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*Source / Izvornik:* **Physical Review B (Condensed Matter), 1991, 44, 6799 - 6802**

**Journal article, Published version**

**Rad u časopisu, Objavljena verzija rada (izdavačev PDF)**

<https://doi.org/10.1103/PhysRevB.44.6799>

*Permanent link / Trajna poveznica:* <https://urn.nsk.hr/urn:nbn:hr:217:287698>

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*Download date / Datum preuzimanja:* **2023-02-08**



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

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(Received 27 February 1991)

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)<sub>2</sub>ClO<sub>4</sub> and (TMTSF)<sub>2</sub>PF<sub>6</sub> under high pressure. Here, TMTSF stands for tetramethyl-tetraselenafulvalene. In an earlier paper,<sup>2</sup> 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,<sup>3</sup> 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  $\epsilon_0$  is the parameter characterizing imperfect nesting.<sup>2</sup> 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  $\Delta_0$  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)<sub>2</sub> 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<sup>3,4</sup>

$$eH = \sum_{p,\alpha} \epsilon(p) C_{p\alpha}^\dagger C_{p\alpha} + U \sum_q n_{q\uparrow} n_{-q\downarrow}, \quad (1)$$

where

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

with

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

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,  $C_{p\alpha}^\dagger, C_{p\alpha}$  are the creation and annihilation operators of the electron with momentum  $\mathbf{p}$  and spin  $\alpha$  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<sup>4</sup>

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

where

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

and  $\Delta$  is the SDW order parameter,  $\omega_n$  is the Matsubara frequency, and the  $\rho_i$ '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

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

where  $\delta\Delta$  is the fluctuation of the order parameter;  $\langle [ ] \rangle$  means the thermal product. In the limit  $\omega_v \rightarrow 0$ , we obtain<sup>4</sup>

$$D_{\phi}^{-1}(0, \mathbf{q}) = (2\Delta)^{-2} N_0 f \{ v^2 q_1^2 + v_2^2 q_2^2 + 2[2t_c \sin(\frac{1}{2} c q_3)]^2 \} \quad (7)$$

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<sup>5,6</sup>

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

where

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

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

where  $\omega_c = vbeB$ , the cyclotron frequency, and subscripts  $\alpha$  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

$$\begin{aligned} K &= \langle [\delta\Delta, \delta\Delta] \rangle(0, \mathbf{q}) \\ &= \pi T N_0 \sum_n \frac{2}{v} \int_{\delta}^{\infty} dx \exp[-2v^{-1}(\omega_n^2 + \Delta^2)^{1/2} x - \Phi] \\ &\quad \times [1 - \frac{1}{4}(\omega_n^2 + \Delta^2)^{-1}(vq_1)^2], \end{aligned} \quad (11)$$

where

$$\begin{aligned} \Phi &= \frac{1}{2} \langle [\phi_1(x) - \phi_1(0) - \phi_2(x) + \phi_2(0)]^2 \rangle \\ &= 2\omega_c^{-2} [(4t_b)^2 \sin^2(\frac{1}{2} b q_2) \sin^2(\frac{1}{2} b e B x) \\ &\quad + \epsilon_0^2 \cos^2(b q_2) \sin^2(b e B x)] \end{aligned} \quad (12)$$

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  $\epsilon_0$  term in Eq. (12) for simplicity. Now expanding  $e^{-\Phi}$  like  $e^{-\Phi} \simeq 1 - \Phi$ , then  $\Phi$  in powers of  $q_2$  and integrating over  $x$ , we obtain

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

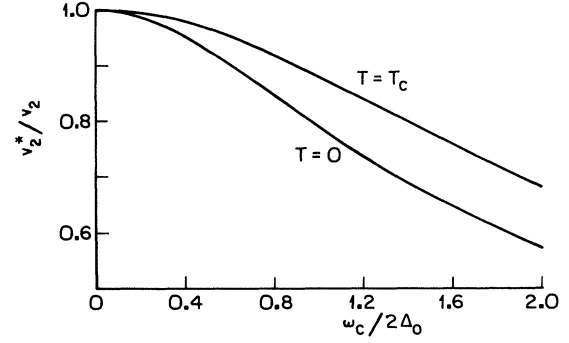


FIG. 1. The field dependence of  $v_2^*/v_2$  is shown as functions of  $\omega_c/2\Delta_0$  for  $T = T_c$  and for  $T = 0$  K.

where

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

$$(v_2^*/v_2)^2 = f_1(\omega_c)/f_1, \quad (15)$$

and

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

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<sup>7</sup> 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

$$\begin{aligned} (v_2^*/v_2)^2 &= (2\Delta_0/\omega_c) [1 + (\omega_c/2\Delta_0)^2]^{-1/2} \\ &\quad \times \text{arcsinh}(\omega_c/2\Delta_0), \quad \text{for } T = 0 \text{ K}, \quad (17) \\ &= [7\zeta(3)]^{-1} (4\pi T_c/\omega_c)^2 \\ &\quad \times \left[ \text{Re} \psi \left[ \frac{1}{2} - i \frac{\omega_c}{4\pi T_c} \right] - \psi \left[ \frac{1}{2} \right] \right], \end{aligned}$$

for  $T = T_c$ ,

(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  $T = T_c$ ),  $v_2^*/v_2$  decreases almost linearly with  $B$ .

### III. TRANSVERSE CORRELATION LENGTH

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

$$D_{\phi}^{-1}(0, \mathbf{q}) = (2\Delta)^{-2} N_0 f [(vq_1)^2 + (v_2^* q_2)^2 + 2(2t_c \sin \frac{1}{2} c q_3)^2], \quad (19)$$

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.<sup>8</sup> 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

$$D_{\phi}^{-1}(\omega, \mathbf{q}) = N_0 \left[ \epsilon + \frac{\pi|\omega_v|}{8T} + \frac{7\xi(3)}{(4\pi T)^2} \times \left\{ v^2 q_1^2 + v_2^* q_2^2 + 2[2t_c \sin(\frac{1}{2}c q_3)]^2 \right\} \right], \quad (20)$$

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

Therefore, the transverse coherence length is given by

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

and  $\xi_2$  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

$$C_{\text{fl}}^> = (2\pi)^{-3} \int d^3q [N_0 D_{\phi}(0, \mathbf{q})]^2 = (4\pi c \xi_1 \xi_2)^{-1} [\epsilon(\epsilon + K)]^{-1/2}, \quad (22)$$

where

$$\xi_1 = [7\xi(3)]^{1/2} v / 4\pi T, \quad (23)$$

$$K = 14\xi(3)(t_c / 2\pi T)^2.$$

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

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

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.<sup>9,10</sup> The correct treatment of the scattering gives,<sup>10</sup> for  $T \geq T_c$ ,

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

where  $\epsilon_0 = 7\xi(3)\Gamma\bar{\Gamma}(2\pi T)^{-2}$ ,  $\sigma_0 = (ev)^2 N_0 \Gamma_2^{-1}$ ,  $\Gamma = \Gamma_1 + \frac{1}{2}\Gamma_2$ ,  $\bar{\Gamma} = \frac{1}{2}(\Gamma_1 + \Gamma_2)$ , and the transport lifetime is given by  $\Gamma_2^{-1}$ . Here  $\Gamma_1$  and  $\Gamma_2$  are the forward and the backward scattering rate due to impurities. Again, the second

term in Eq. (25) is proportional to  $\xi_2^{-1}$ . For  $T < T_c$ , the fluctuation contribution is the same<sup>10</sup> as in Eq. (25), except  $\epsilon$  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.<sup>11</sup>

### B. Fukuyama-Lee-Rice length

Recent experiments on nonohmic transport<sup>12,13</sup> in SDW of  $(\text{TMTSF})_2\text{NO}_3$ ,  $(\text{TMTSF})_2\text{PF}_6$ , and quenched  $(\text{TMTSF})_2\text{ClO}_4$  indicate that the magnitude of the threshold electric field and its temperature dependence of pristine samples are described by 3D weak-pinning theory.<sup>14</sup> In the weak-pinning limit the longitudinal Fukuyama-Lee-Rice (FLR) length is given by<sup>15</sup>

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

Further, in 3D weak-pinning limit  $E_T(T)$  is related to  $v_2^*$  as<sup>14</sup>

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

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

$$L_l \propto (v_2^*/v_2). \quad (28)$$

Finally, since the transverse FLR length is given by

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

$L_t$  decreases in a magnetic field much faster than  $L_l$ . So far, we considered only pristine samples. The SDW in x-ray irradiated samples<sup>12</sup> of  $(\text{TMTSF})_2\text{PF}_6$  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.

## ACKNOWLEDGMENTS

We thank the Laboratoire de Physique des Solides, Université Paris-Sud and Groupe de Physique des Solides, Université Paris-7, where most of this work was done for hospitality. We acknowledge useful discussions with G. Montambaux and G. Kriza and thank D. Jérôme for drawing our attention to the long-standing questions of magnetoresistance in Bechgaard salts. This work was in part supported by the National Science Foundation under Grant No. DMR89-15285.

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

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

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

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

where we have inserted

$$\hat{G}(x - y) = \int \frac{dp}{2\pi} (i\omega_n - \xi p_3 - \Delta \rho_1)^{-1}$$

$$= \frac{1}{2v} \left[ \frac{1}{\sqrt{\omega_n^2 + \Delta^2}} (i\omega_n + \Delta \rho_i) \pm \rho_3 \right]$$

$$\times e^{(-\sqrt{\omega_n^2 + \Delta^2}/v)|x - y|} \quad (\text{A2})$$

and

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

$$= \exp \left\{ -\frac{1}{2} \langle [\phi_1(x) - \phi_1(0) - \phi_2(x) + \phi_2(0)]^2 \rangle \right\}. \quad (\text{A3})$$

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