# Anomalous electric and heat current in charge- and spin-density waves

# Kazumi Maki

Department of Physics, University of Southern California, Los Angeles, California 90089-0484 and Institute of Scientific Interchange, Villa Gualino, Viale Settimio Severo 65, 10133 Torino, Italy

### Xiaozhou Huang

## Department of Physics, University of Southern California, Los Angeles, California 90089-0484 (Received 3 October 1990)

We study theoretically the electric current and the heat current associated with sliding chargedensity waves (CDW's) or spin-density waves (SDW's). In the clean limit (i.e.,  $l \gg \xi$ , where l is the electron mean free path and  $\xi$  is the BCS coherence length), we find large sliding CDW (or SDW) contributions to these currents. The present result is consistent with Artemenko's prediction based on a kinetic equation and describes a peculiar temperature dependence of the condensate density observed in CDW's of NbSe<sub>3</sub> by Richard and Chen.

### I. INTRODUCTION

Within a conventional picture, the charge-density-wave (CDW) or spin-density-wave (SDW) condensate is believed to carry only the electric current in the chain direction.<sup>1</sup> On the other hand, a number of recent experiments on CDW's and SDW's indicate that the sliding CDW (or SDW) condensate carries the Hall current<sup>2-4</sup> as well as the entropy current.<sup>5,6</sup> Recently, making use of a kinetic equation in a quasi-one-dimensional CDW, Artemenko *et al.*<sup>7</sup> calculated contributions to the Hall current and the heat current associated with sliding CDW's which appear to account for these observations at least qualitatively.

The object of the present paper is to calculate both the electric current and the heat current associated with the sliding CDW's within the framework of the standard Green's-function technique. As a model, we use the anisotropic Hubbard model as introduced by Yamaji.<sup>8</sup> Further, we carry out most of our analysis on SDW's, though the most of results are applicable to CDW's as well. For simplicity, we neglect the phonon-drag term in the analysis of the heat current. For numerical analysis, we limit ourselves to  $\epsilon_0 / \Delta_0 \ll 1$ , where  $\epsilon_0$  is the parameter characterizing imperfect nesting and  $\Delta_0$  is the SDW or-der parameter at T=0 K.<sup>9</sup> Unlike earlier analysis, we find large contributions to both electric current and heat current associated with the sliding SDW's (or CDW's) from the anomalous region (i.e.,  $\omega_n \omega_{n+\nu} < 0$ , where  $\omega_n$ and  $\omega_{n+v}$  are two Matsubara frequencies attached to two Green's functions involved in the correlation function), which is proportional to  $l/\xi$ . These anomalous contributions behave like the normal current even though they are generated by moving SDW's (or CDW's). For example, they carry both the transverse current (i.e., the Hall current) in a magnetic field and the entropy. Therefore, we establish the transport equation for the electric and heat current written down by Artemenko:"

$$j = \sigma_0 E - \tilde{a} \dot{\phi} - \eta (\nabla T) T^{-1} , \qquad (1)$$

$$j^{h} = \prod E - \tilde{b} \dot{\phi} - \kappa (\nabla T) T^{-1} , \qquad (2)$$

and

43

5731

$$\dot{\phi} = -\Gamma^{-1}e\left[E - E_T - \frac{\tilde{b}}{\tilde{a}}(\nabla T)T^{-1}\right] \\ \times \theta\left[E - E_T - \frac{\tilde{b}}{\tilde{a}}(\nabla T)T^{-1}\right], \qquad (3)$$

where  $\Pi = \eta T$  and  $\sigma_0$  is the conductivity associated with the quasiparticle and  $\kappa$  is the thermal conductivity. Here  $\Gamma$  is the phason damping coefficient<sup>10</sup> and Eq. (3) is the simplest version of the dynamic equation controlling the sliding motion of the SDW condensate and  $\phi$  is the phase of the order parameter. The parameter  $\tilde{a}$  is expressed in terms of the condensate density f as

$$\tilde{a} = enQ^{-1}f = e(\pi bc)^{-1}f$$
 (4)

while  $\tilde{b}$  may be written in terms of  $\Pi_c$  the Peltier coefficient associated with the moving condensate

$$\Pi_{c} = \widetilde{b} / \widetilde{a} , \qquad (5)$$

where  $Q = 2p_F$  and *n* is the electron density.

In this paper, we limit ourselves to the case without magnetic field. The effect of magnetic field will be described in a future paper.

In addition to the anomalous heat current, we find a large anomalous electric current. When  $l/\xi \simeq 10$ , the condensate density has a broad peak around  $T \simeq 0.8 T_c$ . The broad peak may describe an anomalous temperature dependence of the condensate density observed by Richard and Chen in NbSe<sub>3</sub>.<sup>11</sup>

#### **II. FORMULATION**

Starting from an anisotropic Hubbard model, the quasiparticle Green's function in a SDW within mean-field theory is given by<sup>12</sup>

© 1991 The American Physical Society

5732

$$G^{-1}(\omega_n, p) = i\omega_n - \eta - \xi \rho_3 - \Delta \rho_1 \sigma_3 , \qquad (6)$$

where  $\eta = \epsilon_0 \cos(2bp_2)$ ,  $\omega_n$  is the Matsubara frequency,  $\xi$  is the quasiparticle energy measured from the Fermi surface, and  $\Delta$  is the SDW order parameter. Here,  $\rho_i$  and  $\sigma_i$  are Pauli spin matrices, the former operating on the spinor space formed by the right-going and the left-going quasiparticles, while the latter in the ordinary spin space.

Following Kubo's prescription, the four transport coefficients in Eqs. (1) and (2) are obtained from the retarded product  $\langle [j_x, j_x] \rangle$ ,  $\langle [j_x, \delta\Delta] \rangle$ ,  $\langle [j_x^h, j_x] \rangle$ , and  $\langle [j_x^h, \delta\Delta] \rangle$  where  $j_x = ev\rho_3$ ,  $j^h = \frac{1}{2}(\omega_n + \omega_{n+v})v\rho_3$  (heat current), and  $\delta\Delta = \Delta\rho_2$ , respectively. Making use of standard technique,<sup>13</sup> we obtain

$$\langle [j,j] \rangle / -i\omega = \sigma_0 = 2(ev)^2 N_0 I_1 , \qquad (7)$$

$$\langle [j^h, j] \rangle / -i\omega = \Pi = 2ev^2 N'_0 I_2 , \qquad (8)$$

$$\langle [j, \delta \Delta] \rangle / -i\omega = \tilde{a} = enQ^{-1}I_3$$
, (9)

$$\langle [j^h, \delta \Delta] \rangle / -i\omega = \tilde{b} = 2v N'_0 I_4 , \qquad (10)$$

where

$$I_1 = \frac{1}{2T} \int_0^\infty dz \operatorname{sech}^2(\frac{1}{2}\beta z) \left[ 1 + \frac{|u|^2 - 1}{|u^2 - 1|} \right] D^{-1}(\omega) , \quad (11)$$

$$I_{2} = \frac{1}{2T} \int_{0}^{\infty} dz \, z^{2} \operatorname{sech}^{2}(\frac{1}{2}\beta z) \left[ 1 + \frac{|u|^{2} - 1}{|u^{2} - 1|} \right] D^{-1}(\omega) , \qquad (12)$$

$$I_{3} = f_{1} + \frac{2\Delta}{T} \int_{0}^{\infty} dz \operatorname{sech}^{2}(\frac{1}{2}\beta z) \frac{\operatorname{Im} u}{|u^{2} - 1|} D^{-1}(\omega) , \qquad (13)$$

$$I_4 = \frac{2\Delta}{T} \int_0^\infty dz \, z^2 \mathrm{sech}^2(\frac{1}{2}\beta z) \frac{\mathrm{Im}u}{|u^2 - 1|} D^{-1}(\omega) \,, \qquad (14)$$

$$D(\omega) = 2\Delta \operatorname{Im}(u^2 - 1)^{1/2} - \Gamma'\left[1 + \frac{|u|^2 - 1}{|u^2 - 1|}\right], \quad (15)$$

$$\frac{z}{\Delta} = u \left[ 1 - \frac{\Gamma}{\Delta} (1 - u^2)^{-1/2} \right], \qquad (16)$$

and  $\Gamma = \Gamma_1 + \frac{1}{2}\Gamma_2$ ,  $\Gamma' = \Gamma_1 - \frac{1}{2}\Gamma_2$ , and  $\Gamma_1$  and  $\Gamma_2$  are the forward and backward scattering rate due to the impurity scattering. Here,  $N_0 = (\pi v b c)^{-1}$ ,  $N'_0 = \pm (\sqrt{2}t_a)^{-1}N_0$ , and the sign  $\pm$  corresponds to the  $\frac{1}{4}$ -filled band or  $\frac{3}{4}$ -filled band. Finally,  $f_1$  is the condensed density in the static limit

$$f_1 = 2\pi T \Delta^{-1} \sum_{n=0}^{\infty} \left[ (u_n^2 + 1)^{3/2} - \Gamma / \Delta \right]^{-1}$$
$$\simeq \rho_s(T) / \rho , \qquad (17)$$

which is hardly affected by the impurity scattering. In deriving Eqs. (11)–(16), we assumed  $\epsilon_0=0$  for simplicity. A derivation of Eqs. (7)–(10) is sketched in the Appendix.

### **III. ANOMALOUS TRANSPORT**

Equations (11)–(14) are evaluated numerically for a few  $\Gamma_i / \Delta_0$  and shown in Figs. 1–4 where

$$\sigma_0(T) / \sigma_0(T_c) = I_1(T) / I_1(T_c)$$
  

$$\Pi(T) / \Pi(T_c) = I_2(T) / I_2(T_c) ,$$
  

$$f(T/T_c) = I_3 ,$$

and

$$\Pi_c(T)/\Gamma T_c = I_4(T)/I_3(T)\Gamma T_c .$$

We note that both  $\sigma_0$  and  $\Pi(T)$  decrease monotonically as temperature decreases. Further, they become exponentially small at low temperatures. Especially at low temperatures, we obtain

$$\sigma_0(T) / \sigma_0(T_c) \simeq \frac{4\Gamma_2}{3\Gamma} \left[ \frac{T}{G} \right] e^{-\beta G} \left[ 1 + \frac{4\Gamma'}{3\Gamma} \left[ \frac{T}{G} \right] + \cdots \right]$$
(18)

$$\Pi(T)/\Pi(T_c) \simeq \frac{4}{\pi^2} \frac{\Gamma_2 G}{\Gamma T} e^{-\beta G} \times \left[ 1 + 4 \left[ 1 + \frac{1}{3} \frac{\Gamma'}{\Gamma} \right] \frac{T}{G} + \cdots \right], \quad (19)$$

where  $G = \Delta (1 - \xi^{2/3})^{3/2}$  the energy gap and  $\xi = \Gamma/\Delta$ . Note that  $\sigma_0(T_c) = 2(ev)^2 N_0 \Gamma_2^{-1}$  and  $\Pi(T_c) = \frac{2}{3} \pi^2 ev^2 N'_0 T^2 \Gamma_2^{-1}$ . Perhaps, the most remarkable is the condensed density f in the dynamical limit (see Fig. 3). It has a broad peak around  $T \sim 0.8 T_c$ . Further, this peak increases as  $l/\xi$  increases. At low temperature, f approaches unity as

$$f \simeq 1 - 2 \left[ \frac{2\pi T}{3\Delta} \right]^{1/2} \zeta^{-2/3} e^{-\beta G} \left[ 1 + \frac{\Gamma'}{\Gamma} \frac{T}{G} \right] .$$
 (20)



FIG. 1. The quasiparticle (Ohmic) conductivity  $\sigma_0(T)$  is shown as a function of temperature for a few values of  $\Gamma/\Delta_0=0.01$  (a), 0.05 (b), and 0.1 (c). The solid curves are for  $\Gamma_2=\frac{1}{2}\Gamma_1$  while the dashed curves are for  $\Gamma_2=\Gamma_1$ .



FIG. 2. The Peltier coefficient  $\Pi_c(T)$  is shown as a function of temperature for the same set of  $\Gamma_1$  and  $\Gamma_2$  as in Fig. 1.

The effective Peltier coefficient  $\Pi_c(T)$  associated with condensate first increases with decreasing temperature with a peak value  $(T_c/\Gamma)$  times larger than that at  $T = T_c$  and then decreases with decreasing temperature (see Fig. 4). In particular, at low temperatures

$$\Pi_{c}(T)/\Pi_{c}(T_{c}) \simeq \frac{\pi}{2} \left[ \frac{\pi G}{3T} \right]^{1/2} \left[ \frac{G}{\Gamma} \right] \times \left[ 1 + \frac{7\zeta(3)\Gamma_{2}}{\pi^{3}T_{c}} \right] \zeta^{-2/3} e^{-\beta G}$$
(21)

and

$$\Pi_{c}(T_{c}) = \pm \frac{4\sqrt{2}}{\pi e t_{a}}(\Gamma T) \left[1 - \frac{\pi \Gamma}{4T_{c}}\right] / \left[1 + \frac{7\zeta(3)\Gamma}{\pi^{3}T}\right].$$
(22)

Comparing Eq. (21) with Eq. (19), we conclude that at low temperatures in the non-Ohmic regime, the Peltier coefficient should be dominated by that due to the sliding CDW's or SDW's.

In terms of  $\sigma_0$ ,  $\Pi$ , f, and  $\Pi_c$ , the observed transport coefficients are expressed as

$$\delta j = j (E, \nabla T) - j (E, 0)$$
  
=  $-L_{12}(E) \nabla T / T^2$   
=  $\Gamma^{-1} \tilde{b} \theta (E - E_T) (\nabla T) T^{-1}$   
=  $\frac{\tilde{b}}{\tilde{a}} [J_{\text{CDW}}(E) / E] (\nabla T) T^{-1}$  (23)

or

$$L_{12}(E) = -\frac{\tilde{b}}{\tilde{a}} [J_{\text{CDW}}(E)/E]$$
$$= \mp \frac{\sqrt{2}}{et_a} (I_4/f) \frac{J_{\text{CDW}}(E)}{E} , \qquad (24)$$

while



FIG. 3. The condensate density f(T) is shown as a function of temperature for the same set of  $\Gamma_1$  and  $\Gamma_2$  as in Fig. 1.

$$L_{21}(E) = \mp \frac{\sqrt{2}}{et_s} (I_4/f) \frac{\partial J_{\text{CDW}}(E)}{\partial E} , \qquad (25)$$

where  $J_{CDW}(E)$  is the non-Ohmic current

$$j = \sigma_0 E + J_{\rm CDW}(E) . \tag{26}$$

This is essentially Artemenko's interpretation on the violation of Onsager's relation between  $L_{12}(E)$  and  $L_{21}(E)$  We believe that these new contributions should be considered as the anomalous term associated with moving SDW's (or CDW's) and which can carry both entropy and transverse current in the presence of an external magnetic field. Also, the ordinary CDW current contains the anomalous contribution of which temperature dependence is anomalous, as we have seen already.

### **IV. CONCLUDING REMARKS**

We have extended the nonlinear transport equation for SDW's (or CDW's) involving the heat current. The general form of the equation and the order of magnitudes of the transport coefficient agree with those deduced by Artemenko. The only exception is the sign of the anomalous contribution to the electric current. According to



FIG. 4. The Peltier coefficient associated with condensate  $\Pi_c(T)$  is shown as a function of temperature for the same set of  $\Gamma_1$  and  $\Gamma_2$  as in Fig. 1.

our analysis, the contributions from the regular term  $f_1$ and the anomalous term have the same sign and they have to be added up. Otherwise, the effective condensate density in the vicinity of  $T \simeq T_c$  should be negative since in this region the anomalous term dominates, which is clearly unphysical. In general, we conclude that the contribution of the anomalous term is most important in the vicinity of  $T \simeq T_c$ , though in the case of the Peltier coefficient, the anomalous term appears to dominate even at low temperatures (see Fig. 4).

Note added in proof. Recently Artemenko confirmed

our sign of the anomalous term. Therefore our result agrees completely with his.

### ACKNOWLEDGMENTS

One of us (K.M.) has benefited from stimulating discussions with G. Kriza and A. Janossy. He also thanks them for bringing an unpublished work by Artemenko to his attention. The present work is supported by the National Science Foundation under Grant No. DMR89-15285.

# APPENDIX: EVALUATION OF CORRELATION FUNCTIONS

First thermal products are calculated as

$$\langle [j,j] \rangle (\omega_{\nu}) = 2(ev)^{2} N_{0} T \sum_{n} \int d\xi d_{1}^{-2} d_{2}^{-2} (\xi^{2} - \tilde{\omega} \, \tilde{\omega}' - \tilde{\Delta} \, \tilde{\Delta}') \Lambda$$
  
$$= 2(ev)^{2} N_{0} \pi T \sum_{n} \left[ 1 - \frac{uu' + 1}{(u^{2} + 1)^{1/2} (u'^{2} + 1)^{1/2}} \right] [D(u,u')]^{-1}, \qquad (A1)$$

$$\langle [j^{h}, j] \rangle (\omega_{v}) = 2ev^{2}N_{0}'\pi T \sum_{n} \omega_{n}^{2} \left[ 1 - \frac{uu'+1}{(u^{2}+1)^{1/2}(u'^{2}+1)^{1/2}} \right] [D(u,u')]^{-1} , \qquad (A2)$$

$$\langle [j,\delta\Delta] \rangle(\omega_{\nu}) = 2ev N_0 \Delta \pi T \sum_{n} \frac{u - u'}{(u^2 + 1)^{1/2} (u'^2 + 1)^{1/2}} [D(u,u')]^{-1}, \qquad (A3)$$

$$\langle [j^{h}, \delta \Delta] \rangle(\omega_{v}) = 2v N_{0}' \Delta \pi T \sum_{n} \omega_{n}^{2} \frac{u - u'}{(u^{2} + 1)^{1/2} (u'^{2} + 1)^{1/2}} [D(u, u'1)]^{-1} , \qquad (A4)$$

where

$$d_{1}^{2} = \tilde{\omega}^{2} + \zeta^{2} + \tilde{\Delta}^{2}, \quad d_{2}^{2} = \tilde{\omega}'^{2} + \zeta^{2} + \tilde{\Delta}'^{2}, \quad (A5)$$

$$\Lambda = [\tilde{\Delta}(u^2 + 1)^{1/2} + \tilde{\Delta}'(u'^2 + 1)^{1/2}][D(u, u')]^{-1}$$
(A6)

$$D(u,u') = \Delta[(u^2+1)^{1/2} + (u'^2+1)^{1/2}] - \Gamma' \left[ 1 - \frac{uu'+1}{(u^2+1)^{1/2}(u'^2+1)^{1/2}} \right],$$
(A7)

$$\tilde{\omega} = \omega + \frac{1}{2} (\Gamma_1 + \Gamma_2) \frac{\tilde{\omega}}{(\tilde{\omega}^2 + \tilde{\Delta}^2)^{1/2}}, \quad \tilde{\Delta} = \Delta - \frac{1}{2} \Gamma_1 \frac{\tilde{\Delta}}{(\tilde{\omega}^2 + \tilde{\Delta}^2)^{1/2}}, \quad (A8)$$

and  $\tilde{\omega}$ ,  $\tilde{\omega}'$ , etc., refer to  $\omega_n$  and  $\omega_{n+v}$ , respectively. Then after analytical continuation, we obtain Eqs. (7)–(10) in the text.

- <sup>1</sup>See, for reviews on the CDW transport, P. Monceau, *Electronic Properties of Inorganic Quasi-One Dimensional Materials*, edited by P. Monceau (Reidel, Dordrecht, 1985), p. 139; G. Grüner and A. Zettl, Phys. Rep. **119**, 117 (1985).
- <sup>2</sup>L. Forró, J. R. Cooper, A. Janossy, and K. Kamarás, Phys. Rev. B **34**, 9047 (1986).
- <sup>3</sup>L. Forró, J. R. Cooper, A. Janossy, and M. Maki, Solid State Commun. 62, 715 (1987).
- <sup>4</sup>T. Osada, N. Miura, I. Oguro, and G. Saito, Phys. Rev. Lett. **58**, 1563 (1987).
- <sup>5</sup>G. Mihaly, G. Kriza, and G. Grüner, Solid State Commun. **68**, 993 (1988).
- <sup>6</sup>G. Kriza, A. Janossy, and L. Forró, Phys. Rev. B **41**, 5451 (1990).

- <sup>7</sup>S. N. Artemenko, E. N. Dolgov, A. N. Kruglov, Yu. I. Latshyev, Ya Savistskaya, and V. V. Frolov, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 258 (1985); Fiz. Tverd. Tela (Leningrad) **26**, 2391 (1985); S. N. Artemenko, Synth. Met. **36**, 381 (1990).
- <sup>8</sup>K. Yamaji, J. Phys. Soc. Jpn. 51, 2787 (1982); 52, 1361 (1983).

- <sup>10</sup>In the presence of a Coulomb interaction, Γ is essentially the quasiparticle damping term. See, for phenomenological analysis for CDW's, L. Sneddon, Phys. Rev. B 29, 719 (1984);
  P. B. Littlewood, *ibid.* 36, 3108 (1987).
- <sup>11</sup>J. Richard and J. Chen (private communication).
- <sup>12</sup>A. Virosztek and K. Maki, Phys. Rev. B **37**, 2028 (1988); K. Maki and A. Virosztek, *ibid.* **41**, 557 (1990).
- <sup>13</sup>A. Virosztek and K. Maki, Phys. Rev. B 41, 7055 (1990).

<sup>&</sup>lt;sup>9</sup>X-Z. Huang and K. Maki, Phys. Rev. B 42, 6498 (1990).