Phase Hamiltonian and depinning electric field in the charge-density wave and the spin-density wave

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Making use of the phase Hamiltonian derived from microscopic models, we study theoretically the threshold electric field when the charge-density wave (CDW) or the spin-density wave starts sliding. Unlike earlier phenomenological models, we can describe the temperature dependence of the threshold field. Most of experimental results on the threshold field in quasi-one-dimensional CDW's are interpreted in terms of the three-dimensional CDW. Curious exceptions are the CDW's in $NbSe_3$, which appear to be described better by the two-dimensional CDW.

I. INTRODUCTION

The threshold electric fields associated with depinning of charge-density waves (CDW's) have been studied extensively both theoretically and experimentally.[1] In particular, Fukuyama, Lee, and Rice[2,3] provide an extremely useful theoretical framework to analyze the threshold electric field E_T. They correctly identify the two limiting cases, the strong-pinning limit and the weak-pinning limit. Furthermore, they pointed out that the n_i dependence of E_T gives the key signature to discriminate the strong-pinning limit from the weak-pinning limit[3] where n_i is the impurity concentration. This prediction is used successfully to test the validity of the theory.[4–6] In spite of this remarkable success, Lee and Rice[3] were unable to predict the temperature dependence of E_T, partly due to their confusion[7] on the temperature dependence of the condensate density f and partly due to the fact that the importance of the thermal fluctuation[8] in the phase ϕ of the order parameter is unknown. Further, their analysis of the weak-pinning limit was done only for the three-dimensional (3D) CDW, which appears to be somewhat too restrictive.

More recently, the nonohmic conductivities in spin-density waves (SDW's) in Bechgaard salts like tetramethyl tetraselenfulvalinium nitrate $(TMTSF)_2NO_3$, $(TMTSF)_2PF_6$ and quenched $(TMTSF)_2ClO_4$ have been reported.[9,10] Therefore, it is necessary to extend the early analysis to SDW's and to field-induced spin-density waves (FISDW's) as well.

The object of this paper is to reexamine the threshold electric field within the phase Hamiltonian derived from the microscopic models.[11] Within the present phase Hamiltonian, we can predict the temperature dependence of E_T in both in CDW's and SDW's.[12] In particular, in a CDW E_T diverges at $T=T_c$ like $E_T \propto (T_c-T)^{-\alpha}$ where $\alpha=\frac{1}{2}$ in the strong-pinning limit while $\alpha=2(4-D)^{-1}$ in the weak-pinning limit and D is the spatial dimension of the CDW. The observed E_T of the first CDW in $NbSe_3$ by Fleming[13] is described well in terms of the two-dimensional (2D) weak-pinning limit, while the later result on E_T by Richard *et al.*[14] is described by the strong-pinning limit theory. In a SDW, E_T is almost constant for $T \le \frac{1}{2}T_c$. Then E_T increases monotonically up to $T=T_c$, though there is no divergence at $T=T_c$. The temperature dependence of E_T observed in $(TMTSF)_2NO_3$, $(TMTSF)_2PF_6$ and quenched $(TMTSF)_2ClO_4$ are qualitatively consistent with the present theory.

II. PHASE HAMILTONIAN

As a microscopic model for the CDW, we take the Fröhlich Hamiltonian as considered by Lee, Rice, and Anderson[15] with one exception. We consider the quasi-one-dimensional electron band with the quasiparticle energy given by

$$\varepsilon(p)=-2t_a\cos ap_1-2t\cos bp_2-2t_c\cos cp_3-\mu \tag{1}$$

with say

$$t_a:t_b t_c \simeq 10:1:0.03 \tag{2}$$

and μ is the chemical potential. The present model gives the anisotropic Fermi velocity

$$\mathbf{v}_F=(v,v_2,v_3) \tag{3}$$

with

$$v=2t_a a\sin ap_F,\quad v_2=\sqrt{2}t_b b,\quad v_3=\sqrt{2}t_c c\ . \tag{4}$$

For the SDW, we take the anisotropic Hubbard model as introduced by Yamaji[16] in order to describe the phase diagram of Bechgaard salts. Again, the quasiparticle spectrum in Yamaji's model is given by Eq. (1). Due to the quasi-one-dimensionality the perfect nesting with the nesting vector $\mathbf{Q}=(2p_F,\pi/b,\pi/c)$ is weakly broken. The degree of imperfect nesting is given by[17]

$$\tfrac{1}{2}[\varepsilon(\mathbf{p})+\varepsilon(\mathbf{Q}+\mathbf{p})]$$

$$\simeq t_b \cos ap_F [a(p_1-p_F)]^2-\delta\mu \approx \epsilon_0 \cos(2bp_2) \tag{5}$$

with

$$\epsilon_0=-\tfrac{1}{2}t_b^2\cos(ap_F)(t_a \sin^2 ap_F)^{-1} . \tag{6}$$

In the following, we limit ourselves to the case $|\epsilon_0|/\Delta_0 \ll 1$ for clarity, where Δ_0 is the CDW (or the SDW) order parameter at $T=0$ K. The effect of ϵ_0/Δ_0 on the threshold field will be described elsewhere.[18] From the analysis of the phason propagator[11] the phase Hamiltonian of a CDW (or a SDW) is given by

$$H_\phi=\int d^Dx \left\{ \tfrac{1}{4}N_0 f \left[(m^*/m)\left[\frac{\partial\phi}{\partial t}\right]^2+v^2\left[\frac{\partial\phi}{\partial x}\right]^2 + v_2^2\left[\frac{\partial\phi}{\partial y}\right]^2+v_3^2\left[\frac{\partial\phi}{\partial z}\right]^2\right] - enfQ^{-1}\phi E \right\} + V_{\mathrm{pin}}(\phi) , \tag{7}$$

where $N_0=(\pi vbc)^{-1}$ is the density of states at the Fermi surface per spin, $Q=2p_F$ and the electron density $n=Q/\pi bc$ and f is the condensate density. Further, slow spatio-temporal distortion of the phase ϕ generates the electric charge and current given by

$$n_c=enfQ^{-1}\frac{\partial\phi}{\partial x} , \tag{8}$$

$$j_c=-enfQ^{-1}\frac{\partial\phi}{\partial t} , \tag{9}$$

which satisfy the charge conservation

$$\frac{\partial n_c}{\partial t}+\frac{\partial j_c}{\partial x}=0 . \tag{10}$$

The electric charge carried by the condensate is strictly conserved at all temperatures in the absence of topological defects like phase vortices. Only these topological defects can convert the electric charge carried by the condensate to the one carried by the quasiparticle and vice versa.[19]

The phason mass m^* is given by

$$m^*/m=1+[2\Delta(T)/\omega_Q]^2(\lambda f)^{-1} \tag{11}$$

for a CDW while $m^*/m=1$ in a SDW.[11] Here λ is the dimensionless electron-phonon coupling constant. Equation (11) generalized the result in Ref. 15 for all temperatures.

Finally, the pinning potential $V_{\mathrm{pin}}(\phi)$ for CDW's and SDW's, respectively, is given by

$$V_{\mathrm{pin}}(\phi)=\begin{cases} -2N_0V\lambda^{-1}\Delta(T)\sum_i \cos[\mathbf{Q}\mathbf{x}_i+\phi(x_i)] & \text{(12a)} \\ -[(\pi/2)N_0V]^2\Delta(T)\tanh[\Delta(T)/2T] \times \sum_i \cos\{2[\mathbf{Q}\mathbf{x}_i+\phi(x_i)]\} , & \text{(12b)} \end{cases}$$

where the sum over i is on the impurity site.

Before going to analyze the threshold electric field, it is very important to define the temperature dependence of f. In general, f is a complicate function of ω and q where ω and q are the frequency and the wave vector associated with ϕ. In the adiabatic limit (i.e., ω, $\zeta=vq \ll \Delta_0$) f takes the simple forms[11,20]

$$f=\begin{cases} f_1 & \text{for } \omega/\zeta \ll 1 \\ f_0 & \text{for } \zeta/\omega \ll 1 . \end{cases} \tag{13}$$

The temperature dependences of f_0 and f_1 are given in Fig. 1. In particular, the temperature dependence of f_1 is the same as the superfluid density $\rho_s(T)/\rho$ in a BCS superconductor. In the analysis of the threshold field, we have to take $f=f_1$, since in the vicinity of $E=E_T$ the phase ϕ is dominated by the spatial distortion. Only when $E \gg E_T$ and the narrow band noise frequency ω_c becomes larger than vL^{-1} where L is the Fukuyama-Lee-Rice coherence length, $f=f_0$ will become more appropriate. Further, for the present analysis we do not need the term $(\partial\phi/\partial t)^2$ in Eq. (7). Then it is more convenient to rewrite Eq. (7) in an isotropic form with the help of the scale transformation.[3]

$$H'_\phi=\eta f_1\int d^Dx(\tfrac{1}{4}N_0v^2|\nabla\phi|^2-enQ^{-1}\phi E)+V_{\mathrm{pin}}(\phi) , \tag{14}$$

where $\eta=v_2v_3/v^2$ (or v_2/v) for 3D (or 2D) systems. Note that $V_{\mathrm{pin}}(\phi)$ is not affected by this scale transform, although n_i has to be replaced by $\eta\, n_i$.

Finally, the thermal fluctuation[8] of ϕ modifies the temperature dependence of $V_{\mathrm{pin}}(\phi)$ significantly. This is incorporated into the Hamiltonian (7) or (14) by multiplying

$$\exp(-\tfrac{1}{2}\langle\phi^2\rangle)=\exp(-T/T_0)$$

on $V_{\mathrm{pin}}(\phi)$ for a CDW, while $\exp(-2\langle\phi^2\rangle)$ for a SDW. From the analysis of the short-range fluctuation we obtain

$$T_0=2\pi t_b t_c/\Delta_0 , \tag{15}$$

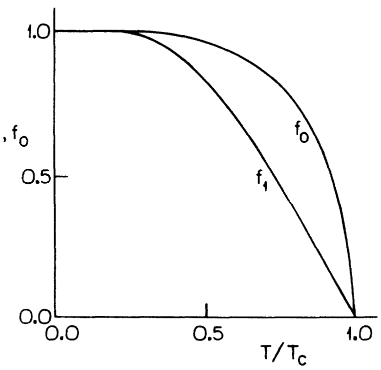

FIG. 1. The dynamic and the static condensate density f_0 and f_1 are shown as functions of the reduced temperature T/T_c.

where we cut off the momentum at $q_c = \Delta_0/v$ the inverse of the BCS coherence length. As we have shown,[12] the observed threshold electric field[13,21] in the second CDW of $NbSe_3$ gives $T_0 = 14.6-15.2$ K. On the other hand, a simple estimate of Eq. (15) appears to give T_0 at least by an order of magnitude larger than the one observed experimentally. The most likely source of this discrepancy is the cutoff momentum. Therefore, in the following, we assume that

$$T_0 = Ct_b t_c/\Delta_0 = \tfrac{1}{2}C\eta v^2/bc\Delta_0 \tag{16}$$

instead of Eq. (15) where C is the numerical constant of the order of $1-10^{-1}$. This means we need a higher cutoff momentum.

As far as the organic conductors are concerned, the effect of the thermal fluctuations is most likely negligible, since most of the SDW transition temperatures lie around 10 K. In contrast, most of the CDW transition temperatures are around 100–300 K.

III. THRESHOLD ELECTRIC FIELD IN CDW

First, we shall consider the threshold electric field in a CDW. Following Fukuyama, Lee, and Rice[2,3] we consider the strong-pinning and the weak-pinning limit separately.

A. Strong-pinning limit

In the strong-pinning limit, individual impurities pin the local phase $\phi(\mathbf{x}_i)$ at the impurity site. The potential is then given by the volume average of the local pinning potential, resulting in the threshold electric field[12]

$$E_T^s(0) = 2Q(e\lambda)^{-1}(n_i/n)(N_0 V)\Delta_0 \tag{17}$$

and

$$E_T^s(T)/E_T^s(0) = e^{-T/T_0}[\Delta(T)/\Delta_0]f_1^{-1} , \tag{18}$$

where $Q = 2p_F$, λ is the electron-phonon coupling constant, n_i is the impurity density and n is the electron density. Here superscript s means the strong-pinning limit. Equation (18) diverges as T approaches T_c like $(T_c - T)^{-1/2}$. The square-root divergence of $E_T(T)$ in CDW's of $NbSe_3$ has been observed in a number of experiments.[13,14] This implies that the pinning in these systems is described by the strong-pinning theory. Also, it is noteworthy that E_T is independent of η except through T_0 in the strong-pinning limit.

B. Weak-pinning limit

In this limit, the single impurity cannot pin the phase. Following the procedure introduced by Fukuyama, Lee, and Rice, we obtain

$$E_T^W(0) = (4-D/4D)\alpha(Q/en)v^2 N_0 L^{-2}(0) \tag{19}$$

and

$$E_T^W(T)/E_T^W(0) = [E_T^s(T)/E_T^s(0)]^{4/4-D} , \tag{20}$$

where $\alpha = \pi^2/3$ and $L(T)$ is the temperature-dependent Fukuyama-Lee-Rice length

$$L(T) = [\alpha v^2 \lambda f_1 e^{T/T_0}/2(\eta^{-1}n_i)^{1/2} DV\Delta(T)]^{2/4-D} \tag{21}$$

and D is the spatial dimension of the CDW. Especially at $T = 0$ K, we have

$$E_T^W(0) \propto (\eta^{-1}n_i)^{2/4-D}\Delta_0^{4/4-D} . \tag{22}$$

Further, as T approaches T_c, $E_T^W(T)$ diverges like $(T_c - T)^{-2/4-D}$. Therefore, we have a variety of indices to discriminate between the strong-pinning limit and the weak-pinning limit. Further, in the latter case we can infer the dimensionality of the CDW. For example, in a recent paper Petravić *et al.*[22] analyzed the pressure dependence of variety of parameters referring to CDW's of $(NbSe_4)_{10/3}I$, $(TaSe_4)_2I$ and TaS_3. We find that the observed E_T scales with T_0 like $E_T \propto (T_0)^{-2}$ or $(T_0)^{-3}$.

Indeed, only $E_T(0)$ and T_0 depend strongly on pressure in the above CDW's. Noting the fact that $T_0 \propto \eta$ [see Eq. (16)], their results can be described in terms of the weak-pinning theory with $D = 3$ where we have $E_T(0) \propto \eta^{-2}$ [Eq. (22)], since the anisotropic parameter η is most sensitive to the pressure. More recently, Mihaly and Canfield[23] observed the pressure dependence of $E_T(0)$ and Δ_0 in blue bronze $K_{0.3}MoO_3$. Their result is $E_T(0) \propto \Delta_0^4$, which is again consistent with the 3D weak-pinning limit.

More generally, the present theory describes most of data on the temperature dependence of $E_T(T)$ compiled in Ref. 1 with exception of CDW's in $OTaS_3$ and $K_{0.3}MoO_3$. In these two systems, it is possible that the commensuration potential given by

$$V_c(\phi) = -C_1[\Delta(T)]^4 W^{-3}\cos[4\phi(\mathbf{x})] \tag{23}$$

should be added to the Hamiltonian (7). Here C_1 is a constant of the order of unity and W is the band width. The commensuration potential of order $N = 4$ gives rise to the pinning energy, which is roughly one order of magnitude smaller than the one due to impurities. When the scale transformation is introduced, $V_c(\phi)$ has to be multiplied by η as the kinetic energy. Further, the thermal fluctuation reduces Eq. (23) by a factor e^{-16T/T_0}. Therefore, the commensurability potential in Eq. (14) is given by

$$V_{c'}(\phi) = -C_1 e^{-16T/T_0}[\Delta(T)]^4 W^{-3}\cos[4\phi(\mathbf{x})] . \tag{24}$$

For example, when the pinning is dominated by the commensurability potential, the threshold electric field is given by

$$E_T^c(T) = C_1 Q(ef_1)^{-1} e^{-16T/T_0}[\Delta(T)]^4 W^{-3} . \tag{25}$$

The threshold field due to the commensurability potential decreases monotonically with increasing temperature and vanishes linearly like $(T_c - T)$ at the transition temperature. We note that Eq. (25) is also consistent with the relation between $E_T(0)$ and Δ_0 established by Mihaly and Canfield.[23]

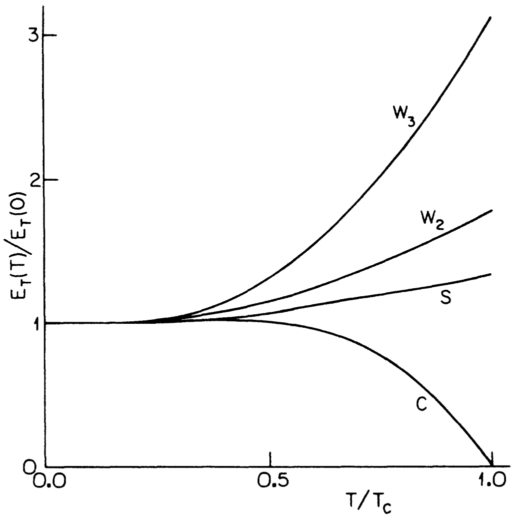

FIG. 2. The temperature dependence of the threshold electric field $E_T(T)$ of a SDW is shown in the strong-pinning limit (s), the weak-pinning limit with $D=3$ and $2(W_3, W_2)$ and when the pinning is due to the commensuration potential (c).

IV. THRESHOLD ELECTRIC FIELD IN SDW

Again, we shall consider the strong-pinning and the weak-pinning limit separately, though, we believe, the weak-pinning limit should apply for a SDW.

A. Strong-pinning limit

Making use of the pinning potential for a SDW [Eq. (12b)], we obtain[12]

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

and

$$E_T^s(T)/E_T^s(0)=[\Delta(T)/\Delta(0)]\tanh[\Delta(T)/2T]f_1^{-1} \tag{27}$$

The temperature dependence of $E_T^s(T)/E_T^s(0)$ is calculated numerically and shown in Fig. 2. Unlike E_T in a CDW, E_T is almost constant for $T\le\frac{1}{2}T_c$ and then increases with the temperature monotonically and reaches

$$E_T^s(T_c)/E_T^s(0)\simeq 1.33$$

at the transition temperature. Further, since Eq. (26) is proportional to $(N_0V)^2$ and since Δ_0 in a SDW is smaller than the one in a CDW by an order of magnitude, $E_T^s(0)$ in a SDW is smaller by a factor of 10^{-2} to the one corresponding to a CDW. As already mentioned, we neglect the effect of the thermal fluctuation in Eq. (27), which appears to be quite small.

B. Weak-pinning limit

The threshold field in the weak-pinning limit is given by

$$E_T^W(T)=(4-D/2D)\alpha(Q/en)v^2N_0L^{-2}(0) \tag{28}$$

and

$$E_T^W(T)/E_T^W(0)=[E_T^s(T)/E_T^s(0)]^{4/4-D}\ , \tag{29}$$

where the Fukuyama-Lee-Rice length is given

$$L(T)=[\alpha v^2N_0f_1/\tfrac{1}{2}(\eta^{-1}n_i)^{1/2}D(\pi N_0V)^2 \times\Delta(T)\tanh(\Delta/2T)]^{2/4-D}\ . \tag{30}$$

The temperature dependences of $E_T(T)/E_T(0)$ in the weak-pinning limit with $D=3$ and 2 are also calculated numerically and shown in Fig. 2.

C. Commensurability potential

For completeness, we consider the effect of the commensurability potential in a SDW. For the commensurability $N=4$, the potential is again given by Eq. (23). The corresponding threshold field is given by

$$E_T^C(0)=4C_1Qe^{-1}\Delta_0^4W^{-3} \tag{31}$$

and

$$E_T^C(T)/E_T^c(0)=[\Delta(T)/\Delta_0]^4f_1^{-1}\ . \tag{32}$$

Here we neglect again the effect of the thermal fluctuation. We show Eq. (32) again in Fig. 2.

V. CONCLUDING REMARKS

Making use of the phase Hamiltonian derived from microscopic models, we have analyzed the threshold electric field in CDW's and SDW's. The present theory describes quantitatively the observed threshold electric field in a variety of quasi-one-dimensional CDW systems. In particular, both from the temperature and the impurity concentration dependence of the threshold electric field we conclude that most of the CDW's are three dimensional and in the weak-pinning limit. The only curious exceptions are CDW's in $NbSe_3$, where the 2D weak-pinning prediction appears to be more appropriate. This is most likely due to the size effect. One of the transverse dimensions of the sample is less than the corresponding Fukuyama-Lee-Rice length $L(T)$. This assignment of the CDW is consistent with a recent theory[24] of the fluctuation-induced resistivity in CDW where the resistance diverges like $\rho\propto(T-T_c)^{-\alpha}$ with $\alpha=\frac{1}{2}(4-D)$ and D is the spatial dimension of the CDW.

The observed pressure dependence[22,23] of E_T in CDW's gives further support to the present theory. In the case of SDW's, the observed temperature dependence of E_T's in $(TMTSF)_2NO_3$, $(TMTSF)_2PF_6$ and quenched $(TMTSF)_2ClO$ appears to agree in general with the present theory. However, the higher-temperature value (i.e., $T>\frac{1}{2}T_c$) of E_T in $(TMTSF)_2NO_3$ is not available.[9] Furthermore, $E_T(T_c)/E_T(0)$ in $(TMTSF)_2PF_6$ appears to lie between the 3D weak pinning and the 2D weak pinning theory predicts.[9] Moreover, E_T for clumped samples of $(TMFSF)_2PF_6$ behaves quite differently from the other samples.[9] Indeed the observed $E_T(T)$ for the clumped sample is consistent with pinning solely due to the commensurability. Clearly, more work in this direction is desirable.

We add that the present phase Hamiltonian gives simple relation between the pinning frequency ω_p, the dielectric constant ϵ in the limit ω tends to zero and the threshold electric field E_T

$$\omega_p^2 = 4ev(m/m^*)E_T \quad (33)$$

and

$$\epsilon(\omega \to 0) = 2ef_1(bcE_T)^{-1} , \quad (34)$$

which generalizes the standard relation for a CDW to a SDW as well, though in the SDW $m^*/m=1$ has to be taken.

For example, from Eq. (33) we see that though E_T in a SDW in the cleanest sample is by order of magnitude smaller than that in a CDW, the corresponding pinning frequency ω_p in a SDW is of the same order of magnitude as in a CDW due to the absence of the phason mass renormalization in a SDW.

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