Magnetic-field dependence of phase correlation length in spin- and charge-density waves

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Within a simple quasi-two-dimensional model, we study the phason propagator in both spin- and charge-density waves in the presence of a magnetic field perpendicular to the conducting plane. We find, though the magnetic field has little effect in the longitudinal correlation length (i.e., the correlation length in the chain direction), the magnetic field reduces significantly the transverse correlation length. This effect is most easily observable as increases in the fluctuation-induced specific heat and the resistivity in the chain direction in magnetic fields.

I. INTRODUCTION

As is well known, a magnetic field perpendicular to the most conductive plane of charge- and spin-density waves (CDW and SDW) in quasi-two-dimensional conductors exhibits a number of peculiar effects. The most remarkable is the appearance of magnetic-field induced SDW's (Ref. 1) in $(TMTSF)_2ClO_4$ and $(TMTSF)_2PF_6$ under high pressure. Here, TMTSF stands for tetramethyltetraselenafulvalene. In an earlier paper,[2] we have analyzed the effects of magnetic field on thermodynamics and transport properties of CDW and SDW and we find these effects are rather small. Also, some of the transport coefficients can be interpreted in terms of the longitudinal correlation length, implying that a magnetic field has little effect on the longitudinal correlation length.

The object of the present paper is to study the phason propagator in the presence of a magnetic field perpendicular to the conducting plane. As a model, we take anisotropic Hubbard model as introduced by Yamaji,[3] and we concentrate our analysis on phason propagator in SDW, though most of our results are applicable to CDW as well. For simplicity, we limit ourselves to the case $\epsilon_0=0$, where ϵ_0 is the parameter characterizing imperfect nesting.[2] In this limit, the longitudinal correlation length is independent of the magnetic field. On the other hand, the transverse correlation (i.e., the correlation length in the direction perpendicular to both the chain direction and the magnetic field) decreases as the magnetic field is increased. The magnetic-field dependence is scaled by $\omega_c/2\Delta_0$ where $\omega_c=vbeB$ is the cyclotron frequency and Δ_0 is the quasiparticle energy gap at $T=0$ K. In CDW's, most of the experiments are done in the field region $\omega_c/2\Delta_0\ll 1$, while in SDW of $(TMTSF)_2$ salts (Bechgaard salts), this parameter can be easily much larger than unity. This means that the energy associated with spatial distortion of the phase or the kinetic energy associated the phase fluctuation is reduced, which results in an increase in the fluctuation contribution to the thermodynamic and the transport properties in magnetic fields.

II. FORMULATION

Let us start with Hamiltonian[3,4]

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

where

$$\begin{aligned}\epsilon(p)&=-2t_a\cos(ap_1)-2t_b\cos(bp_2)-\mu\\ &\simeq v(p_1-p_F)-2t_b\cos(bp_2)-\epsilon_0\cos(2bp_2)\ ,\end{aligned} \tag{2}$$

with

$$\epsilon_0=-\tfrac{1}{2}t_b^2\cos(ap_F)[t_a\sin^2(ap_F)]^{-1}\ , \tag{3}$$

and $v=2t_a a\sin(ap_F)$ is the Fermi velocity in the chain direction, and we neglected the transfer integral t_c in the third direction. Here, $C^{\dagger}_{p\alpha},C_{p\alpha}$ are the creation and annihilation operators of the electron with momentum $\mathbf{p}$ and spin α and we assume $t_b/t_a, t_c/t_b\ll 1$. In the absence of magnetic field, the quasiparticle Green's function in SDW is given by[4]

$$G^{-1}(\omega_n,\mathbf{p})=i\omega_n-\eta-\xi\rho_3-\Delta\rho_1\sigma_3\ , \tag{4}$$

where

$$\begin{aligned}\xi&=v(p_1-p_F)-2t_q\cos(bp_2)\ ,\\ \eta&=\epsilon_0\cos(2bp_2)\ ,\end{aligned} \tag{5}$$

and Δ is the SDW order parameter, ω_n is the Matsubara frequency, and the ρ_i's Pauli matrices operating on the spinor space consisting of the right-going electron and the left-going electron. (Note in the limit $t_b/t_a\ll 1$, the Fermi surface consists of two separate sheets located around $p_1=\pm p_F$.) The phason propagator is then obtained from

$$D_\phi^{-1}(\omega,\mathbf{q})=2U^{-1}(1-U\langle[\delta\Delta,\delta\Delta]\rangle)\ , \tag{6}$$

where $\delta\Delta$ is the fluctuation of the order parameter; $\langle[\ \ ]\rangle$ means the thermal product. In the limit $\omega_\nu\to 0$, we obtain[4]

$$D_\phi^{-1}(0,\mathbf{q})=(2\Delta)^{-2}N_0 f\{v^2q_1^2+v_2^2q_2^2+2[2t_c\sin(\tfrac{1}{2}cq_3)]^2\} \tag{7}$$

where N_0 is the electron density of states at the Fermi surface, f is the static condensate density, $v_2=\sqrt{2}t_b b$, and we inserted the third transfer integral t_c for completeness.

Now the effect of a magnetic field B perpendicular to the conducting plane is incorporated by replacing p_2 in Eq. (2) by p_2+eBx. This effect is incorporated into the quasiparticle Green's function by introducing an extra phase factor[5,6]

$$G_{\alpha\beta}(x-x')\to G_{\alpha\beta}(x-x')\exp\{i[\phi_\alpha(x)-\phi_\beta(x')]\} , \tag{8}$$

where

$$\begin{aligned}\phi_1(x)&=v^{-1}\int_{-\infty}^{x}dx\,\{2t_b\cos[b(p_2+eBx)]\\&\qquad+\epsilon_0\cos[2b(p_2+eBx)]\}\\&=\omega_c^{-1}\{2t_b\sin[b(p_2+eBx)]\\&\qquad+\tfrac{1}{2}\epsilon_0\sin[2b(p_2+eBx)]\} ,\end{aligned} \tag{9}$$

$$\begin{aligned}\phi_2(x)&=-v^{-1}\int_{-\infty}^{x}dx\,\{2t_b\cos[b(p_2+eBx)]\\&\qquad-\epsilon_0\cos[2b(p_2+eBx)]\}\\&=-\omega_c^{-1}\{2t_b\sin[b(p_2+eBx)]\\&\qquad-\tfrac{1}{2}\epsilon_0\sin[2b(p_2+eBx)]\} ,\end{aligned} \tag{10}$$

where $\omega_c=vbeB$, the cyclotron frequency, and subscripts α and $\beta=1,2$ [Eq. (8)] refer to the matrix element in the spinor space.

The phason dispersion is calculated from Eq. (6), where now the thermal product $\langle[\delta\Delta,\delta\Delta]\rangle(0,\mathbf{q})$ is given by

$$\begin{aligned}K&=\langle[\delta\Delta,\delta\Delta]\rangle(0,\mathbf{q})\\&=\pi TN_0\sum_n\frac{2}{v}\int_\delta^\infty dx\,\exp[-2v^{-1}(\omega_0^2+\Delta^2)^{1/2}x-\Phi]\\&\qquad\times[1-\tfrac{1}{4}(\omega_n^2+\Delta^2)^{-1}(vq_1)^2] ,\end{aligned} \tag{11}$$

where

$$\begin{aligned}\Phi&=\tfrac{1}{2}\langle[\phi_1(x)-\phi_1(0)-\phi_2(x)+\phi_2(0)]^2\rangle\\&=2\omega_c^{-2}[(4t_b)^2\sin^2(\tfrac{1}{2}bq_2)\sin^2(\tfrac{1}{2}beBx)\\&\qquad+\epsilon_0^2\cos^2(bq_2)\sin^2(beBx)]\end{aligned} \tag{12}$$

and $\langle\;\rangle$ means the average over p_2.

A derivation of Eqs. (11) and (12) is given in the Appendix. In the following, we neglect the ϵ_0 term in Eq. (12) for simplicity. Now expanding $e^{-\Phi}$ like $e^{-\Phi}\simeq 1-\Phi$, then Φ in powers of q_2 and integrating over x, we obtain

$$\begin{aligned}K&=\pi TN_0\sum_n(\omega_n^2+\Delta^2)^{-1/2}[1-\tfrac{1}{4}(\omega_n^2+\Delta^2)^{-1}(vq_1)^2]\\&\qquad\times[1-\tfrac{1}{4}(\omega_n^2+\Delta^2+\tfrac{1}{4}\omega_c^2)^{-1}(v_2q_2)^2]\\&=\{U^{-1}-N_0(2\Delta)^{-1}f_1[(vq_1)^2+(v_2^*q_2)^2]\} ,\end{aligned} \tag{13}$$

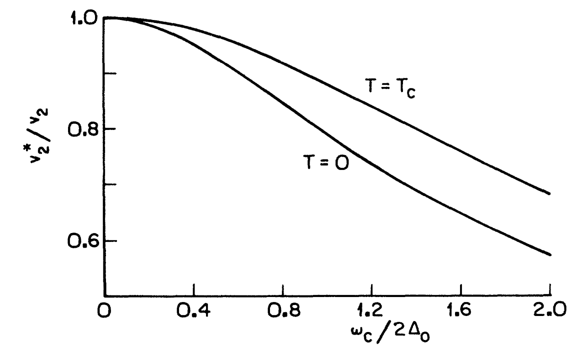

FIG. 1. The field dependence of v_2^*/v_2 is shown as functions of $\omega_c/2\Delta_0$ for $T=T_c$ and for $T=0$ K.

where

$$f_1=2\pi T\Delta^2\sum_{n=0}^{\infty}(\omega_n^2+\Delta^2)^{-3/2} , \tag{14}$$

$$(v_2^*/v_2)^2=f_1(\omega_c)/f_1 , \tag{15}$$

and

$$f_1(\omega_c)=2\pi T\Delta^2\sum_{n=0}^{\infty}(\omega_n^2+\Delta^2)^{-1/2}(\omega_n^2+\Delta^2+\tfrac{1}{4}\omega_c^2)^{-1} , \tag{16}$$

where $f_1=\rho_s(T)/\rho$, and $\rho_s(T)$ is essentially the superfluid density in the BCS theory. We have already encountered $f(\omega_c)$ in the analysis of the magnetoresistance[7] in SDW. Since $f(\omega_c)$ decreases with increasing magnetic field, v_2^* decreases with increasing field. At $T=0$ K and $T=T_c$, Eq. (15) is further simplified as

$$\begin{aligned}(v_2^*/v_2)^2&=(2\Delta_0/\omega_c)[1+(\omega_c/2\Delta_0)^2]^{-1/2}\\&\qquad\times\operatorname{arcsinh}(\omega_c/2\Delta_0) ,\quad\text{for } T=0\text{ K} ,\end{aligned} \tag{17}$$

$$\begin{aligned}&=[7\zeta(3)]^{-1}(4\pi T_c/\omega_c)^2\\&\qquad\times\left[\operatorname{Re}\psi\left[\frac{1}{2}-i\frac{\omega_c}{4\pi T_c}\right]-\psi\left[\frac{1}{2}\right]\right] ,\\&\qquad\text{for } T=T_c ,\end{aligned} \tag{18}$$

where $\psi(x)$ is the digamma function. The field dependence of v_2^*/v_2 is evaluated numerically for $T=0$ K and $T=T_c$ and shown in Fig. 1 as function of $\omega_c/2\Delta_0$. For the intermediate-field region (e.g., $\omega_c/2\Delta_0>0.8$ for $T=T_c$), v_c^*/v_2 decreases almost linearly with B.

III. TRANSVERSE CORRELATION LENGTH

Now putting back Eq. (13) into Eq. (6), we find that

$$\begin{aligned}D_\phi^{-1}(0,q)&=(2\Delta)^{-2}N_0 f[(vq_1)^2+(v_2^*q_2)^2\\&\qquad+2(2t_c\sin\tfrac{1}{2}cq_3)^2] ,\end{aligned} \tag{19}$$

where we have already determined v_2^* in the preceding section. Reduction of v_2^* in a magnetic field means that the energy associated with the spatial distortion or the fluctuation in phase is reduced in a magnetic field. There are two important length scales associated with phase: the coherence length near $T \simeq T_c$ and the Fukuyama-Lee-Rice coherence length.[8] The former controls the thermal fluctuation of the phase, and the latter the pinning of SDW.

A. Coherence length

The phason fluctuation propagator in the vicinity of $T \geq T_c$ is given by

$$D_\phi^{-1}(\omega_\nu,\mathbf{q})=N_0\left[\epsilon+\frac{\pi|\omega_\nu|}{8T}+\frac{7\zeta(3)}{(4\pi T)^2}\times\{v^2q_1^2+v_2^*q_2^2+2[2t_c\sin(\tfrac{1}{2}cq_3)]^2\}\right], \tag{20}$$

where $\epsilon=\ln(T/T_c)$.

Therefore, the transverse coherence length is given by

$$\xi_2=[7\zeta(3)]^{1/2}v_2^*(4\pi T)^{-1}, \tag{21}$$

and ξ_2 decreases in a magnetic field as v_2^* does. For example, the fluctuation contribution to the specific heat just above T_c is given by

$$\begin{aligned}C_{\mathrm{fl}}^{>}&=(2\pi)^{-3}\int d^3q[N_0D_\phi(o,\mathbf{q})]^2\\&=(4\pi c\xi_1\xi_2)^{-1}[\epsilon(\epsilon+K)]^{-1/2},\end{aligned} \tag{22}$$

where

$$\begin{aligned}\xi_1&=[7\zeta(3)]^{1/2}v/4\pi T,\\K&=14\zeta(3)(t_c/2\pi T)^2.\end{aligned} \tag{23}$$

For $T<T_c$, we have a similar expression for the specific heat:

$$C_{\mathrm{fl}}^{<}=(4\pi c\xi_1\xi_2)^{-1}[|\epsilon|(|\epsilon|+\tfrac{1}{2}K)]^{-1/2}. \tag{24}$$

Therefore, the fluctuation contribution to the specific heat increases with magnetic field and this increase is proportional to v_2/v_2^*.

Similarly, the electric conductivity decreases near $T=T_c$ because of the increased electron scattering due to the fluctuation.[9,10] The correct treatment of the scattering gives,[10] for $T \geq T_c$,

$$\sigma(T)=\sigma_0-(ev)^2[16c\xi_1\xi_2\tilde{\Gamma}(\Gamma+\tilde{\Gamma})]^{-1}\epsilon_0(\epsilon-\epsilon_0)^{-1}\times\ln\left[\frac{\sqrt{\epsilon}+\sqrt{\epsilon+K}}{\sqrt{\epsilon_0}+\sqrt{\epsilon_0+K}}\right], \tag{25}$$

where $\epsilon_0=7\zeta(3)\Gamma\tilde{\Gamma}(2\pi T)^{-2}$, $\sigma_0=(ev)^2N_0\Gamma_2^{-1}$, $\Gamma=\Gamma_1+\frac{1}{2}\Gamma_2$, $\tilde{\Gamma}=\frac{1}{2}(\Gamma_1+\Gamma_2)$, and the transport lifetime is given by Γ_2^{-1}. Here Γ_1 and Γ_2 are the forward and the backward scattering rate due to impurities. Again, the second term in Eq. (25) is proportional to ξ_2^{-1}. For $T<T_c$, the fluctuation contribution is the same[10] as in Eq. (25), except ϵ is replaced by $2|\epsilon|$. The magnetoresistance increases with magnetic field and this increase is almost linear in B in the intermediate field range. This term is most likely the origin of anomalous magnetoresistance observed in Bechgaard salts at low temperatures.[11]

B. Fukuyama-Lee-Rice length

Recent experiments on nonohmic transport[12,13] in SDW of $(TMTSF)_2NO_3$, $(TMTSF)_2PF_6$, and quenched $(TMTSF)_2ClO_4$ indicate that the magnitude of the threshold electric field and its temperature dependence of pristine samples are described by 3D weak-pinning theory.[14] In the weak-pinning limit the longitudinal Fukuyama-Lee-Rice (FLR) length is given by[15]

$$L_l(T)=\frac{\pi}{3}[v/eE_T(T)]^{1/2}. \tag{26}$$

Further, in 3D weak-pinning limit $E_T(T)$ is related to v_2^* as[14]

$$E_T \propto (v_2^*/v_2)^{-2}. \tag{27}$$

Therefore, the threshold electric field in the weak-pinning limit increases with magnetic field. Further, through Eq. (26) the longitudinal FLR length decreases as

$$L_l \propto (v_2^*/v_2). \tag{28}$$

Finally, since the transverse FLR length is given by

$$L_t=(v_2^*/v)L_l \propto (v_2^*/v_2)^2, \tag{29}$$

L_t decreases in a magnetic field much faster than L_1. So far, we considered only pristine samples. The SDW in x-ray irradiated samples[12] of $(TMTSF)_2PF_6$ has the threshold field $E_T(T)$ which exhibits much weaker T dependence and is therefore consistent with strong-pinning limit theory. Then crossover concentration of irradiation-induced defects is determined when E_T in the strong-pinning limit is equal to that in the weak-pinning limit. Since E_T in the strong-pinning limit is independent of the elastic energy, it is independent of magnetic field. On the other hand, we have seen that E_T in the weak-pinning limit increases with magnetic field, implying that the crossover concentration of defects decreases with increasing magnetic field.

IV. CONCLUDING REMARKS

We show that a magnetic field perpendicular to the conducting plane strongly reduces the elastic constant associated with the transverse phase distortion $(\partial\phi/\partial y)$. This has a number of consequences. In the vicinity of the transition temperature T_c, the thermal fluctuation of the order parameter is increased in a magnetic field. Second, in SDW the change in the elastic constant increases the threshold electric field in the weak-pinning limit. This reduces both the longitudinal and transverse FLR length in the magnetic field.

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APPENDIX: DERIVATION OF EQUATIONS (11)–(13)

The function K in Eq. (11) is obtained from

$$K=T\sum_n \int T_x[\rho_2\hat{G}(x,y)\rho_2\hat{G}(x,y)]dy$$

$$=T\sum_n \frac{2}{v^2}\int dx \exp\left[-\frac{2}{v}\sqrt{\omega_n^2+\Delta^2}|x-y| - iq(x-y)-i\Phi\right], \tag{A1}$$

where we have inserted

$$\hat{G}(x-y)=\int \frac{dp}{2\pi}(i\omega_n-\xi\rho_3-\Delta\rho_1)^{-1}$$

$$=\frac{1}{2v}\left[\frac{1}{\sqrt{\omega_n^2+\Delta^2}}(i\omega_n+\Delta\rho_i)\pm\rho_3\right] \times e^{(-\sqrt{\omega_n^2+\Delta^2/v})|x-y|} \tag{A2}$$

and

$$\langle e^{i[\phi_1(x)-\phi_1(0)-\phi_2(x)+\phi_2(0)]}\rangle$$

$$=\exp\{-\tfrac{1}{2}\langle[\phi_1(x)-\phi_1(0)-\phi_2(x)+\phi_2(0)]^2\rangle\} . \tag{A3}$$

[1]For early works on FISDW, see *Physics and Chemistry of Quasi One-Dimensional Conductors,* edited by S. Tanaka and K. Uchinokura (Elsevier, Amsterdam, 1986).

[2]A. Bjeliš and K. Maki, Phys. Rev. B **42**, 10 275 (1990).

[3]K. Yamaji, J. Phys. Soc. Jpn. **51**, 2787 (1982).

[4]A. Virosztek and K. Maki, Phys. Rev. B **37**, 2028 (1988).

[5]L. P. Gor'kov and A. G. Lebed, J. Phys. (Paris) Lett. **45**, L433 (1984).

[6]K. Maki, Phys. Rev. B **33**, 4826 (1986); A. Virosztek, L. Chen, and K. Maki, *ibid.* **34**, 3371 (1986).

[7]A. Virosztek and K. Maki, Phys. Rev. B **39**, 616 (1989).

[8]H. Fukuyama and P. A. Lee, Phys. Rev. B **17**, 535 (1978); P. A. Lee and T. M. Rice, *ibid.* **19**, 3970 (1979).

[9]P. M. Horn and D. Guiddoti, Phys. Rev. B **16**, 491 (1977).

[10]K. Maki, Phys. Rev. B **41**, 9308 (1990).

[11]See some articles in Ref. 1.

[12]S. Tomić, J. R. Cooper, D. Jérome, and K. Bechgaard, Phys. Rev. Lett. **62**, 462 (1989); W. Kang, S. Tomić, J. R. Cooper, and D. Jérome, Phys. Rev. B **41**, 4862 (1990); W. Kang, S. Tomić, and D. Jérome, *ibid.* **43**, 1264 (1991).

[13]T. Sambongi *et al.*, Solid Sate Commun. **72**, 817 (1989); K. Nomura *et al.*, *ibid.* **72**, 1123 (1989).

[14]K. Maki and A. Virosztek, Phys. Rev. B **42**, 655 (1990).

[15]K. Maki, in *Microscopic Aspect of Nonlinearity in Condensed Matter,* edited by V. Tognetti (Plenum, New York, in press).