Comment on “Quasiclassical Transport at a van Hove Singularity in Cuprate Superconductors”

In a recent Letter, Newns et al. [1] proposed that standard transport theory (STT) applied to a model of weakly interacting quasiparticles moving in a two-dimensional band structure with a van Hove singularity (VHS) close to the Fermi energy can explain the anomalous transport properties observed in the normal phase of the cuprate superconductors. However, we wish to point out that the weighting factors that enter STT (which are proportional to the change of the transported variable) are very important in this model and can change completely the predictions for transport coefficients.

The decay rate of a quasiparticle due to electron-electron interactions is anomalous as the energy separation $\mu$ of the VHS from the Fermi energy vanishes. However, in STT it is not this lifetime which is relevant. We have to consider weighted scattering probabilities [2]

$$p_{ij}^{el} = \frac{2\pi}{\hbar T} \sum_{k_1,...,k_G} V_{k_1-k_2} f_{k_1} f_{k_2} (1-f_{k_1}) (1-f_{k_2}) \left( \Phi_{k_1}^{(i)} + \Phi_{k_2}^{(i)} - \Phi_{k_1}^{(j)} - \Phi_{k_2}^{(j)} \right) \delta (\varepsilon_{k_1} + \varepsilon_{k_2} - \varepsilon_{k_1} - \varepsilon_{k_2}),$$

where $V_{k_1-k_2}$ is the scattering amplitude from $k_1, k_2$ to $k_3, k_4$, $\varepsilon_k$ is the quasiparticle dispersion, and $G$ is a reciprocal lattice vector. The weighting functions $\Phi_k^{(i)}$ describe the deviation of the electron distribution from its equilibrium value $f_k$. We consider $\Phi_k^{(i)} = v_k \cdot n$ and $\Phi_k^{(2)} = (\varepsilon_k - \mu) v_k \cdot n$ as the simplest descriptions of states carrying predominantly electric and heat current, respectively [2]; $n$ is a unit vector in the direction of the external field and $v_k = \partial \varepsilon_k / \partial k$. A state described by $\Phi_k^{(i)}$ carries both an electric current $J_i = \sum_k \Phi_k^{(i)} (\partial f_k / \partial \varepsilon_k)$ and a heat current $U_i = \sum_k \Phi_k^{(i)} (\partial f_k / \partial \varepsilon_k)$.

In STT the resistivity $\rho$ is given by $\rho = P_{1,1}/J_1^2$ [2]. If one considers intra-saddle-point electron-electron scattering and assumes a quadratic dispersion around the saddle point $\varepsilon_k = k_x k_y$, then the form of $\Phi_k^{(i)}$ leads to vanishing of $P_{1,1}$ and of resistivity. This result is exact due to the variational principle for the resistivity [2] and therefore we have to study inter-saddle-point scattering. The cuprates are modeled with two VHS located at $(\pm \pi, 0)$ and $(0, \pm \pi)$ in a square Brillouin zone. The resistivity in such a band structure is $\rho \propto T^2 \ln^2(1/T)$ [3].

Similarly, the treatment of the thermopower $S$ needs to be modified. In STT one finds [2]

$$S = \frac{1}{T} \sum_{i,j} J_i (P^{-1})_{i,j} U_j.$$

For intra-saddle-point electron-electron scattering, the only nonvanishing matrix element of $P_{i,j}$ is $P_{2,2}$ and the thermopower becomes independent of scattering: $S = U_1/TJ_1$. Assuming that $\mu_0 = \mu(T = 0) \ll D$ where $D = 10000$ K is the half bandwidth [1], we thus find

$$\frac{S}{S_0} = \begin{cases} \frac{2\pi^2}{3} \mu_0 D & , T \ll \mu_0, \\
\frac{2\pi}{D} \ln |D/\mu_0| & , T \gg D, \end{cases}$$

where $S_0 = k_B |\varepsilon_l| \approx 86 \mu V/K$. Numerical results smoothly interpolate between these two limits and there are no features in $S$ at intermediate temperatures. Thus, in agreement with Newns et al., $S$ changes sign with $\mu_0$. There are, however, two important differences with respect to Ref. [1]: (i) the magnitude of $S$ is substantially smaller (e.g., for $\mu_0/D = 0.05$ and $T/D < 0.05$, $S < 2 \mu V/K$) and (ii) the saturation of $S$ as a function of $T$ occurs only at very high temperatures (e.g., for $\mu_0/D = 0.05$, at $T/D = 1$). Both of these features disagree with the experimental results shown in Fig. 1 of Ref. [1]. It remains to be seen whether including the inter-saddle-point processes (not present in the model considered in Ref. [1]) changes the results for $S$.

Another difficulty with the VHS model concerns the effect of impurities. This will be discussed elsewhere [4].

In conclusion, we are led to question the proposal that standard transport theory applied to a VHS model yields results in agreement with experiment for the normal-state properties of the cuprate superconductors.

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