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Indications of coherence-incoherence crossover in layered metallic transport

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For many strongly correlated metals with layered crystal structure the temperature dependence of the interlayer resistance is different to that of the intralayer resistance. We consider a small polaron model which exhibits this behavior, illustrating how the interlayer transport is related to the coherence of quasiparticles within the layers. Explicit results are also given for the electron spectral function, interlayer optical conductivity, and the interlayer magnetoresistance. All these quantities have two contributions: one coherent (dominant at low temperatures) and the other incoherent (dominant at high temperatures).

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Many of the most interesting strongly correlated electron materials have a layered crystal structure and highly anisotropic electronic properties. Examples include the cuprates,[1] colossal magnetoresistance materials,[2] organic molecular crystals,[3,4] strontium ruthenate,[5] and cobalt oxides.[6] One poorly understood property is that the resistivity perpendicular to the layers can have quite a different temperature dependence to that parallel to the layers.[7] This is in contrast to what is expected for an anisotropic Fermi liquid: the parallel and perpendicular resistivities then have the same temperature dependence, being determined by the intralayer scattering rate $\Gamma(T)$. In many of these materials the interlayer resistivity is a nonmonotonic function of temperature with a maximum at some temperature $T_\perp^{\max}$. In some of the materials the intralayer resistivity also has a maximum as a function of temperature, but at a higher temperature $T_\parallel^{\max} > T_\perp^{\max}$.[2,4,5] An important question concerns how the interlayer transport is effected by the coherence (or existence) of quasiparticles within the layers.[6,7] Recent angle-resolved photoemission spectroscopy (ARPES) experiments on two different layered cobalt oxide compounds[6] found that peaks were only observed in the electronic spectral function (corresponding to coherent quasiparticle excitations within the layers) below a temperature T^{coh} that was comparable to $T_\perp^{\max}$. Although many theoretical papers have considered the problem of interlayer transport (see Ref. 8 and references therein) we are unaware of any theory which starts with a many-body Hamiltonian and produces the three temperature scales T^{coh}, $T_\perp^{\max}$, and $T_\parallel^{\max}$.[9,10]

In this Rapid Communication we consider a simple microscopic model which elucidates the connection between interlayer transport and the coherence of quasiparticles. We find that the interlayer conductivity has two contributions. The coherent (incoherent) contribution is characterized by the intralayer momentum of the quasiparticle being (not being) conserved in the interlayer tunneling process and is dominant at low (high) temperatures. We show that experimentally the two different contributions could be clearly distinguished at finite frequencies or in a magnetic field parallel to the layers. The model is a layered version of Holstein's molecular crystal model where the electrons strongly couple to bosonic excitations to produce small polarons. We are not claiming that the charge transport involves small polarons in *all* of the above materials. Rather, we suggest that this model can provide insight into the relevant physics associated with these temperature scales and its connection to coherence.[11]

We consider the regime where $\Gamma > t_\perp$ and so we need to only consider two layers. Within each layer the electrons can hop but there is a coupling to a bosonic degree of freedom in each layer. The bosons can be phonons, or any boson coupling to the charge. We only consider a single bosonic frequency ω_0 since it allows us to express our results in analytical form. The two layers are coupled via interlayer hopping $t_\perp$. The Hamiltonian is

$$\begin{aligned}\mathcal{H} = {} & \hbar\omega_0 \sum_i a_i^\dagger a_i + t_\parallel \sum_{\langle i\eta\rangle} c_\eta^\dagger c_i + M \sum_i c_i^\dagger c_i (a_i + a_i^\dagger) \\ & + \hbar\omega_0 \sum_j b_j^\dagger b_j + t_\parallel \sum_{\langle j\delta\rangle} d_\delta^\dagger d_j + M \sum_j d_j^\dagger d_j (b_j + b_j^\dagger) \\ & + t_\perp \sum_i (c_i^\dagger d_i + \mathrm{H.c.}).\end{aligned}$$

Electrons and bosons at site i in the first layer are created by $c_i^\dagger$ and $a_i^\dagger$, respectively. $d_i^\dagger$ and $b_i^\dagger$ are the corresponding operators for the second layer. $t_\parallel$ is the hopping integral between nearest-neighbor sites i and η within the same layer ($t_\parallel \gg t_\perp$) and M is the coupling between the bosons and the electrons. We introduce a dimensionless coupling $g = (M/\hbar\omega_0)^2$ and assume that $g \gg 1$ in order for small polaronic effects to be important. It should be stressed that the Hamiltonian is such that the intralayer momentum of electrons is conserved in interlayer hopping. However, we will see below that due to many-body effects the intralayer momentum of quasiparticles is not always conserved.

First we focus on the properties of the two individual layers. We perform a Lang-Firsov transformation[12,13] to remove the coupling of the electrons to the bosons. Then $c_i \to \tilde{c}_i = c_i X_i$ and $a_i \to a_i - (M/\hbar\omega_0) c_i^\dagger c_i$, where X is a polaron operator.[17] The Hamiltonian is transformed to $\bar{\mathcal{H}} = e^S \mathcal{H} e^{-S}$ where $S = (M/\hbar\omega_0)\Sigma_i c_i^\dagger c_i (a_i^\dagger - a_i)$. A similar transformation is made for the second layer. This diagonalizes the electron-boson part of the Hamiltonian, but introduces extra X-operators in the hopping parts of the Hamiltonian. The intralayer term is treated by adding and subtracting from the Hamiltonian a term which describes a tight-binding band of small polarons within each layer,[12,14] $\epsilon_{\mathbf{k}} = \mu - e^{-g(1+2n_B)} t_{\parallel}[\cos(k_x a) + \cos(k_y a)]$, where μ is the chemical potential, a is the lattice constant within the layers, and $n_B(T) = [\exp(\hbar\omega_0/k_B T) - 1]^{-1}$ is the Bose function. There is then a residual interaction[14] between the polarons and the bosons, which leads to scattering of the polarons. The first nonzero contribution to the imaginary part of the polaron self-energy comes when the polaron emits one boson and absorbs one boson. For an energy independent density of states (DOS) one finds that[14]

$$\Gamma(T) = W g^2 n_B(T)[1 + n_B(T)] \equiv W[\tilde{g}(T)]^2, \tag{1}$$

where W is the renormalized bandwidth, $W = 4t_{\parallel} e^{-g(1+2n_B)} \equiv 4t_{\parallel} Z(T)$,[12,14,17] and we have defined a temperature-dependent coupling $\tilde{g}(T)$ and a renormalization factor $Z(T)$.

Note that the small polarons are composite particles (quasiparticles). They consist of an electron bound to a "cloud" of bosons. This coherent quantum state can move freely within the layers producing coherent charge transport. In contrast, ARPES involves ejection of electrons rather than polarons from the crystal. Similarly, the interlayer charge transport involves the tunneling of electrons between layers. In order for this to occur the bosons bound to the electron in the polaron must be removed, the electron tunnels, and a new set of bosons is bound to the electron.

Electronic spectral function within a single layer. The electron GF $G(\mathbf{k}, i\omega_n)$ involves a convolution of the polaron GF $G^0(\mathbf{k},\omega) = (\omega - \epsilon_{\mathbf{k}} + i\Gamma)^{-1}$ with the Fourier transformed X-operators.[15] The electronic spectral function $A(\mathbf{k},\omega) = \mathrm{Im}[G(\mathbf{k},\omega)]$ can be expressed in terms of the polaron spectral function $A^0(\mathbf{k},\omega)$ and the density of states $\rho^0(\omega) = \Sigma_{\mathbf{k}'} A^0(\mathbf{k}',\omega)$ for the polaron band,

$$A(\mathbf{k},\omega) = Z(T)\Bigg\{ A^0(\mathbf{k},\omega) + \{I_0[2\tilde{g}(T)] - 1\}\rho_0(\omega) + \sum_{l \neq 0} I_l[2\tilde{g}(T)] e^{-l\hbar\omega_0\beta/2} \rho_0(\omega + l\hbar\omega_0) \Bigg\}. \tag{2}$$

I_l is a modified Bessel function of order l. Note that the spectral function is a sum of a coherent and a incoherent part, i.e., the second term in the first row and in the second row are *independent* of $\mathbf{k}$.[15] In Fig. 1 we plot the electron spectral function, Eq. (2), for different temperatures. With increasing temperature the boson modes become populated, $n_B(T)$ increases, and the spectral weight shifts from the coherent part of the spectral function to the incoherent part. Qualitatively similar behavior was seen in recent ARPES (Ref. 6) measurements. This behavior does not change much qualitatively when g is changed. From plots we estimated that the crossover takes place at

$$k_B T^{\mathrm{coh}} \sim \frac{\hbar\omega_0}{2g}. \tag{3}$$

This can also be justified using Eq. (2) when $W < \hbar\omega_0$.

Interlayer conductivity. Standard techniques can be used to derive an expression for the current perpendicular to the layers.[16,17] Since the bosons in separate layers are independent of one another we can decouple the X polaron operators corresponding to the first and second layers. This means that the Fourier transformed averages of the electron operators give rise to two GF's. These GF's describe polaron bands within each layer. The final result is

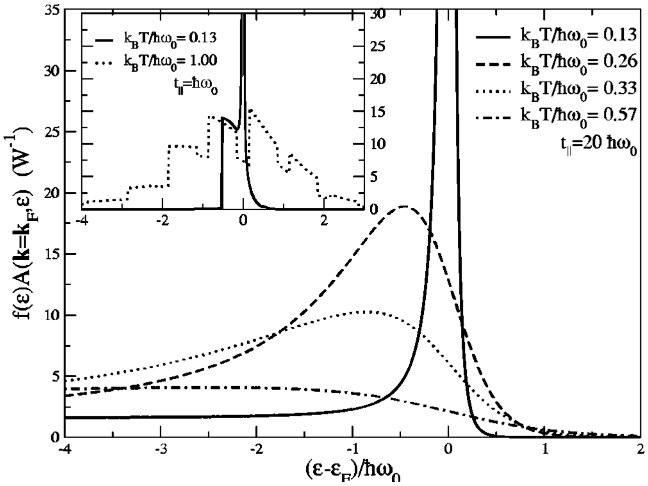

FIG. 1. Energy dependence of the electron spectral function at a wave vector on the Fermi surface, using a constant DOS. The product of the spectral function $A(\mathbf{k}_F, \epsilon)$ with the Fermi-Dirac distribution function $f(\epsilon)$ is shown because this can be compared with ARPES spectra. Note that the well-defined quasiparticle peak which occurs for $k_B T \ll \hbar\omega_0$ disappears at higher temperature. The results are shown for $g = 1$. The inset shows the same quantities for a smaller bandwidth.

$$\sigma_{\perp} = \frac{2e^2}{h} t_{\perp}^2 \frac{d}{S} Z(T)^2 \Bigg\{ \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \left[\frac{-df(\epsilon)}{d\epsilon} \right] \times \left(\sum_{\mathbf{k}} A^0(\mathbf{k},\epsilon)^2 + \{I_0[4\tilde{g}(T)] - 1\}\rho^0(\epsilon)^2 \right) + \sum_{\substack{l \neq 0 \\ l=-\infty}}^{\infty} I_l[4\tilde{g}(T)] e^{-l\hbar\omega_0\beta/2} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \rho^0(\epsilon) \times \left(\frac{d\rho^0(\epsilon + l\hbar\omega_0)}{d\epsilon} [f(\epsilon) - f(\epsilon + l\hbar\omega_0)] + \rho^0(\epsilon + l\hbar\omega_0) \left[\frac{-df(\epsilon)}{d\epsilon} \right] \right) \Bigg\}, \tag{4}$$

where d is the distance between the two layers and S is the area of the unit cell. Note the similarity in structure between Eqs. (2) and (4). The first term corresponds to tunneling where the momentum of the polaron parallel to the layers is conserved. In the second, third and fourth terms the intralayer momentum is not conserved. The second line has an energy difference, of $l\hbar\omega_0$ between the polarons in the two layers because there is a nonzero difference l between the net number of bosons that are absorbed and emitted in the two layers. At low temperature the coherent part dominates but at

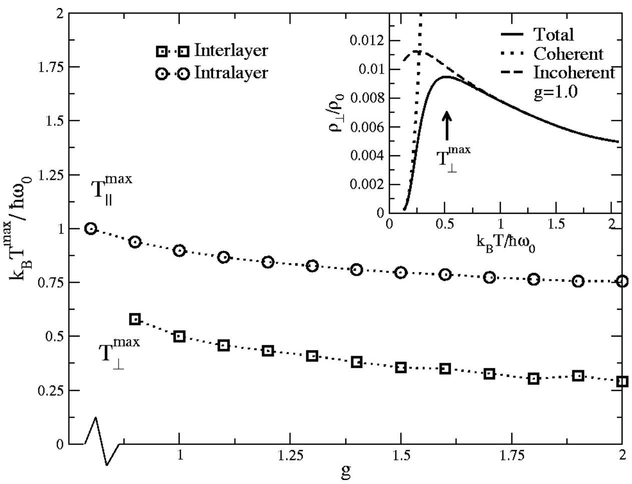

FIG. 2. Peak temperature in the resistivity as a function of coupling. Results obtained using a tight-binding DOS (no major change was seen when using a constant DOS). The two sets of data points are for the intralayer and the interlayer crossover temperatures, respectively. The intralayer crossover occurs at much higher temperatures than the interlayer. The inset shows the interlayer conductivity as a function of temperature when $g=1$ and $t_\parallel=20\hbar\omega_0$. $\rho_0=h/[2e^2(d/S)(t_\perp/t_\parallel)^2]$.

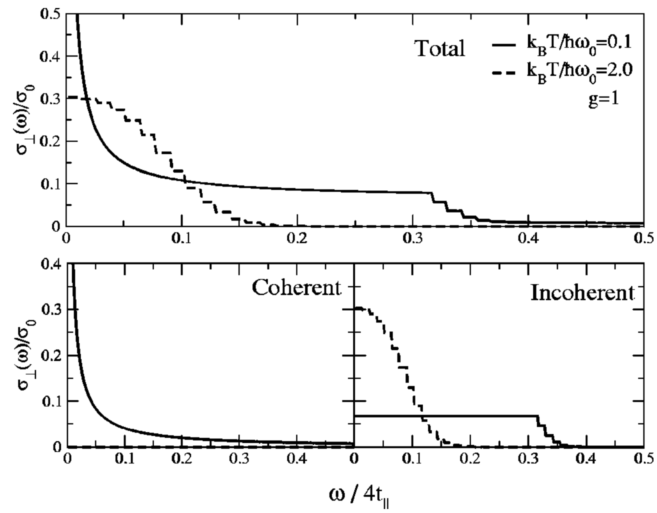

FIG. 3. Optical conductivity divided into the two contributions, coherent and incoherent, plotted for two different temperatures. In the lower left panel we plot the coherent part and in the right the incoherent part. $\sigma_0=2e^2(d/S)(t_\perp/t_\parallel)^2/h$.

high temperature ($k_BT>\hbar\omega_0$) the incoherent mechanism of transport will dominate. Thus, there is a *crossover* from coherent to incoherent transport.

We can estimate the temperature of the crossover in the conductivity. If we look at the conductivity there is a minimum (maximum in the resistivity, $\rho_\perp=\sigma_\perp^{-1}$), corresponding to the crossover (see inset of Fig. 2). Ignoring the contribution from the $l\neq 0$ terms in Eq. (4) we can get an approximate expression

$$k_BT_\perp^{\max}\sim 0.6\frac{\hbar\omega_0}{g}. \tag{5}$$

This expression compares quite well to the crossover temperature extracted from a numerical plot of the resistivity versus temperature in Fig. 2. Hence, we see that T^{coh} and $T_\perp^{\max}$ are comparable. At these temperatures, $\Gamma\sim 0.3W$, justifying the assumption of a band of polarons within each layer (see below). Note that the coherent and incoherent contributions are actually comparable at a temperature *lower* than $T_\perp^{\max}$, as can be seen in the inset of Fig. 2. This is because the $l\neq 0$ terms depend only weakly on temperature.

Intralayer conductivity. When we calculated the current between the layers we assumed that the small polaron band was well defined. However, it is known that even within the layer, as the temperature increases, there is a crossover from coherent to incoherent transport, occurring at $T_\parallel^{\max}$, and there is a maximum in the resistivity associated with this crossover.[17] An important question is the size of $T_\parallel^{\max}$ relative to $T_\perp^{\max}$.

Many authors have previously considered the crossover from band to hopping transport in an isotropic crystal, and this work has been reviewed by Appel.[18] At low temperatures ($\Gamma\ll W$) the transport in the layers is coherent, and decided by standard expressions derived from Boltzmann theory. We assume that we have well-developed quasiparticles in the layers and the polaron-boson interaction acts as a small perturbation.[12,14] At high temperatures ($\Gamma\gg W$) the electrons are localized at the lattice sites and the concept of a wave vector for the small polaron is meaningless. The intralayer hopping term in the Hamiltonian should then be treated as the perturbation. We make use of Holstein's expression [Eq. (13.66) in Ref. 18]. The conductivity for the low- and high-temperature regions were plotted and the crossover extracted. The intralayer crossover occurs at higher temperatures than the interlayer crossover and so the assumption made above that for the interlayer calculation we have well-developed quasiparticles within each layer is justified. This result was still valid even when we used $t_\parallel<\hbar\omega_0$.[13]

Optical conductivity. The frequency dependence of the interlayer optical conductivity $\sigma_\perp(\omega)$ has been suggested to be a probe of interlayer coherence in the metallic state.[19] The optical conductivity can be found from a straightforward generalization of the techniques used for the dc conductivity.[17,20] Figure 3 shows how at low temperatures there is a well-defined Drude peak at zero frequency due to coherent interlayer transport of small polarons. The width of this feature is approximately Γ. Note that this feature occurs even though $\Gamma>t_\perp$, as has been pointed out previously.[20] As the temperature increases the spectral weight of this feature decreases and is replaced with a broader feature associated with incoherent interlayer transport and with a width that is determined by the small polaron bandwidth *within* the layers. The incoherent part becomes narrower with increasing temperature because of the polaron narrowing of the bands. Changing g and $t_\parallel$ does not qualitatively change this behavior.

Magnetoresistance. If we apply a magnetic field B parallel to the layers (the x-y plane) we have an orbital effect on the paths of the electrons. This can be described by a shift in the Bloch wave vector $\mathbf{k}\rightarrow\mathbf{k}-(e/\hbar)\mathbf{A}$, where $\mathbf{A}$ is the vector potential for the magnetic field. For a magnetic field in the x direction, when an electron tunnels between adjacent layers it undergoes a shift in the y component of its wave vector by $-dB$.[16] In the derivation of $\sigma_\perp$ $A^2(\mathbf{k},\epsilon)$ is replaced with $A(\mathbf{k},\epsilon)A(\mathbf{k}+(e/\hbar)dB\vec{y})$.[16] However, since the incoherent part of the conductivity contains separate summations over $\mathbf{k}$ space for the two layers this will be unaffected by the magnetic field. Thus, we will have two contributions to the interlayer conductivity and one is B independent:

$$\sigma_\perp(B)=\sigma_\perp^{\mathrm{coh}}(B)+\sigma_\perp^{\mathrm{incoh}}(B=0). \qquad (6)$$

$\sigma^{\mathrm{coh}}(B)$ decreases with increasing magnetic field.[21] If we increase B, the coherent part decreases, and, therefore, $T_\perp^{\max}$ would shift to lower values. A separation of the conductivity in two parts, as in Eq. (6), has been proposed previously on a phenomenological basis, in order to describe the magnetoresistance of Sr_2RuO_4 (Ref. 5) (Except there a weak-field dependence is associated with the incoherent contribution due to Zeeman splitting).[22]

We have shown that a small polaron model for transport in layered systems shows a crossover from coherent to incoherent transport at different temperatures for intralayer and interlayer transports. The crossover can be observed in ARPES, as well as in measurements of magnetoresistance and optical conductivity. It is sometimes suggested (or assumed) that the maximum in the interlayer resistivity as a function of temperature occurs at a temperature $T_\perp^{\max}$ determined by the strength of the interlayer hopping $t_\perp$, either by $k_BT_\perp^{\max}\sim t_\perp$ or $\Gamma(T_\perp^{\max})\sim t_\perp$ where $\Gamma(T)$ is the temperature-dependent scattering rate within the layers. However, we find that $T_\perp^{\max}$ can occur at a higher temperature, which is actually independent of $t_\perp$, and instead closely related to T^{coh}.

Note added. After completion of this work we became aware of related work by Ho and Schofield concerning a small polaron model for interlayer transport (Ref. 23).

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