

Transport Theory Cookbook for Cuprates

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This document summarize the mathematical relations between electronic transport coefficients, and shows how to compute them in the semi-classical approximation. We start with Chamber's formula and give the steps and approximations needed to get back to the Drude formula, and we obtain many useful intermediate special cases results in between. All transport coefficient ultimately depend on only two parameters: the lifetime $\tau_{\mathbf{k}}$ and the dispersion $E(\mathbf{k})$ describing the material. The last section define such a dispersions and lifetime appropriate to evaluate baseline transport results in cuprates.

CONTENTS

I. Conductivity tensors	2
A. Resistivity & Hall effect	3
B. Thermoelectricity: Seebeck, Pelletier & Nernst effects	4
C. Thermal conductivity & Righi-Leduc effect	4
D. Example of interpretation for the Seebeck effect	4
E. Note on the strongly correlated case	5
II. Complete Semi-classical formulas	6
III. Simplifications	7
A. Equi-energy surfaces	7
B. Zero Magnetic field	8
C. Effective mass and Drude results	8
D. Zero temperature	9
IV. For cuprates	10
A. Bare dispersion	10
B. Approximation for the pseudogap	10
C. Lifetime	11
References	12

I. CONDUCTIVITY TENSORS

Three conductivity tensors L_{11} , L_{12} , and L_{22} suffice to determine all electronic transport coefficients. They are tensors because they express the relations between x, y, z components of: the electric current \mathbf{j}_e , the heat current \mathbf{j}_Q , the electric field \mathbf{E} , and the Temperature gradient ∇T [1, 2]:

$$\mathbf{j}_e = L_{11} \mathbf{E} + L_{12} (-\nabla T), \quad (1)$$

$$\mathbf{j}_Q = L_{21} \mathbf{E} + L_{22} (-\nabla T). \quad (2)$$

These tensors depend on temperature T and magnetic field \mathbf{B} , satisfying the Onsager relations: $L_{11}(\mathbf{B}) = L_{11}^\top(-\mathbf{B})$, $L_{22}(\mathbf{B}) = L_{22}^\top(-\mathbf{B})$, and $L_{12}(\mathbf{B}) = -TL_{21}^\top(-\mathbf{B})$. Since the latter defines L_{21} from L_{12} , we can disregard L_{21} . These tensors' components are usually written:

$$[L_{11}]_{ij} = \sigma_{ij}, \quad (3)$$

$$[L_{12}]_{ij} = \alpha_{ij}, \quad (4)$$

$$[L_{22}]_{ij} = \beta_{ij}, \quad (5)$$

with i, j denoting x, y, z . In almost all cases, these can be computed as energy integrals of the same energy function $\sigma_{ij}(\epsilon)$, which we view here as a *density of conductivity*:

$$\sigma_{ij} = \int_{-\infty}^{\infty} d\epsilon \left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \sigma_{ij}(\epsilon) \quad (6)$$

$$\alpha_{ij} = \int_{-\infty}^{\infty} d\epsilon \left[\left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \frac{\epsilon}{T} \right] \frac{\sigma_{ij}(\epsilon)}{-e} \quad (7)$$

$$\beta_{ij} = \int_{-\infty}^{\infty} d\epsilon \left[\left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \frac{\epsilon^2}{T} \right] \frac{\sigma_{ij}(\epsilon)}{e^2} \quad (8)$$

$$C_V = \int_{-\infty}^{\infty} d\epsilon \left[\left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \frac{\epsilon^2}{T} \right] N(\epsilon). \quad (9)$$

with $-e$ as the electron charge. The name “density of conductivity” for $\sigma_{ij}(\epsilon)$ is not standard. I chose it because, as seen above, the specific heat C_V can be computed from an identical integral, but with the density of states $N(\epsilon)$ taking the place of this $\sigma_{ij}(\epsilon)$. In the integrals above, $\sigma_{ij}(\epsilon)$ is always weighted by the derivative of the Fermi-Dirac distribution $f(\epsilon)$:

$$f(\epsilon) = \frac{1}{e^{\epsilon/k_B T} + 1}. \quad (10)$$

The various functions seen in the brackets of (6), (7), (8), and (9) are illustrated in Fig. 1 for various temperature T . Here are useful identities regarding these functions:

$$\frac{\partial f(\epsilon)}{\partial \epsilon} = -\frac{T}{\epsilon} \frac{\partial f(\epsilon)}{\partial T} = \frac{1}{4 \cosh^2(\epsilon/k_B T)}. \quad (11)$$

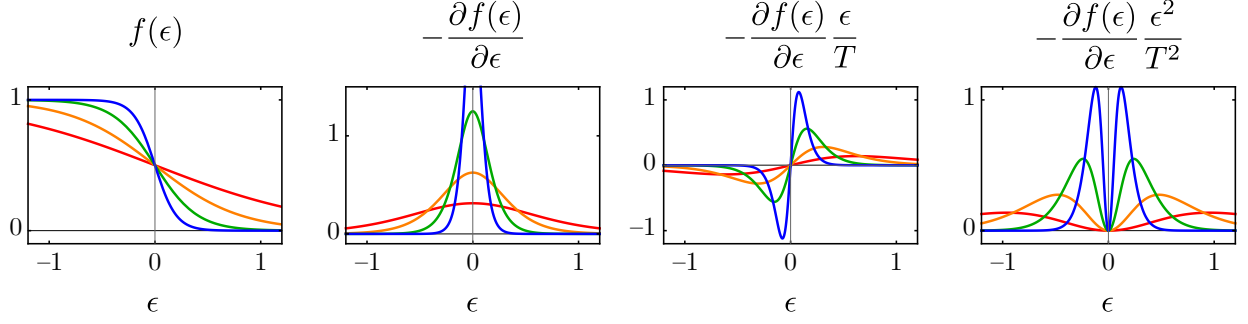


FIG. 1. Weighting functions involved in the expressions of transport coefficients, shown at temperatures $k_B T = 0.8$ (red), $k_B T = 0.4$ (orange), $k_B T = 0.2$ (green), $k_B T = 0.1$ (blue)

Such functions are non-zero only in a narrow window surrounding the Fermi level (at $\epsilon = 0$ in our convention). This is why we often only care about the Fermi surface when studying transport. We can displace the Fermi energy by considering $\epsilon = E_{\mathbf{k}} - \mu$, where the chemical potential μ controls the expected number of particles n filling the band $E_{\mathbf{k}}$ (with hole doping $p = 1 - n$).

The remaining sections of this document explain how to compute $\sigma_{ij}(\epsilon)$ in various limit of the semi-classical approximation. First, however, let us define the usual measurable transport coefficients (resistivity, Hall coefficient, Seebeck coefficient, etc.) in 2D, and give an example of how one can use the above formulation to think about those coefficients in cuprates, by comparing the resistivity and the Seebeck coefficient.

A. Resistivity & Hall effect

The resistivity tensor $\boldsymbol{\rho}$ is defined as L_{11}^{-1} .

$$\boldsymbol{\rho} \equiv L_{11}^{-1} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}^{-1} = \frac{1}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \begin{pmatrix} \sigma_{yy} & -\sigma_{xy} \\ -\sigma_{yx} & \sigma_{xx} \end{pmatrix} \quad (12)$$

with longitudinal resistivity is then given as:

$$\rho_{xx} = \frac{\sigma_{yy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \approx \boxed{\frac{1}{\sigma_{xx}}}, \quad (13)$$

where σ_{xy} and σ_{yx} are usually only non-zero under magnetic field \mathbf{B} , are usually very small, and give rise to the transverse resistivity:

$$\rho_{xy} = \frac{-\sigma_{xy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \approx \boxed{\frac{-\sigma_{xy}}{\sigma_{xx}\sigma_{yy}}}. \quad (14)$$

From the latter, the Hall coefficient, R_H and the Hall number, n_H , are defined as:

$$R_H = \frac{-\rho_{xy}}{B} \quad n_H = \frac{1}{-eR_H}. \quad (15)$$

B. Thermoelectricity: Seebeck, Pelletier & Nernst effects

The thermoelectricity tensor \mathbf{Q} is defined as:

$$\mathbf{Q} \equiv L_{11}^{-1} L_{12} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}^{-1} \begin{pmatrix} \alpha_{xx} & \alpha_{xy} \\ \alpha_{yx} & \alpha_{yy} \end{pmatrix} = \begin{pmatrix} \frac{\sigma_{yy}\alpha_{xx} - \sigma_{xy}\alpha_{yx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} & \frac{\sigma_{yy}\alpha_{xy} - \sigma_{xy}\alpha_{yy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \\ \frac{\sigma_{xx}\alpha_{yx} - \sigma_{yx}\alpha_{xx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} & \frac{\sigma_{xx}\alpha_{xy} - \sigma_{yx}\alpha_{yy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \end{pmatrix} \quad (16)$$

Therefore, the Seebeck coefficient corresponds to:

$$S_x \equiv Q_{xx} = \frac{\sigma_{yy}\alpha_{xx} - \sigma_{xy}\alpha_{yx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \approx \boxed{\frac{\alpha_{xx}}{\sigma_{xx}}} \quad (17)$$

And the Nernst coefficient is given by:

$$N \equiv Q_{xy} = \frac{\sigma_{yy}\alpha_{xy} - \sigma_{xy}\alpha_{yy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \approx \boxed{\frac{\alpha_{xy}}{\sigma_{xx}} - S_y \frac{\sigma_{xy}}{\sigma_{xx}}} \quad (18)$$

C. Thermal conductivity & Righi-Leduc effect

In the same way, the thermal conductivity κ can be obtained from:

$$\kappa \equiv -L_{22} + T L_{12} L_{11}^{-1} L_{12} \quad (19)$$

which yields thermal conductivity:

$$\kappa_{xx} = T \left(\frac{\alpha_{xx}\sigma_{yy}\alpha_{xx} - \alpha_{xx}\sigma_{xy}\alpha_{yx} - \alpha_{xy}\sigma_{yx}\alpha_{xx} + \alpha_{xy}\sigma_{xx}\alpha_{yx}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \right) - \beta_{xx} \quad (20)$$

$$\approx T \left(\frac{\alpha_{xx}^2}{\sigma_{xx}} + \frac{\alpha_{xy}\alpha_{yx}}{\sigma_{yy}} \right) - \beta_{xx} \quad (21)$$

and the Righi-Leduc (or thermal Hall) coefficient:

$$\kappa_{xy} = T \left(\frac{\alpha_{xx}\sigma_{yy}\alpha_{xy} - \alpha_{xx}\sigma_{xy}\alpha_{yy} - \alpha_{xy}\sigma_{yx}\alpha_{xy} + \alpha_{xy}\sigma_{xx}\alpha_{yy}}{\sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx}} \right) - \beta_{xy} \quad (22)$$

$$\approx T \left(\frac{\alpha_{xx}\alpha_{xy}}{\sigma_{xx}} + \frac{\alpha_{xy}\alpha_{yy}}{\sigma_{yy}} \right) - \beta_{xy} \quad (23)$$

D. Example of interpretation for the Seebeck effect

When substituting the expressions the resistivity (13) for ρ_{xx} and (7) for α_{xx} in the reduced expression for the Seebeck coefficient (17), one gets a particularly revealing expression regarding

the density of conductivity $\sigma_{xx}(\epsilon)$:

$$S_x = \frac{\alpha_{xx}}{\sigma_{xx}} = \frac{\rho_{xx}}{-eT} \int_{-\infty}^{\infty} d\epsilon \left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \epsilon \sigma_{xx}(\epsilon). \quad (24)$$

In this expression, we can see that if $\sigma_{xx}(\epsilon)$ is even with respect to the Fermi-level, *i.e.* $\sigma_{xx}(-\epsilon) = \sigma_{xx}(\epsilon)$ within the narrow energy window determined by $-\frac{\partial f(\epsilon)}{\partial \epsilon}$, then, because of the extra ϵ in the integral, the integrand is perfectly odd and the Seebeck coefficient should be zero. Thus, any non-zero Seebeck effect must come from an assymetry in the density of conductivity $\sigma_{xx}(\epsilon)$ with respect to the Fermi level.

Equation 24 is particularly relevant to cuprates, regarding the pseudogap transition occuring at doping p^* . At low temperature, an abrupt augmentation of the resistivity ρ_{xx} is observed at p^* . Since resistivity explicetely enters expression (24), an equivalent augmentation is expected in the Seebeck effect, given the latter is non-zero. However, a comparison between the augmentation in ρ_{xx} and the augmentation in S_x might reveal a lot more. Namely, if the p^* transition causes $\sigma_{xx}(\epsilon)$ to change symetrically in energy with respect to the Fermi level, then the only effect in S_x will come from ρ_{xx} , because the ϵ would make the symmetric changes of the transition an odd contribution in the integral of (24), which would cancel out. In that case, the Seebeck augmentation should track the resistivity augmentation exactly. On the other hand, if the change in $\sigma_{xx}(\epsilon)$ is assymetric with respect to the Fermi level, then there will be a difference between the augmentations in S_x and that in ρ_{xx} . Note that in either cases, the Seebeck effect can remain nonzero at all times, given a sufficiently assymetric $\sigma_{xx}(\epsilon)$; only the evenness or oddness of *the changes* brought by the transition are relevant.

E. Note on the strongly correlated case

The above analysis remains mostly valid in the strongly correlated case. As we we will see in the next section, the non-interacting, zero-field $\sigma_{xx}(\epsilon)$ is:

$$\sigma_{xx}(\epsilon) = e^2 \iiint_{\text{BZ}} \frac{d^3k}{(2\pi)^3} v_x(\mathbf{k})^2 \tau_{\mathbf{k}} \delta(\epsilon - E(\mathbf{k})), \quad (25)$$

In the strongly correlated case, $\sigma_{xx}(\epsilon)$ would be the current-current correlation function, given in first approximation by:

$$\sigma_{xx}(\epsilon) = e^2 \iiint_{\text{BZ}} \frac{d^3k}{(2\pi)^3} v_x(\mathbf{k})^2 \pi \hbar A(\mathbf{k}, \epsilon)^2, \quad (26)$$

where $A(\mathbf{k}, \epsilon)$ is the spectral weight.

The above correspondence for the longitudinal conductivity has an analogous one for the transverse conductivity (not shown here, please refer to [3]). These correspondence between non-interacting and interacting transport functions suggests the following heuristic:

$$\tau_{\mathbf{k}}\delta(\epsilon - E(\mathbf{k})) \longleftrightarrow \pi\hbar A(\mathbf{k}, \epsilon)^2 \quad (27)$$

$$\tau_{\mathbf{k}}^2\delta(\epsilon - E(\mathbf{k})) \longleftrightarrow \frac{\pi^2\hbar^2}{3}A(\mathbf{k}, \epsilon)^3 \quad (28)$$

to go from one to the other. This might be useful to guide more rigorous derivation of strongly correlated formulas.

II. COMPLETE SEMI-CLASSICAL FORMULAS

To get full magnetic field dependence in $\sigma_{ij}(\epsilon)$, one must use the Chambers Formula [1]:

$$\sigma_{ij}(\epsilon) = e^2 \iiint_{\text{BZ}} \frac{d^3k}{(2\pi)^3} v_i(\mathbf{k}) \bar{v}_j(\mathbf{k}) \delta(\epsilon - E(\mathbf{k})), \quad (29)$$

which is an integral on all \mathbf{k} -states in the first Brillouin zone (BZ). The Dirac delta indicates that each states only contributes to this “density of conductivity” at the energy $E(\mathbf{k})$. The weight of this contribution is given by a component of the group velocity $\mathbf{v}(\mathbf{k})$:

$$v_i(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial E(\mathbf{k})}{\partial k_i}, \quad (30)$$

multiplied by a “decaying” or “travelling” velocity, $\bar{v}_j(\mathbf{k})$:

$$\bar{v}_j(\mathbf{k}) = \int_0^\infty dt \exp \left[- \int_0^t dt' / \tau_{\mathbf{k}(t')} \right] v_j(\mathbf{k}(t)), \quad (31)$$

where we find the lifetime $\tau_{\mathbf{k}}$ (which is not only \mathbf{k} -dependent, but can also be ϵ - and T -dependent, as discussed in section IV C). Both $\tau_{\mathbf{k}}$ and $v_j(\mathbf{k})$ are evaluated on a trajectory $\mathbf{k}(t)$, in \mathbf{k} -space. This trajectory starts at $\mathbf{k}(0) = \mathbf{k}$, and is governed by the semiclassical equation of motion:

$$\hbar \frac{d\mathbf{k}(t)}{dt} = -e(\mathbf{v}(\mathbf{k}(t)) \times \mathbf{B}) \quad (32)$$

where \mathbf{B} is the magnetic field. To compute conductivity tensors, one must thus solve this differential equation (32) for each starting point \mathbf{k} contained the integral of (29).

All-in-one equation

We can reduce all the tensors into a single expression. We substitute (31) and (30) in (29), and then substitute the result in (6), (7), and (8), unifying them in the following monster:

$$\begin{aligned} \sigma_{ij}^{(n)} = & \int_{-\infty}^{\infty} d\epsilon \left[\left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \frac{\epsilon^n}{T^n} \right] (-e)^{2-n} \iiint_{\text{BZ}} \frac{d^3k}{(2\pi)^3} \frac{1}{\hbar} \frac{\partial E(\mathbf{k})}{\partial k_i} \\ & \times \int_0^{\infty} dt \exp \left[-\int_0^t dt' / \tau_{\mathbf{k}(t')} \right] \frac{1}{\hbar} \frac{\partial E(\mathbf{k})}{\partial k_j} \Big|_{\mathbf{k}(t)} \delta(\epsilon - E(\mathbf{k})) \end{aligned} \quad (33)$$

with:

$$\sigma_{ij} = \sigma_{ij}^{(0)} \quad (34)$$

$$\alpha_{ij} = \sigma_{ij}^{(1)} \quad (35)$$

$$\frac{\beta_{ij}}{T} = \sigma_{ij}^{(2)}. \quad (36)$$

The semiclassical movement equation (32) must be used to find $\mathbf{k}(t)$. The only free paramters associated to the material under study are $E(\mathbf{k})$ and $\tau_{\mathbf{k}}$.

III. SIMPLIFICATIONS

A. Equi-energy surfaces

The Dirac delta $\delta(\epsilon - E(\mathbf{k}))$ allow to change the three-dimensional \mathbf{k} integral to a two-dimensional surface integral, on the surface defined by $E(\mathbf{k}) = \epsilon$ (see equation 8.57 and 8.62 of Ashcroft & Mermin [1] for a similar statement). Take an arbitrary function $F(\mathbf{k})$, for example:

$$\iiint d^3k F(\mathbf{k}) \delta(\epsilon - E(\mathbf{k})) = \iint_{E(\mathbf{k})=\text{cst.}} d^2k_{\parallel} \int dk_{\perp} F(\mathbf{k}) \delta(\epsilon - E(\mathbf{k})) \quad (37)$$

$$= \iint_{E(\mathbf{k})=\text{cst.}} d^2k_{\parallel} \int \frac{dE(\mathbf{k})}{|\nabla_{\mathbf{k}} E(\mathbf{k})|} F(\mathbf{k}) \delta(\epsilon - E(\mathbf{k})) \quad (38)$$

$$= \iint_{E(\mathbf{k})=\epsilon} d^2k_{\epsilon} \frac{F(\mathbf{k}_{\epsilon})}{|\nabla_{\mathbf{k}} E(\mathbf{k})|_{\mathbf{k}=\mathbf{k}_{\epsilon}}}. \quad (39)$$

where \mathbf{k}_{ϵ} are the wave vectors belonging to this equi-energy surface $E(\mathbf{k}) = \epsilon$. The integral on the Brillouin zone therefore reduces to a surface integral for each value of ϵ , and (29) becomes:

$$\sigma_{ij}(\epsilon) = e^2 \iint_{\substack{E(\mathbf{k})=\epsilon \\ \text{in BZ}}} \frac{d^2k_{\epsilon}}{(2\pi)^3} \frac{v_i(\mathbf{k}_{\epsilon}) \bar{v}_j(\mathbf{k}_{\epsilon})}{\hbar |\mathbf{v}(\mathbf{k}_{\epsilon})|}. \quad (40)$$

B. Zero Magnetic field

In the limit of zero magnetic field, $\mathbf{B} \rightarrow 0$, the differential equation (32) becomes trivial, and $\mathbf{k}(t) = \mathbf{k}$ at all t . In that case, (31) simply reduces to:

$$\bar{v}_j(\mathbf{k}) = v_j(\mathbf{k}) \int_0^\infty dt e^{-t/\tau_{\mathbf{k}}} \quad (41)$$

$$= v_j(\mathbf{k}) \tau_{\mathbf{k}}. \quad (42)$$

However, in the case of $i \neq j$, $\sigma_{ij}(\omega)$ is zero at zero field, so we shall keep the linear term in \mathbf{B} in this case (see [4] for details). This allows to write (29) as:

$$\lim_{\mathbf{B} \rightarrow 0} \sigma_{ij}(\epsilon) = e^2 \iiint_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} v_i(\mathbf{k}) \left[\delta_{ij} v_i(\mathbf{k}) \tau_{\mathbf{k}} - \varepsilon_{ijk} (-e B_k) \left[v_i(\mathbf{k}) \frac{\partial v_j(\mathbf{k})}{\partial k_j} - v_j(\mathbf{k}) \frac{\partial v_i(\mathbf{k})}{\partial k_j} \right] \tau_{\mathbf{k}}^2 \right] \delta(\epsilon - E(\mathbf{k})), \quad (43)$$

where δ_{ij} is the Kronecker symbol and ε_{ijk} is the Levi-Cevita symbol (which is 0 if $i = j$). The first term of this equation corresponding to (25).

C. Effective mass and Drude results

We can carry out explicitly the integral over energy in the all-in-one equation (33) and reorganize it as:

$$\sigma_{ij}^{(n)} = -\frac{(-e)^{2-n}}{\hbar T^n} \iiint_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} E(\mathbf{k})^n \frac{\partial f(\epsilon)}{\partial E(\mathbf{k})} \frac{\partial E(\mathbf{k})}{\partial k_i} \bar{v}_j(\mathbf{k}) \quad (44)$$

$$= -\frac{(-e)^{2-n}}{\hbar T^n} \iiint_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} E(\mathbf{k})^n \frac{\partial f(E(\mathbf{k}))}{\partial k_i} \bar{v}_j(\mathbf{k}). \quad (45)$$

This allow to integrate by parts as follows:

$$\begin{aligned} \int_{-\pi/a_i}^{\pi/a_i} dk_i E(\mathbf{k})^n \frac{\partial f(E(\mathbf{k}))}{\partial k_i} \bar{v}_j(\mathbf{k}) &= \left[E(\mathbf{k})^n f(E(\mathbf{k})) \bar{v}_j(\mathbf{k}) \right]_{-\pi/a_i}^{\pi/a_i} \\ &\quad - \int_{-\pi/a_i}^{\pi/a_i} dk_i n E(\mathbf{k})^{n-1} \frac{\partial E(\mathbf{k})}{\partial k_i} f(E(\mathbf{k})) \bar{v}_j(\mathbf{k}) \\ &\quad - \int_{-\pi/a_i}^{\pi/a_i} dk_i E(\mathbf{k})^n f(E(\mathbf{k})) \frac{\partial \bar{v}_j(\mathbf{k})}{\partial k_i}. \end{aligned} \quad (46)$$

Since n only takes the values 0, 1, 2, and under the conditions $E(-\mathbf{k}) = E(\mathbf{k})$, and $\bar{v}_j(-\mathbf{k}) = -\bar{v}_j(\mathbf{k})$, then the first and second terms of (46) are zero, and (45) becomes:

$$\sigma_{ij}^{(n)} = (-e)^{2-n} \iiint_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} \frac{E(\mathbf{k})^n}{T^n} \frac{1}{\hbar} \frac{\partial \bar{v}_j(\mathbf{k})}{\partial k_i} f(E(\mathbf{k})). \quad (47)$$

Taking explicitly the derivative of (31):

$$\begin{aligned} \frac{1}{\hbar} \frac{\partial \bar{v}_j(\mathbf{k})}{\partial k_i} = \int_0^\infty dt \left[e^{-\int_0^t dt' / \tau_{\mathbf{k}(t')}} \frac{1}{\hbar^2} \frac{\partial^2 E(\mathbf{k}(t))}{\partial k_i \partial k_j} \right. \\ \left. + e^{-\int_0^t dt' / \tau_{\mathbf{k}(t')}} \left(\int_0^t \frac{dt'}{\tau_{\mathbf{k}(t')}^2} \frac{\partial \tau_{\mathbf{k}(t')}}{\partial k_i} \right) \frac{1}{\hbar^2} \frac{\partial E(\mathbf{k}(t))}{\partial k_j} \right] \end{aligned} \quad (48)$$

we find the effective mass:

$$M_{ij}^{-1}(\mathbf{k}) \equiv \frac{1}{\hbar^2} \frac{\partial^2 E(\mathbf{k})}{\partial k_i \partial k_j}. \quad (49)$$

Note that if the lifetime is independent of \mathbf{k} , then the second term of (48) disappears, and only the first term remains. In that case, carrying the zero magnetic field manipulations of IIIB and restituting of the integral in energy lead to:

$$\begin{aligned} \lim_{\substack{\mathbf{B} \rightarrow 0 \\ \tau_{\mathbf{k}} \rightarrow \tau}} \sigma_{ij}^{(n)} = \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \frac{\epsilon^n}{T^n} (-e)^{2-n} \iiint_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} \left[\delta_{ij} M_{ii}^{-1}(\mathbf{k}) \tau \right. \\ \left. + \varepsilon_{ijk} (-e B_k) \left(M_{ii}^{-1}(\mathbf{k}) M_{jj}^{-1}(\mathbf{k}) - M_{ij}^{-2}(\mathbf{k}) \right) \tau^2 \right] \delta(\epsilon - E(\mathbf{k})), \end{aligned} \quad (50)$$

The above is an all-in-one equation expressed with the mass instead of the velocities. Note in particular the longitudinal electric conductivity case $\sigma_{ii} = \sigma_{ii}^{(0)}$:

$$\lim_{\substack{\mathbf{B} \rightarrow 0 \\ \tau_{\mathbf{k}} \rightarrow \tau}} \sigma_{ii} = \iiint_{\text{BZ}} \frac{d^3 k}{(2\pi)^3} f(E(\mathbf{k})) e^2 M_{ii}^{-1}(\mathbf{k}) \tau_{\mathbf{k}}, \quad (51)$$

which reduces to the Drude formula when $M_{ij}^{-1}(\mathbf{k}) = \delta_{i,j} \frac{1}{m_i^*}$:

$$\lim_{\substack{\mathbf{B} \rightarrow 0, \tau_{\mathbf{k}} \rightarrow \tau \\ M_{ij}(\mathbf{k}) \rightarrow \delta_{ij} m_i^*}} \sigma_{ij} = \delta_{i,j} \frac{n e^2 \tau}{m_i^*} \quad (52)$$

D. Zero temperature

In the zero temperature limit, the electrical conductivity tensor (6) becomes:

$$\lim_{T \rightarrow 0} \sigma_{ij} = \int_{-\infty}^{\infty} d\epsilon \lim_{T \rightarrow 0} \left(-\frac{\partial f(\epsilon)}{\partial \epsilon} \right) \sigma_{ij}(\epsilon) \quad (53)$$

$$= \int_{-\infty}^{\infty} d\epsilon \delta(\epsilon - \mu) \sigma_{ij}(\epsilon) \quad (54)$$

$$\boxed{\lim_{T \rightarrow 0} \sigma_{ij} = \sigma_{ij}(\mu)}. \quad (55)$$

Unfortunately, this simplification does not extend to α_{ij} and β_{ij} for which one must instead turn to Sommerfeld expansions (very well explained at Appendix C of Ashcroft & Mermin [1]). Note

that together with the simplification III A for energy surfaces, the zero-temperature simplification implies that the conductivity at $T = 0$ is entirely given by the Fermi Surface:

$$\lim_{T \rightarrow 0} \sigma_{ij} = \frac{e^2}{(2\pi)^3} \iint_{\text{FS}} d^2 k_F \frac{v_i(\mathbf{k}_F) \bar{v}_j(\mathbf{k}_F)}{\hbar |\mathbf{v}(\mathbf{k}_F)|}. \quad (56)$$

IV. FOR CUPRATES

When working with cuprates, we consider two candidates for $E(\mathbf{k})$: (i) the bare dispersion $\epsilon_{3\text{D}}(\mathbf{k})$, and (ii) the antiferromagnetic approximation for the pseudogap $E_{3\text{D}}^\pm(\mathbf{k})$. Both are introduced in what follow.

A. Bare dispersion

To simulate overdoped cuprates, we use the one-band three-dimensional dispersion measured by ARPES [5] in Eu-LSCO:

$$\epsilon_{3\text{D}}(\mathbf{k}) = \epsilon_{\mathbf{k}} + \epsilon_{\perp}(\mathbf{k}) \quad (57)$$

where $\epsilon_{\mathbf{k}}$ is the plane dispersion:

$$\epsilon_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y b)) - 4t' \cos(k_x a) \cos(k_y b) - 2t''(\cos(2k_x a) + \cos(2k_y b)) \quad (58)$$

and $\epsilon_{\perp}(\mathbf{k})$ is the inter-plane dispersion:

$$\epsilon_{\perp}(\mathbf{k}) = -2t_z \cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{k_y b}{2}\right) \cos\left(\frac{k_z c}{2}\right) (\cos(k_x a) - \cos(k_y b))^2. \quad (59)$$

We use parameters $a = b = 3.75 \text{ \AA}$, $c = 13.20 \text{ \AA}$, $t = 190 \text{ meV}$, and $(t', t'', t_z) = (-0.14t, 0.07t, 0.07t)$. The chemical potential μ is obtained by solving the integral equation for a given doping p :

$$p = 1 - n \quad (60)$$

$$= 1 - \iiint_{BZ} \frac{d^3 k}{4\pi^3} f(\epsilon_{3\text{D}}(\mathbf{k}) - \mu) \quad (61)$$

B. Approximation for the pseudogap

To fit the results for the pseudogap regime at $p < p^*$, we start from a two-dimensional antiferromagnetic (AF) reconstruction of the bare band (following recent success of such a model for the Hall number [3, 6]):

$$E^\pm(\mathbf{k}) = \frac{1}{2}(\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{Q}}) \pm \sqrt{\frac{1}{4}(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}})^2 + M^2} \quad (62)$$

We cannot extend this model straightforwardly to the three-dimensional dispersion, because taking $\epsilon_{\mathbf{k}} \rightarrow \epsilon_{3D}(\mathbf{k})$ in the above equation results in C4 rotational symmetry breaking. This is because of the body-centered structure of Nd-LSCO, which is fully taken into account in $\epsilon_{\perp}(\mathbf{k})$, and in for which antiferromagnetism is not the same for $\mathbf{Q} = (\pi/a, \pi/a, 0)$ than for $\mathbf{Q} = (\pi/a, -\pi/a, 0)$. Therefore, we can instead suppose that the 2D planes contain independent antiferromagnetic orders, and add the z -dispersion after the reconstruction:

$$E_{3D}^{\pm}(\mathbf{k}) = E^{\pm}(\mathbf{k}) + \epsilon_{\perp}(\mathbf{k}) \quad (63)$$

This may be interpreted as antiferromagnetism uncorrelated between planes.

Note on numerical optimization: The bottleneck when evaluating equations (56) at zero temperature or (40) at finite temperature is the repeated evaluation of the velocity required to solve the semiclassical equation (32). In practice, we can save a lot of computation time by noting that $\epsilon_{\mathbf{k}+\mathbf{Q}}$ and $\mathbf{v}(\mathbf{k} + \mathbf{Q})$ are simply linked to $\epsilon_{\mathbf{k}}$. We first split the latter as:

$$\epsilon_{\mathbf{k}} = \zeta_{\mathbf{k}} + \xi_{\mathbf{k}} \quad (64)$$

$$\xi_{\mathbf{k}} \equiv -2t(\cos(k_x a) + \cos(k_y b)), \quad (65)$$

$$\begin{aligned} \zeta_{\mathbf{k}} \equiv & -4t' \cos(k_x a) \cos(k_y b) \\ & - 2t''(\cos(2k_x a) + \cos(2k_y b)) \end{aligned} \quad (66)$$

and note that for $\mathbf{Q} = (\pi/a, \pi/a)$:

$$\epsilon_{\mathbf{k}+\mathbf{Q}} = \zeta_{\mathbf{k}} - \xi_{\mathbf{k}} \quad (67)$$

C. Lifetime

The various lifetime $\tau_{\mathbf{k}}$ we consider are those of previous work on Hall and Seebeck effects [3], and those of the review by Hussey [7]. The lifetime is the inverse of the total scattering rate:

$$\tau_{\mathbf{k}} = \frac{\hbar}{2\Gamma(\mathbf{k})}, \quad (68)$$

and the scattering rate can have various contributions:

$$\begin{aligned} \Gamma(\mathbf{k}) = & \eta_0 + \eta_{\ell}|\mathbf{v}(\mathbf{k})| + \eta_N/|\mathbf{v}(\mathbf{k})| \\ & + \eta_{FLa}(\omega^2 + \pi^2 T^2) + \eta_{PL}T \\ & + \eta_{FLb}(\omega^2 + \pi^2 T^2)/|\mathbf{v}(\mathbf{k})| \\ & + \eta_{an}(\cos k_x - \cos k_y)^2. \end{aligned} \quad (69)$$

In this expression, small numerical values might be needed to prevent divergence. Respectively taken alone, η_0 would yield constant lifetime, η_ℓ would yield constant mean-free path, η_N would yield scattering proportional to the density of state, and η_{an} yields a phenomenological increase of the anti-nodal scattering. There can be various reasons to consider each terms separately, or combined.

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