Imperfect nesting in quasi-one-dimensional charge- and spin-density waves

Xiaozhou Huang and Kazumi Maki
Department of Physics, University of Southern California, Los Angeles, Los Angeles, California 90089-0484
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In quasi-one- and two-dimensional charge- and spin-density-wave systems, the imperfect nesting plays the crucial role in their thermodynamics and transport properties. We study systematically the effects of the imperfect nesting on the condensate density in both static and dynamic limit and related transport properties in charge- and spin-density waves.

I. INTRODUCTION

Since the discovery of the Fröhlich conduction in the charge-density wave (CDW) of $NbSe_3$, a large class of both inorganic and organic CDW-supporting materials were found.[1] A number of low-temperature properties of these materials are well described in terms of mean-field theory starting from the quasi-one-dimensional Fröhlich model for the CDW (Ref. 2) and the quasi-one-dimensional Hubbard model for the spin-density wave (SDW).[3–6] Central to these models is the notion of imperfect nesting, which does not exist in the one-dimensional model. In the limit of perfect nesting (i.e., in the limit of small imperfect nesting) the thermodynamics of the system within mean-field theory is identical to the one for a BCS superconductor. Then the imperfect nesting depresses the CDW (SDW) transition temperature and destroys completely the CDW (SDW), when the imperfect nesting becomes larger than a critical value. Indeed Yamaji[3] was able to describe the remarkable phase diagram of Bechgaard salt $(TMTSF)_2PF_6$ under pressure established by Jerome *et al.*[7] by assuming that ε_0, the unnesting parameter, increases linearly with pressure. Very similar depressions of the CDW transition temperatures in $NbSe_3$ under pressure have been observed by Briggs *et al.*,[6] which is also described in terms of the pressure dependence of the imperfect nesting.[2] Further, in the presence of imperfect nesting the quasiparticle energy gap is no longer the same as $\Delta(T)$, the order parameter, as first shown by Yamaji.[3] More recently, we have shown[2] that a similar model for the CDW accounts for the electron density of states of CDW's in $NbSe_3$ observed by the electron tunneling technique.[9,10]

We emphasize here that a large ratio of $\Delta_a(0)/k_BT_c$, where $\Delta_a(0)$ is the apparent energy gap at $T=0$ K in CDW's of $NbSe_3$ and in SDW's of Bechgaard salts is due to the imperfect nesting and not due to the strong electron-phonon interaction as commonly assumed until now, though the strong electron-phonon coupling was originally invoked[11,12] to interpret the anomalies in the layered compounds.

The object of this paper is to study a variety of physical quantities that characterize the transport properties of the CDW and SDW in the presence of imperfect nesting. Since the effects of imperfect nesting in a CDW is parallel to those in a SDW, we consider mostly the anisotropic Hubbard model introduced by Yamaji.[3] The Hamiltonian is given by

$$H=\sum_{\rho,\alpha}\varepsilon(p)C^{\dagger}_{\rho\alpha}C_{\rho\alpha}+U\sum_{q}n_{q\uparrow}n_{-q\downarrow}\ , \tag{1}$$

where

$$\varepsilon(p)=-2t_a\cos(ap_1)-2t_b\cos(bp_2)-2t_c\cos(cp_3)-\mu \tag{2}$$

and μ is the chemical potential, $C^{\dagger}_{p\alpha}$ and $C_{p\alpha}$ are the electron-creation and -annihilation operators with momentum $\mathbf{p}$ and spin α ($=\uparrow$ or $\downarrow$), and $n_{q\uparrow}$ and $n_{q\downarrow}$ are corresponding number operators. In the vicinity of the Fermi surface, $\varepsilon(p)$ is well approximated as[3,4]

$$\varepsilon(p)=v(|p|-p_F)-2t_b\cos(bp_2)-\varepsilon_0\cos(2bp_2)-2t_c\cos(cp_3)\ ,$$

with

$$\varepsilon_0=-\tfrac{1}{2}t_b^2\cos(ap_F)[t_a\sin^2(ap_F)]^{-1}\ . \tag{3}$$

Here we assumed that

$$t_a\gg t_b\gg t_c\ . \tag{4}$$

Then, for not too large ε_0, the ground state of the Hamiltonian is a SDW with the nesting vector $\mathbf{Q}=(2p_F,\pi/b,\pi/c)$, and the quasiparticle Green's function in a SDW is given by

$$G^{-1}(\mathbf{p},\omega_n)=i\omega_n-\eta-\xi\rho_3-\Delta\rho_1\sigma_3\ , \tag{5}$$

where

$$\xi=v(|p_1|-p_F)-2t_b\cos\phi-2t_c\cos(cp_3)\ ,\qquad \eta=\varepsilon_0\cos(2\phi),\quad \phi=bp_2 \tag{6}$$

and ω_n is the Matsubara frequency and ρ_i's are the Pauli matrices operating on the spinor space formed by the right-going and the left-going electrons.

The gap equation is now given by[3,4]

$$1=\bar{U}\pi T\sum_n \langle [(\omega_n+i\eta)^2+\Delta^2]^{-1/2}\rangle$$
$$=\bar{U}\int_0^{x_c} dx\,\langle \tanh[\tfrac{1}{2}\beta(\Delta\cosh x-\eta)]\rangle$$
$$=\tfrac{1}{2}\bar{U}\left[\ln(2E_c/\Delta)-2\sum_{n=1}^{\infty}(-1)^{n+1}K_0(n\beta\Delta)I_0(n\beta\varepsilon_0)\right], \quad (7)$$

where $\bar{U}=UN_0$, $N_0=(\pi v bc)^{-1}$ is the electron density of states at the Fermi surface per spin and $\langle\ \rangle$ means the average over ϕ, $E_c=\sqrt{2}t_a$ is the cutoff energy I_0 and K_0 are modified Bessel functions, and $\beta=(k_BT)^{-1}$ is the inverse temperature. Equation (7) is somewhat simplified as

$$\ln(\Delta/\Delta_0)=-2\sum_{n=1}^{\infty}(-1)^{n+1}K_0(n\beta\Delta)I_0(n\beta\varepsilon_0), \quad (8)$$

where $\Delta_0=2E_c\exp[-2(\bar{U})^{-1}]$ is the energy gap at $T=0$ K and $\varepsilon_0=0$. We see immediately from Eq. (8) the order parameter Δ at $T=0$ K is $\Delta=\Delta_0$ independent of ε_0.

Although the temperature-dependent Δ is already discussed by Yamaji,[3] we calculate $\Delta(T,\varepsilon_0)$ numerically, which is shown in Fig. 1 for several ε_0/Δ_0. $\Delta(T,\varepsilon_0)$ thus obtained describes quite well the width of the NMR in the SDW of $(TMTSF)_2PF_6$ measured at several pressures by Takahashi *et al.*[13]

The transition temperature T_c is given, on the other hand, by

$$\ln(\varepsilon_0/\Delta_0)=-2\sum_{n=1}^{\infty}(-1)^{n+1}K_0(n\beta_c\varepsilon_0), \quad (9)$$

where now $\beta_c=(k_BT_c)^{-1}$. Comparing this with Eq. (8) with $\varepsilon_0=0$, we conclude that T_c is determined from

$$\varepsilon_0=\Delta(T_c), \quad (10)$$

where $\Delta(T)$ is the BCS energy gap for $\varepsilon_0=0$. This implies that T_c tends to zero as ε_0 approaches Δ_0.

II. CONDENSATE DENSITY

As is well known, the collective transport of the CDW and SDW is characterized by the condensate density f, which takes two limiting values f_0 (dynamic) and f_1 (static) as given by[6]

$$f_0=1-2\sum_{n=1}^{\infty}(-1)^{n+1}\tilde{K}(n\beta\Delta)I_0(n\beta\varepsilon_0) \quad (11)$$

and

$$f_1=1-2\beta\Delta\sum_{n=1}^{\infty}(-1)^{n+1}nK_1(n\beta\Delta)I_0(n\beta\varepsilon_0), \quad (12)$$

where K_1 and I_0 are again modified Bessel functions while

$$\tilde{K}(z)=\int_0^{\infty}dx\, e^{-z\cosh x}\operatorname{sech}^2 x. \quad (13)$$

For example, the phase Hamiltonian for a SDW is given by

$$H(\phi)=f\int d^Dx\left\{\tfrac{1}{4}N_0\left[\left(\frac{\partial\phi}{\partial t}\right)^2+\tilde{v}^2\left(\frac{\partial\phi}{\partial x}\right)^2+v_2^2\left(\frac{\partial\phi}{\partial y}\right)^2+v_3^2\left(\frac{\partial\phi}{\partial z}\right)^2\right]-enQ^{-1}\phi E\right\}-V_{\text{pinning}}(\phi), \quad (14)$$

where

$$(\tilde{v},v_2,v_3)=(2(1+\bar{U})^{1/2}t_a a\sin(ap_F),\ \sqrt{2}t_b b,\ \sqrt{2}t_c c) \quad (15)$$

and the pinning potential $V_{\text{pinning}}(\phi)$ is given by[14]

$$V_{\text{pinning}}(\phi)=-\frac{\pi^2}{2}(N_0V)^2T\sum_n\langle\Delta[(\omega_n+i\eta)^2+\Delta^2]^{-1/2}\rangle^2\sum_i\cos\{2[\mathbf{Q}\cdot\mathbf{x}_i+\phi(\mathbf{x}_i)]\} \quad (16)$$

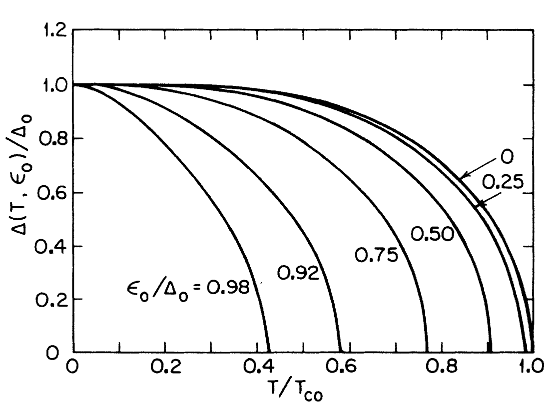

FIG. 1. The temperature-dependent order parameter $\Delta(T,\epsilon_0)$ is shown as a function of the reduced temperature T/T_{c0} for several values of ϵ_0's.

and the sum is over the impurity sites $\mathbf{x}_i$.

Here, f is the condensate density which also describes the electric charge and the current associated with a slow spatiotemporal variation of ϕ,

$$n_c=enfQ^{-1}\frac{\partial\phi}{\partial x}, \quad (17)$$

$$j_c=-enfQ^{-1}\frac{\partial\phi}{\partial t}, \quad (18)$$

with $nQ^{-1}=(\pi bc)^{-1}$. In the adiabatic limit, (i.e., $\omega, vq \ll \Delta_0$), f reduces to

$$f=\begin{cases} f_0, & \text{for } \omega\gg vq_1 & (19a)\\ 1, & \text{for } \omega=vq_1 & (19b)\\ f_1, & \text{for } \omega\ll vq_1\,. & (19c)\end{cases}$$

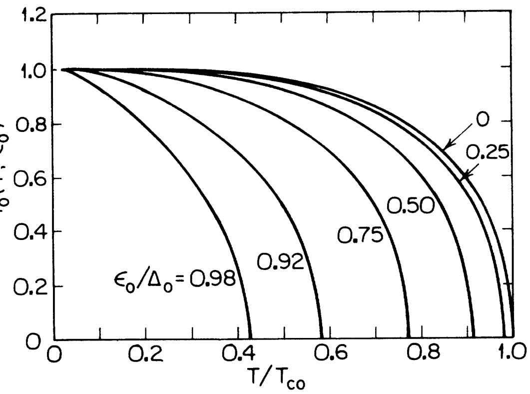

FIG. 2. The dynamic condensate density f_0 is shown as a function of the reduced temperature for several ϵ_0's.

The fact that f takes two different limiting values is first recognized by Rice *et al.*[15] However, its implication on Eqs. (17) and (18) appears to be still largely ignored even now.

The temperature dependence of f_0 and f_1 for several ε_0's are calculated numerically and shown in Figs. 2 and 3. In the vicinity of the transition temperature T_c, f_0 vanishes like $(T_c - T)^{1/2}$ while f_1 vanishes like $(T_c - T)$. Further, this linear slope of f_1 decreases very fast as ε_0/Δ_0 approaches unity.

We also note that f_0 describes the condensate density of the microwave conductivity[9] while f_1 describes the dc conductivity, the elastic constant, and the static spin susceptibility.

III. THRESHOLD ELECTRIC FIELD

As the most direct application of the phase Hamiltonian (14), we shall consider the threshold electric field that depins the CDW or SDW. In the following, we shall consider the CDW and SDW separately.

A. Charge-density wave

Following Fukuyama, Lee, and Rice[16] it is important to distinguish the strong-coupling limit and the weak-

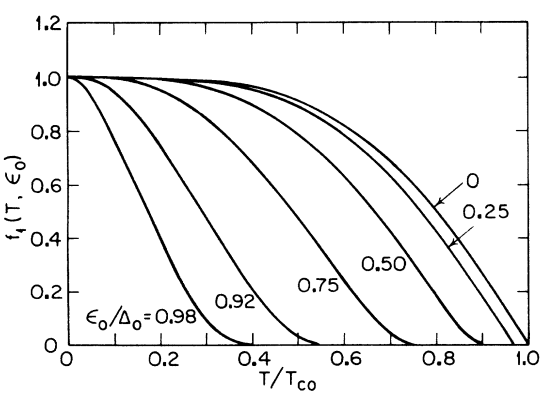

FIG. 3. The static condensate density f_1 is shown as a function of the reduced temperature for several ϵ_0's.

coupling limit though there are accumulating evidences that in most cases the CDW is in the weak-pinning limit.[17] In the strong-pinning limit, we obtain[18]

$$E_T^S(0) = 2Q(e\lambda)^{-1}(n_i/n)(N_0 V)\Delta_0 \tag{20}$$

and

$$E_T^S(T)/E_T^S(0) = e^{-T/T_0}[\Delta(T)/\Delta_0] f_1^{-1} , \tag{21}$$

where n_i is the impurity concentration and λ is the electron-phonon coupling constant. In Eq. (21), we include the effect of thermal fluctuation[19] (i.e., the Debye-Waller factor).

In a CDW, $E_T^S(0)$ is independent of ε_0 within the present model. Further, $E_T^S(T)/E_T^S(0)$ is rather insensitive to ε_0 except when ε_0 is very close to Δ_0 (i.e., $\varepsilon_0 \gtrsim 0.8\Delta_0$). In particular, $E_T^S(T)/E_T^S(0)$ diverges like

$$E_T^S(T)/E_T^S(0) \simeq e^{-T_c/T_0} A(1-T/T_c)^{-1/2} \tag{22}$$

as T approaches T_c. The coefficient A is evaluated numerically and shown in Fig. 4. In this circumstance, T_0 in Eq. (22) should be most sensitive to the pressure since $T_0 \propto \eta = v_2 v_3/\bar{v}^2$, the anisotropic factor. On the other hand, in the weak-pinning limit we have[18]

$$E_T^W(0) = [(4-D)/4D]\alpha(Q/en)\bar{v}^2 N_0 \times [2(\eta^{-1} n_i)^{1/2} D V \Delta_0/\alpha \bar{v}^2 \lambda f_1]^{4/(4-D)} \tag{23}$$

and

$$E_T^W(T)/E_T^W(0) = [E_T^S(T)/E_T^S(0)]^{4/(4-D)} , \tag{24}$$

where $\alpha = \pi^2/3$ and D is the spatial dimension of the phase fluctuation. We have shown recently[18] that most of the observed $E_T(T)$ in CDW's of $NbSe_3$, etc., are described by the weak-pinning model with $D=2$ or 3. In particular, $D=2$ in $NbSe_3$ should imply[17] rather large Fukuyama-Lee-Rice coherence length $L(T)$;

$$L(T) = [\alpha \bar{v}^2 \lambda f_1 e^{T/T_0}/2(\eta^{-1} n_i)^{1/2} D V \Delta(T)]^{2/(4-D)} . \tag{25}$$

For example, in clean $NbSe_3$ samples the maximal value of $L(T)$ can be as large as 0.1 mm. This implies

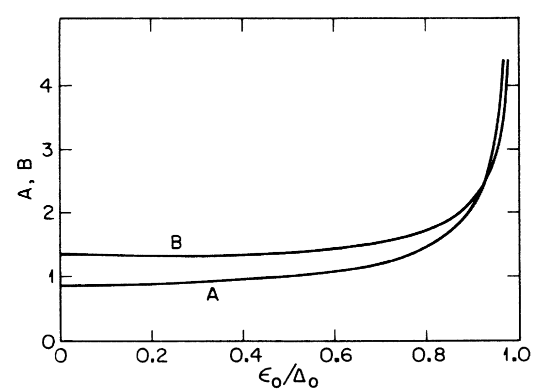

FIG. 4. The coefficients A and B which appear in the expressions of the threshold field for the CDW [Eq. (22)] and for the SDW [after Eq. (30)] are shown as a function of ϵ_0.

that the transverse coherence length $L_{tr}(T)=(v_2/\bar{v})L(T)$ is of the order of 10 μm. Note that $L(T)$ takes the maximum value immediately below $T=T_c$ where $E_T(T)$ takes the minimum value. $L(T)$ vanishes like $(T-T_c)^{1/(4-D)}$ as T approaches T_c.

B. Spin-density wave

Due to the weakness in the pinning potential in a SDW in comparison with that in a CDW, the weak-pinning limit appears to be much more appropriate here. However, for completeness we first describe the strong-pinning limit. In this limit the threshold field is given by

$$E_T^S(0)=(Q/e)(n_i/n)(\pi N_0 V)^2 F_0(0,\,\varepsilon_0/\Delta_0) \tag{26}$$

and

$$E_T^S(T)/E_T^S(0)=[F_0(T,\,\varepsilon_0/\Delta_0)/F_0(0,\,\varepsilon_0/\Delta_0)]f_1^{-1} \ , \tag{27}$$

where

$$F_0(T,\varepsilon_0/\Delta_0) =\pi T\Delta^2(T)\sum_{n=0}^{\infty}\langle[(\omega_n+i\eta)^2+\Delta^2(T,\varepsilon_0)]^{-1/2}\rangle^2 \ . \tag{28}$$

At $T=0$ K, F_0 is given by

$$F_0(0,x)=\frac{\pi}{2}\Delta_0\sum_{n=0}^{\infty}\left[\frac{(2n-1)!!}{2^n n!}\right]^4 x^{2n} \ , \tag{29}$$

while at $T\simeq T_c$,

$$F_0(T,\varepsilon_0/\Delta_0)=\frac{\pi}{2}\Delta^2(T,\varepsilon_0)\varepsilon_0^{-1}\tanh(\tfrac{1}{2}\varepsilon_0/k_B T_c) \ . \tag{30}$$

We evaluate Eq. (27) numerically, as shown in Fig. 5 for a few ε_0's. As ε_0 increases, $E_T^S(T_c)/E_T^S(0)=B$ increases from 1.33 monotonically to ∞ as ε_0 tends to Δ_0. The constant B is evaluated as a function of ε_0 shown in Fig. 4. Now, in the weak-pinning limit we have[18]

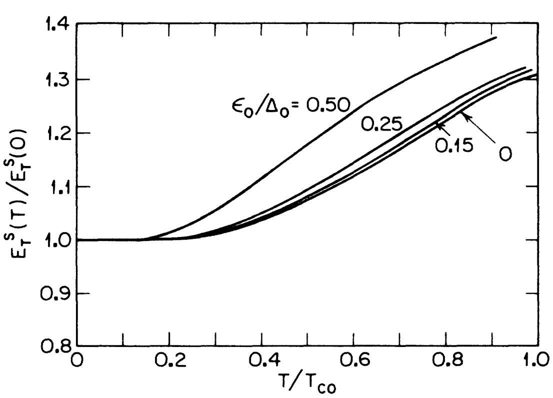

FIG. 5. The temperature dependence of the threshold field $E_T(T)$ in the SDW in the strong-pinning limit is shown as a function of the reduced temperature for a few ϵ_0's.

$$E_T^W(0)=[(4-D)/2D](Q/en)[\tfrac{1}{2}D(\pi N_0 V)^2]^{4/(4-D)} \times(\alpha\bar{v}^2 N_0)^{-D/(4-D)}(\eta^{-1}n_i)^{2/(4-D)} \times(F_0)^{4/(4-D)} \tag{31}$$

and

$$E_T^W(T)/E_T^W(0)=[E_T^S(T)/E_T^S(0)]^{4/(4-D)} \ . \tag{32}$$

In both Eqs. (27) and (32), we neglected the effect of the thermal fluctuations since in SDW's of Bechgaard salts like $(TMTSF)_2NO_3$, $(TMTSF)_2PF_6$, and $(TMTSF)_2ClO_4$ this effect is rather small due to the small spin-density-wave transition temperature. Making use of Eq. (32), we can describe quantitatively the observed temperature dependence of the threshold field in SDW's in $(TMTSF)_2PF_6$ with conventional silver paints,[20] if we assume that the SDW is the two-dimensional (2D) weak-coupling limit and $\epsilon_0/\Delta_0\simeq0.6$. However, unfortunately this interpretation is not unique. The threshold electric field of SDW's in $(TMTSF)_2PF_6$ with clamped contacts exhibits completely different temperature dependence,[20] which is more consistent with the pinning due to the commensurability with $N=4$. If this is the case, it is natural to expect that the threshold field in the sample with conventional contacts is influenced by commensurability as well. Then the 3D weak-pinning model with $\epsilon_0/\Delta_0\simeq0$ may not be inconsistent after all. Clearly, more systematic study on this point is desirable.

Now, as to the Fukuyama-Lee-Rice (FLR) coherence length in a SDW we obtain

$$L(0)=[2\alpha\bar{v}^2 N_0/(\eta^{-1}n_i)^{1/2}D(\pi N_0 V)^2 F_0]^{2/(4-D)} \tag{33}$$

and

$$L(T)/L(0)=[E_T^S(T)/E_T^S(0)]^{-2/(4-D)} \ . \tag{34}$$

Unlike to the case of the CDW, $L(T)$ in a SDW depends only weakly on temperature; $L(T)$ decreases monotonically with increasing temperature. In the cleanest samples, we expect $L(T)\sim1$ mm. This implies in the cleanest samples we have only a few FLR domains unlike in a CDW of $NbSe_3$. Perhaps, the rather peculiar noise spectrum observed in the non-Ohmic regime of SDW's in $(TMTSF)_2ClO_4$ by Nomura *et al.*[21] is due to few FLR domains in the sample.

IV. CONCLUDING REMARKS

We have analyzed systematically the transport properties of the CDW and SDW related to imperfect nesting. The model was already successful in describing the phase diagram of SDW's in Bechgaard salts and that of CDW's in $NbSe_3$ under pressure. A systematic study of the condensate density f_0 and f_1 in SDW's and CDW's will throw more light on effects of imperfect nesting.

ACKNOWLEDGMENTS

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