Confinement of Electrons in Layered Metals

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We analyze the out of plane hopping in models of layered systems where the in-plane properties deviate from Landau's theory of a Fermi liquid. We show that the hopping term acquires a nontrivial energy dependence, due to the coupling to in-plane excitations, and the resulting state, at low temperatures, can be either conducting or insulating in the third direction. The latter is always the case if the Fermi level lies close to a saddle point in the dispersion relation.

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Layered materials have been the object of intensive study because they present important physics. Unusual properties are derived from the anisotropy and periodicity along the axis perpendicular to the planes [1]. Among the most studied layered materials are the high-temperature cuprate superconductors. In the normal state the transport properties within the CuO_2 planes are very different from those along the c axis: electron motion in the c direction is incoherent in contrast with the metallic behavior of the in-plane electrons as probed by the different ρ_c and ρ_{ab} resistivities [2,3]. The relevance of the nature of the conductance in the direction perpendicular to the CuO_2 planes has been noted on both theoretical [4–6] and experimental [7] grounds.

Graphite is another layered material which presents unconventional properties, such as the linear increase with energy of the inverse lifetime. These results suggest deviations from the conventional Fermi liquid behavior, which could be due to strong Coulomb interaction, which remains unscreened because of the lack of states at the Fermi level [8,9]. It is interesting to note that, as different experiments suggest, the conductivity of graphite shows an insulating behavior in the direction perpendicular to the layers, while it is metallic along the layers [10]. Other experiments show evidence of anomalous behavior in other properties [11].

The anomalous out of plane behavior of the cuprates has led to the suggestion that conventional Fermi liquid theory fails in these compounds [4]. An alternative explanation of the emergence of incoherent behavior in the out of plane direction has been proposed in terms of the coupling of the interlayer electronic motion to charge excitations of the system [6]. This approach implicitly assumes that electron-electron interactions modify the in-plane electron propagators in a nontrivial way.

In the following, we show that, even in the clean limit, many body effects can suppress the coherent contribution to the out of plane electron hopping. We define the clean limit as that in which the length scale, L, over which electrons remain coherent within the layers diverges. We first apply the method to the well understood problem of interchain tunneling in an array of clean Luttinger liquids. We recover known results, and show that the method is equivalent to lowest order scaling, which, in turn, gives the renormalization of the interchain tunneling with logarithmic accuracy [12–15]. Then, we extend the calculation to layered models where the intralayer properties show deviations from Fermi liquid behavior [9,16].

The method of calculation.—The influence of inelastic scattering on electron tunneling has been studied, using equivalent methods, in mesoscopic devices which show Coulomb blockade [17], Luttinger liquids [13–15,18], and dirty metals [19]. The simplest formulation of the method replaces the excitations of the system (such as electron-hole pairs) by a bath of harmonic oscillators with the same excitation spectrum. This approach can be justified rigorously in one dimension, and is always an accurate description of the response of the system when the coupling of the quasiparticles to each individual excitation is weak [20].

In the following, we will assume a local interaction between electrons close to the Fermi level, and the charge fluctuations of the system:

$$\mathcal{H}_{\rm int} = c_i^\dagger c_i \sum_{\vec{\mathbf{k}}} V_i(\vec{\mathbf{k}}) \hat{\boldsymbol{\rho}}_{\vec{\mathbf{k}}}, \tag{1}$$

where c_i creates an electron at site i, and $\hat{\boldsymbol{\rho}}_{\vec{\mathbf{k}}}$ describes the charge fluctuations of the environment, which are to be described as a set of harmonic modes. The Hamiltonian of the system is approximated as:

$$\begin{aligned}\mathcal{H}_{e-b} &= \mathcal{H}_{\rm elec} + \mathcal{H}_{\rm env} + \mathcal{H}_{\rm int} \\ &= \sum \mathbf{t}_{ij} c_i^\dagger c_j + \sum \omega_k b_k^\dagger b_k + \sum g_{k,i} c_i^\dagger c_i (b_k^\dagger + b_k),\end{aligned} \tag{2}$$

where $\mathcal{H}_{\rm elec}$ describes the individual quasiparticles, $\mathcal{H}_{\rm env}$ stands for the set of harmonic oscillators which describe the environment, and $\mathcal{H}_{\rm int}$ defines the (linear) coupling between the two. The $b_k^\dagger$ are boson creation operators, the $\mathbf{t}_{ij}$ describe the electronic hopping processes, and the information about the interaction between the electron in state i and the system is defined by the function [20] $J_i(\omega) = \sum_k |g_{k,i}|^2 \delta(\omega - \omega_k)$.

Using second order perturbation theory and Eq. (1), we can write [17,20]

$$J_i(\omega) = \sum_{\vec{k}} V_i^2(\vec{k}) \mathrm{Im}\chi(\vec{k}, \omega), \tag{3}$$

where $\chi(\vec{k}, \omega)$ is the Fourier transform of the density-density response of the system, $\langle \hat{\rho}_{\vec{k}}(t) \hat{\rho}_{-\vec{k}}(0) \rangle$. The interaction in Eq. (1) is spin independent. Other, more complicated, couplings can also be taken into account, provided that the appropriate response function is used.

The influence of the electron-boson coupling on the electron propagators can be calculated to all orders if the state i is localized, that is, neglecting the hopping terms in Eq. (3). We find

$$\langle c_i^\dagger(t) c_i(t') \rangle \sim \langle c_i^\dagger(t) c_i(t') \rangle_0 \times \exp\left\{ - \int d\omega [1 - e^{i\omega(t-t')}] \frac{J_i(\omega)}{\omega^2} \right\}, \tag{4}$$

where $\langle c_i^\dagger(t) c_i(t') \rangle_0 \sim e^{i\varepsilon_i (t-t')}$ is the Green's function in the absence of the interaction. The method that we use assumes that Eq. (4) also holds in a system with extended states. For a standard metallic system, we must insert $\langle c_i^\dagger(t) c_i(t') \rangle_0 \sim 1/(t-t')$ in Eq. (4). It can be shown that this approximation is exact at short times, $W \ll (t-t')^{-1} \ll \Lambda$, where W is an energy scale related to the dynamics of the electrons, and Λ is the upper cutoff in the spectrum of the environment.

The time dependence in Eq. (4) is determined by $\lim_{\omega \to 0} \chi(\vec{k}, \omega)$. In a gapless, metallic system, we have $\chi(\vec{k}, \omega) \sim \alpha(\vec{k}) |\omega|$. This behavior, when inserted in Eq. (4), leads to

$$\langle c_i^\dagger(t) c_i(t') \rangle \sim \frac{1}{(t-t')^{(1+\alpha)}}, \tag{5}$$

where

$$\alpha = \int_{|\vec{k}| \ll L^{-1}} d\vec{k} \, V^2(\vec{k}) \alpha(\vec{k}), \tag{6}$$

where L is the scale of the region where the tunneling process takes place. The value of L is limited by the length over which the phase of the electronic wave functions within the layers is well defined. We assume that, in a translationally invariant system, there is no dependence on the position of the local orbital, i. This result implies that the frequency dependence of the Green's function, in a continuum description, can be written as

$$\lim_{|\vec{r} - \vec{r}'| \to 0} G(\vec{r} - \vec{r}', \omega) \propto |\omega|^\alpha. \tag{7}$$

We can now use Eq. (5) to analyze the interlayer tunneling by applying renormalization group methods. The simplest case where this procedure has been used is for the problem of an electron tunneling between two states, i and j, which has been intensively studied [21,22]. We integrate out the high energy bosons, with energies $\Lambda - d\Lambda \le \omega_k \le \Lambda$, and rescaled hopping terms are defined. As mentioned earlier, Eq. (5) is valid for this range of energies. The renormalization of the hoppings is such that the properties of the effective Hamiltonian at energies $\omega \ll \Lambda$ remain invariant. If the hoppings $\mathbf{t}_{ij}$ are small, any physical quantity which depends on them can be expanded, using time dependent perturbation theory, in powers of

$$\mathbf{t}_{ij}^2 \langle c_i^\dagger(t) c_j(t) c_j^\dagger(t') c_i(t') \rangle \approx \mathbf{t}_{ij}^2 \langle c_i^\dagger(t) c_i(t') \rangle \langle c_j(t) c_j^\dagger(t') \rangle. \tag{8}$$

The integration of the high energy modes implies that the terms in Eq. (8) are restricted to $t \le \Lambda^{-1}$, or, alternatively, the time units have to be rescaled [23], $\tau' = \tau e^{d\Lambda/\Lambda}$, where $\tau \sim \Lambda^{-1}$. Using Eq. (5), the condition of keeping the perturbation expansion in powers of the terms in Eq. (8) invariant implies that

$$\mathbf{t}_{ij}^2 \to \mathbf{t}_{ij}^2 e^{(d\Lambda/\Lambda)(2+2\alpha)}, \tag{9}$$

which can also be used to define the scaling dimension of the hopping terms. Finally,

$$\frac{\partial(\mathbf{t}_{ij}/\Lambda)}{\partial l} = -\alpha \frac{\mathbf{t}_{ij}}{\Lambda}, \tag{10}$$

where $l = \log(\Lambda_0/\Lambda)$, and Λ_0 is the initial value of the cutoff.

This approach has been successfully used to describe inelastic tunneling in different situations in [6,13–19].

The analysis that leads to Eq. (10) can be generalized to study hopping between extended states, provided that we can estimate the long time behavior of the Green's function, $G(\vec{k}, t-t') = \langle c_{\vec{k}}^\dagger(t) c_{\vec{k}}(t') \rangle$. This function is related to the local Green's function, Eq. (7), by

$$\lim_{|\vec{r} - \vec{r}'| \to 0} G(\vec{r} - \vec{r}', \omega) = \int d^D \vec{k} \, G(\vec{k}, \omega), \tag{11}$$

where D is the spatial dimension. In the cases discussed below, the interaction is instantaneous in time, and the noninteracting Green's function can be written as

$$G_0(\vec{k}, \omega) \propto \frac{1}{\omega} \mathcal{F}\left(\frac{k_i^z}{\omega} \right), \tag{12}$$

where $z = 1, 2$. In the following, we assume that the interacting Green's function has the same scaling properties, with the factor ω^{-1} replaced by $\omega^{-\delta}$ in Eq. (12), where δ depends on the interactions. This can be shown to be correct in perturbation theory to all orders, in the models studied below, because the corrections depend logarithmically on ω (it is a well known fact for the Luttinger liquid). Then, using Eqs. (7), (11), and (12), we obtain

$$G(\vec{k}, \omega) \propto |\omega|^{\alpha - D/z} \mathcal{F}\left(\frac{k_i^z}{\omega} \right), \tag{13}$$

and $\mathcal{F}(u)$ is finite. Thus, from the knowledge of the real space Green's function, using Eq. (4), we obtain α, which, in turn, determines the exponent $\alpha + D/z$ which characterizes $G(\vec{k}, \omega)$. Generically, we can write

$$G_{l,e}(\omega) \sim |\omega|^{\delta_{l,e}}, \tag{14}$$

where the subindices l, e stand for localized and extended wave functions. In terms of these exponents, we can generalize Eq. (10) to tunneling between general states to

$$\frac{\partial(\mathbf{t}_{ij}^{l,e}/\Lambda)}{\partial l} = -\delta_{l,e} \frac{\mathbf{t}_{ij}}{\Lambda}. \tag{15}$$

Before proceeding to calculations of δ_l and δ_e for various

models, it is interesting to note that, in general, the response function of an electron gas in dimension $D > 1$ behaves as $\lim_{\omega\to 0,|\vec{\mathbf{k}}|\to 0} \chi(\vec{\mathbf{k}}, \omega) \sim |\omega|/|\vec{\mathbf{k}}|$, so that, from Eq. (6), $\lim_{L\to\infty} \alpha \sim L^{(1-D)}$. Thus, for $D > 1$, the contribution of the inelastic processes to the renormalization of the tunneling vanishes for delocalized states, $L \to \infty$.

One dimensional systems.—We assume a smooth, short range interaction parametrized by U. Using second order perturbation theory, Eq. (4), becomes

$$\lim_{L\to\infty} \int_{|\vec{\mathbf{k}}|\ll L^{-1}} d\vec{\mathbf{k}} \frac{d\omega}{\omega^2} e^{i\omega(t-t')} U^2 \mathrm{Im}\chi(\vec{\mathbf{k}}, \omega) \sim U^2 \log[v_F(t-t')/L]. \quad (16)$$

This logarithmic divergence remains in higher order perturbation theory, because of the scaling properties of the response function of a Luttinger liquid.

Equation (16) leads to a Green's function like that in Eq. (4), with $\alpha = \delta_l \sim (U/E_F)^2$. For this model, $D = 1$ and $z = 1$. Then, using Eq. (13), $\delta_e = \alpha - 1$. Tunneling between localized states is suppressed at low temperatures, while tunneling between delocalized states is not, unless $\alpha \geq 1$ [13].

Graphene planes.—The simplest two-dimensional model for interacting electrons where it can be rigorously shown that the couplings acquire logarithmic corrections in perturbation theory is a system of Dirac fermions ($\epsilon_k = v_F|\vec{\mathbf{k}}|$), with Coulomb, $1/|\vec{\mathbf{r}} - \vec{\mathbf{r}}'|$, interaction. This model can be used to describe isolated graphene planes [9,24].

In order to apply the procedure outlined in the previous section, one needs the Fourier transform of the coupling between quasiparticles and the density fluctuations, $V(\vec{\mathbf{k}}) = e^2/(\epsilon_0|\vec{\mathbf{k}}|)$, where e is the electronic charge, and ϵ_0 is the dielectric constant, and the response function of the system. For a single graphene plane, this quantity is

$$\mathrm{Im}\chi_0(\vec{\mathbf{k}}, \omega) = \frac{1}{8} \frac{|\vec{\mathbf{k}}|^2}{\sqrt{v_F^2|\vec{\mathbf{k}}|^2 - \omega^2}}. \quad (17)$$

These expressions need to be inserted in Eq. (6). Alternatively, we can use the RPA, and include the effects of interplane screening, as described in [24]. As the long range properties of the screening potential remain unchanged, we expect no qualitative changes. Hence, for simplicity, we consider the expression in Eq. (17). Using Eq. (6), we obtain an expression similar to Eq. (16), except that the local potential U has to be replaced by $e^2/(\epsilon_0|\vec{\mathbf{k}}|)$. The integral in Eq. (16) also diverges logarithmically in the present case, with a prefactor $\alpha \sim e^4/(\epsilon_0 v_F)^2$ which does not depend on L. The main difference with the previous case is that Eq. (7) has to be replaced by

$$\lim_{|\vec{\mathbf{r}}-\vec{\mathbf{r}}'|\to 0} G(\vec{\mathbf{r}} - \vec{\mathbf{r}}', \omega) \propto |\omega|^{1+\alpha}, \quad (18)$$

where $\alpha \sim e^4/v_F^2$. In the absence of interactions, $\alpha = 0$, the density of states vanishes at the Fermi level, because of the semimetallic nature of graphene. Equation (18) gives $\delta_l = 1 + \alpha$. For this system, $D = 2$ and $z = 1$, so that $\delta_e = \alpha - 1$. Tunneling between localized states is always strongly suppressed at low temperatures, while tunneling between extended states is suppressed only if $\alpha \geq 1$.

In graphite, the dimensionless coupling constant, e^2/v_F, is of order unity. Under renormalization, it flows towards zero [9], so that α becomes scale dependent, and vanishes at low energies. Thus, interplane tunneling increases at low energies, leading to interlayer coherence. Note, however, that in a dirty system with a finite mean free path, short range interactions can grow at low energies, leading to the suppression of interplane tunneling [24].

Saddle point in the density of states.—The Fermi surface of most hole-doped cuprates is close to a Van Hove singularity. The possible relevance of this fact to the superconducting transition as well as to the anomalous behavior of the normal state was put forward in the early times of the cuprates and gave rise to the so-called Van Hove scenario [25]. We will assume that the metallic layers are well described by electrons in a square lattice, and that the Fermi level is close to the $(\pi, 0)(A)$ and $(0, \pi)(B)$ points of the Brillouin zone (BZ). Close to these points, the dispersion relation can be parametrized as

$$\varepsilon_{A,B}(\vec{\mathbf{k}}) \approx \frac{k_x^2}{2m_{x,y}} \mp \frac{k_y^2}{2m_{y,x}}, \quad (19)$$

where m_x and m_y are parameters which can be estimated from the band structure of the model. In the following, we will consider the renormalization of the interlayer tunneling associated with these regions in the Brillouin zone. Note that in the case of the cuprate superconductors matrix elements suppress the interlayer tunneling at points close to the diagonal of the BZ.

The response function at low energies and small wave vectors has been computed in [16]:

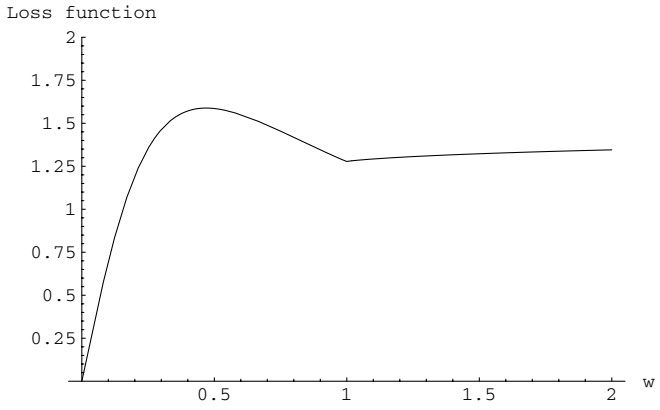

FIG. 1. Effective potential as a function of the energy for fixed $\mathbf{k}$ for a system of Van Hove layers coupled by Coulomb interaction.

$$\mathrm{Im}\chi(\vec{\mathbf{k}}, \omega) = \sum_{i=A,B} \frac{1}{4\pi\varepsilon_i(\vec{\mathbf{k}})} (|\omega + \varepsilon_i(\vec{\mathbf{k}})| - |\omega - \varepsilon_i(\vec{\mathbf{k}})|), \tag{20}$$

where $\varepsilon_i(\vec{\mathbf{k}})$ is the dispersion relation (19).

The long time dependence of the Green's function is determined by the low energy behavior of χ: $\lim_{\omega\to 0} \mathrm{Im}\chi(\vec{\mathbf{k}}, \omega) \sim \sum_{i=A,B} |\omega|/\varepsilon_i(\vec{\mathbf{k}})$. We assume that the interaction between the electrons and the density fluctuations is short ranged as before. The divergence of $\mathrm{Im}\chi$ when $\varepsilon_{A,B} = 0$ implies that the integral in Eq. (6) diverges logarithmically as $L \to \infty$, as in the two previous cases, irrespective of the details of the interaction, $V(\vec{\mathbf{k}})$. Because of this divergence, it is convenient to shift slightly the chemical potential, μ away from the saddle point [16], ε_{vH}. A finite value of $|\mu - \varepsilon_{vH}|$ implies the existence of a length scale, $L_0 \sim [\mathrm{Max}(m_x, m_y)|\mu - \varepsilon_{vH}|]^{-1/2}$, which regularizes the $\vec{\mathbf{k}}$ integrals in Eq. (6).

Using a local potential as in the $D = 1$ case, we find $\alpha \sim (U/E_F)^2 \log^2(L/L_0)$, where E_F is an energy scale of the order of the width of the conduction band. The dependence of α on L goes as $\log^2(L/L_0)$, as in other physical quantities in this model [16].

Figure 1 compares well with the effective potential [3] obtained numerically for a system of Van Hove layers. Figure 1 compares well with the experimental plots of the loss function given in [26] which reveals that the Van Hove model is also compatible with transport experiments [27].

In this model, $D = 2$ and $z = 2$, so that $\delta_l = \alpha$, as estimated above, and $\delta_e = \alpha - 1$. The divergence of α implies that tunneling between localized and also between extended states is suppressed at low temperatures. In addition, the effective electron-electron coupling, U, grows at low energies or temperatures, until a scale at which the system is unstable and a phase transition takes place [16]. This effect enhances the suppression of interlayer hopping.

Conclusions.—We have discussed the suppression of interlayer tunneling by inelastic processes in two-dimensional systems in the clean limit. Our results suggest that, when perturbation theory for the in-plane interactions leads to logarithmic divergences, the out of plane tunneling acquires a nontrivial energy dependence. The conductance goes to zero as $T \to 0$ if the Fermi level of the interacting electrons lies at a Van Hove singularity. Thus, we have shown that insulating behavior in the out of plane direction is not incompatible with gapless or even superconducting in-plane properties, although the in-plane properties are also markedly different from those of an ordinary Fermi liquid.

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Note added in proof.—Recent experiments [28] are consistent with the existence of confinement within layers analyzed in this work.

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