_0, p, \omega_n) \qquad (2')$$

with $\omega_n \equiv (2n+1)\pi T$, $\tilde{p} \equiv p - q x_0/b$ and p is the transverse wave number. $\mathcal{G}_0$ is the propagator in absence of magnetic field,

$$\mathcal{G}_0(k, \tilde{p}, \omega_n) = \left[i\omega_n + \hbar v_F \phi'/2 + 2t'_b \cos(2\tilde{p}b) - \sigma_3 (\hbar vk + \dot{\phi}/2) - \sigma_1 \Delta \right]^{-1}, \qquad (3)$$

where σ_1 and σ_3 are Pauli matrices. We introduce also ϕ' and $\dot{\phi}$, the uniform strain and velocity of CDW respectively, which are convenient for later calculations of corresponding densities f_1 and f_0.

In the perturbative treatment of eq.(2) we determine iteratively the series $\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_1 + \ldots$, with $\mathcal{G}_p \sim (t'_b)^p$, and expand $\mathcal{G}_0(k \pm 2q)$ in the Taylor series with respect to q. Limiting the expansion up to the quadratic terms in q, we get

$$\mathcal{G}_1 = 2iq\varepsilon_0 \sin(2\tilde{p}b)\, \mathcal{G}_0 \mathcal{G}'_0 - 2q^2 \varepsilon_0 \cos(2\tilde{p}b)\, \mathcal{G}_0 \mathcal{G}''_0 + O(q^3),$$

$$\mathcal{G}_2 = -4 q^2 \varepsilon_0^2 \sin^2(2\tilde{p}b)\, \mathcal{G}_0 (\mathcal{G}'_0 \mathcal{G}_0)' + O(q^3), \qquad (4)$$

$$\mathcal{G}_3 = O(q^3), \text{ etc.},$$

where $\mathcal{G}'_0 \equiv \partial \mathcal{G}_0/\partial k$ and $\varepsilon_0 \equiv 2t'_b$. $\mathcal{G}_1$ and $\mathcal{G}_2$ contain all corrections up to the second order in the magnetic field. The quantities to be considered below are integrals of the function $\mathcal{G}$. The above procedure is valid under the assumption that the Taylor expansion in q and those integrations are commutative.

Results and conclusion. The result (4) enables the calculation of thermodynamic quantities in the whole temperature range below T_P.[9] For illustration we discuss here mainly the limit of almost perfect nesting ($t'_b \ll \Delta_0$) in the low temperature range ($T \ll \Delta$). The equilibrium value of the order parameter, which follow straightforwardly from the integration of $\mathrm{Tr}(\sigma_1 \mathcal{G})$ with $\phi' = \dot{\phi} = 0$, is in this regime given by

$$\log\left[\Delta/\Delta(T,B{=}0)\right] = -\frac{1}{3}(\varepsilon_0 q/\Delta^2)^2 \left[1 + \frac{\Delta^2}{2\varepsilon_0 T^2} \sum_{n \geq 1} (-1)^n n^2 \left[K_1 + \frac{2T}{n\Delta} K_2\right] I_1\right], \qquad (5)$$

with

$$\log\left[\Delta(T,B{=}0)/\Delta_0\right] = 2 \sum_{n \geq 1} (-1)^n K_0\, I_0 ,$$

where $K_j \equiv K_j(n\Delta/T)$ and $I_j \equiv I_j(n\,\varepsilon_0/T)$ are Bessel functions, and Δ_0 is the Peierls gap at T=0 and B=0. Thus at T=0 the magnetic field causes the decrease of the order parameter. By increasing temperature this decrease is gradually compensated by the last term in eq.(5). The more detailed analysis[9] shows that $\Delta(T,B) - \Delta(T,B{=}0)$ becomes positive above the temperature determined by the relation $\varepsilon_0 T \simeq [\Delta(T)]^2$.

The densities f_1 and f_0 follow from the integrations of $\mathrm{Tr}(\mathcal{G})$ and $\mathrm{Tr}(\sigma_3 \mathcal{G})$, respectively linearized in terms of ϕ' and $\dot{\phi}$. Both of them increase in the magnetic field at finite temperatures. The leading quadratic corrections at low temperatures are given by

$$f_1(T,B) = f_1(T,B=0) + \delta f_1 = n_0 \left[1 + \frac{2\Delta}{T} \sum_{n\geq 1} (-1)^n K_1 I_0\right] -$$

$$- \frac{n_0 q^2 \varepsilon_0}{3 T^3} \sum_{n\geq 1} (-1)^n n^3 K_2 I_1 , \qquad (6)$$

$$f_0(T,B) = f_0(T,B=0) + \delta f_0 = n_0 \left[1 + 2 \sum_{n\geq 1} (-1)^n \tilde{K} I_0\right] -$$

$$- \frac{n_0 q^2 \varepsilon_0}{3 T^2 \Delta} \sum_{n\geq 1} (-1)^n n^2 \left[K_1 + 3 \frac{T}{n\Delta} K_0 + 3 (\frac{T}{n\Delta})^2 \tilde{K}'\right] , \qquad (7)$$

where

$$\tilde{K} \equiv \int_0^\infty \mathrm{sech}^2(x) \exp\left[- \frac{n\Delta}{T} \cosh(x)\right] dx$$

and $\tilde{K}' \equiv \partial\tilde{K}/\partial(n\Delta/T)$. As follows from eqs. (6) and (7), f_0 is less sensitive to the magnetic field than f_1, the ratio of two corrections being

$$\delta f_0/\delta f_1 \simeq T/\Delta \quad . \qquad (8)$$

The results (6) and (7) have to be taken with caution since at temperatures below $\hbar\omega_c$ the increase due to the magnetic field is larger than the decrease of $f_{0,1}(T,0)$, so that the total densities $f_{0,1}$ become larger than the band density n_0. This indicates that at $T \leq \hbar\omega_c'$ some CDW properties depend on details of the $G(k)$ dependence on the scale smaller than q. Then the magnetic field in eq.(2) has to be treated nonperturbatively.

The experiments on $NbSe_3$ show that the number of collective carriers in the frequency range of narrow band noise is weakly affected by the magnetic field,[6] in contrast to the magnetoresistance in the regime of linear transport which is positive and rather large.[4,6] Since the densities which correspond to these regimes are f_0 and f_1 respectively, the result (8) is in a qualitative agreement with these observations.

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