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Excess thermal conductivity at the charge- and spin-density-wave transitions

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The fluctuation contribution to the thermal conductivity in the vicinity of charge- and spin-density-wave (CDW and SDW) transitions is analyzed within microscopic models. We find a new term associated with the heat current, which gives rise to a cusp in the thermal conductivity in the chain direction at the CDW (or SDW) transition. Within the mean-field approximation the cusp is described as $\kappa(T)=\text{const}-\{32\pi^3T^2/[7\zeta(3)]^{3/2}\}(v_a/v_cv_b)\sqrt{\varepsilon}$ for the three-dimensional SDW system for $T>T_c$ where $\varepsilon=|1-T/T_c|$, $\zeta(3)=1.202\ldots$, and v_a,v_b,v_c are the Fermi velocities in the a (chain), b, and c directions. A similar expression is obtained for CDW, where the size of the cusp is $\frac{1}{2}$ of that for SDW. The present expression describes quite well the cusps in the thermal conductivity at the CDW transition of $K_{0.3}MoO_3$ and $(TaSe_4)_2I$ reported recently.

The fluctuation effect in the electric conductivity in the vicinity of the charge-density-wave (CDW) transition is now well established.[1-4] In particular, the sharp peaks in the temperature derivative of the electric conductivity $d\sigma/dT$ near the CDW transition in $NbSe_3$ and orthorhombic TaS_3 appear to be described in terms of the three-dimensional (3D) fluctuation, if they are interpreted in terms of the theory which includes the vertex renormalization.[4]

Recently it has been reported[5,6] that the thermal conductivity in the most conducting direction exhibits a peak at the CDW transition in $K_{0.3}MoO_3$ and $(TaSe_4)_2I$. This is somewhat surprising since application of the Wiedermann-Franz law would appear to predict a dip rather than a peak, if the conductivity is dominated by electron scattering[7] due to the fluctuation of the order parameter.

In order to solve this puzzle we examine the heat current in the chain direction associated with spin-density-wave (SDW) and CDW fluctuations within the quasi-one-dimensional model.[4] Following the standard procedure we find the heat current in the chain direction given by

$$j^h(\mathbf{x},t)=\frac{\pi}{8T_c}v_aN_0\sum_i\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial t'}\right)\Delta_i(\mathbf{x},t)\Delta_i(\mathbf{x},t')|_{t'=t}\,, \tag{1}$$

where N_0 is the electron density of states at the Fermi surface per spin and the suffix i on the order parameter runs from 1 to 4 for SDW (corresponding to 4 independent fluctuations; the real and imaginary parts of the SDW order parameter and 2 spin waves) and from 1 to 2 for CDW (there is no spin wave in CDW). This heat current gives rise to excess thermal conductivity where the entropy is carried by the fluctuation itself, like the Aslamazov-Larkin term[8] in the fluctuation-induced electric conductivity in a superconductor. The other term corresponding to the anomalous term,[9] which would give the term expected from the Wiedermann-Franz law, is absent, since the fluctuation affects only the quasiparticle in the immediate vicinity of the Fermi surface. We note that a very similar cancellation occurs in the thermal conductivity in the gapless superconductors.[10] Therefore we shall concentrate on the regular term.[8]

Making use of the fluctuation propagator[4] for $T>T_c$

$$D^{-1}(\mathbf{q},\omega_\nu)=N_0^{-1}\left(\varepsilon+\lambda(q)+\frac{\pi}{8T}|\omega_\nu|\right)^{-1} \tag{2}$$

we obtain for SDW

$$\begin{aligned}\langle[j^h,j^h]\rangle&=4\left(\frac{\pi}{8T_c}v_a\right)^2T\sum_n\int\frac{d^3q}{(2\pi)^3}(\omega_n+\omega_{n+\nu})^2\left(\varepsilon+\lambda(q)+\frac{\pi}{8T}|\omega_n|\right)^{-1}\left(\varepsilon+\lambda(q)+\frac{\pi}{8T}|\omega_{n+\nu}|\right)^{-1}\\&=2\pi\omega_\nu v_a^2\int\frac{d^3q}{(2\pi)^3}\left(\varepsilon+\lambda(q)+\frac{\pi}{8T}\omega_\nu\right)^{-1}\\&=\frac{\omega_\nu v_a^2}{\pi\xi_a\xi_b\xi_c}\left(1-\frac{\pi}{2}\sqrt{\varepsilon}\right)\ \text{for 3D}\end{aligned} \tag{3}$$

$$= \frac{\omega_v v_a^2}{2\pi\xi_a\xi_b C}\left[\sinh^{-1}\left(\frac{1}{\sqrt{K}}\right) - \sinh^{-1}\left(\frac{\varepsilon}{K}\right)^{1/2}\right] \quad \text{for 2D}\,, \tag{4}$$

where $\varepsilon = \ln(T/T_c)$, $K = (2\xi_c/c)^2$,

$$\lambda(q) = \xi_a^2 q_a^2 + \xi_b^2 q_b^2 + (2\xi_c/c)^2 \sin^2(\tfrac{1}{2} c q_3)\,,$$

and

$$\xi_i = [7\zeta(3)]^{1/2} v_i / 4\pi T\,. \tag{5}$$

The last term in $\lambda(q)$ can describe the two-dimensional limit when $K \leq 1$. Finally making use of the Kubo formula the excess thermal conductivity due to the fluctuation is given by

$$\kappa = \langle [j^h, j^h] \rangle / \omega_v T$$

$$= \text{const} - \frac{32\pi^3 T^2}{[7\zeta(3)]^{3/2}} \frac{v_a}{v_c v_b}\sqrt{\varepsilon} \quad \text{for 3D} \tag{6}$$

$$= \text{const} - \frac{8\pi T}{7\zeta(3)} \frac{v_a}{c v_b} \ln(\sqrt{\varepsilon} + \sqrt{K+\varepsilon}) \quad \text{for 2D}\,. \tag{7}$$

In CDW, the above expression has to be multiplied by $\frac{1}{2}$, since there are only two fluctuation modes. The cusps in the thermal conductivity at the CDW transition in $K_{0.3}MoO_3$ and $(TaSe_4)_2I$ appear to be well described by the 3D expression.

Now let us consider $T < T_c$. In SDW there are three gapless modes and one mode with a fluctuation propagator similar to the one given in Eq. (2) (i.e., the amplitude mode), while in CDW there are one gapless mode (phason) and the amplitude mode. Since these gapless modes give an almost temperature-independent contribution near $T \cong T_c$, we concentrate here on the amplitude mode. Within mean-field approximation the fluctuation propagator of the amplitude mode (or amplitudon) is given by Eq. (2) but ε is now given by[4]

$$\varepsilon = 2\ln(T_c/T)\,. \tag{8}$$

Therefore in CDW, the coefficient of $\sqrt{\varepsilon}$ for $T > T_c$ in Eq. (6) is reduced to $\sqrt{\varepsilon/2}$ for $T < T_c$, while in SDW it is reduced to $\frac{1}{2}\sqrt{\varepsilon/2}$. Again, this change in the cusp for $T > T_c$ and $T < T_c$ appears to be consistent with observation.[5,6]

In summary we obtain a new heat current associated with the SDW and CDW fluctuation, which gives rise to the square-root cusps in the thermal conductivity at the CDW and the SDW transition. On the other hand, the quasiparticle scattering due to the fluctuation does not give any singular term in the vicinity of the phase transition. The former term appears to account for the cusps observed in $K_{0.3}MoO_3$ and $(TaSe_4)_2I$. The present work indicates also that there will be new terms in the thermal conductivity associated with heat transport due to phasons. In order to analyze this we have to first generalize Eq. (1) for all temperatures for $T < T_c$.

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