

Baber scattering and resistivity of a two-dimensional two-band model

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We investigate the Baber scattering problem in two dimensions, for the resistivity of a two-band model. The circular Fermi surface is two sheeted, light s electrons scatter against heavy d electrons characterized by a Fermi temperature $T_F(d)$. For $T \gg T_F(d)$ a saturation of the temperature dependence is expected, whereas for $T \ll T_F(d)$ a Fermi-liquid behavior is recovered. The details of the crossover are studied by analytical and numerical methods. At low temperatures we show the existence of a $T^2 \ln(T^*/T)$ behavior for the case of commensurate density, $k_s = k_d$, and calculate the T^* analytically. In the generic case of noncommensurate density, $k_s \neq k_d$, there is no logarithmic correction. We study the region of validity of the low-temperature expansion by comparing with exact numerical evaluations and find, in many cases, an extremely small domain of validity for the low-temperature expansion. We discuss the possible application of these ideas to high- T_c systems.

I. INTRODUCTION

The discovery of high- T_c superconductivity¹ has stimulated intense research activity on two-dimensional systems. One of the most striking features of these compounds is the linear temperature dependence of the resistivity down to the superconducting transition temperature in all compounds. An extreme example² is the 2:2:0:1 compound $\text{Bi}_2\text{Sr}_2\text{CuO}_6$, having very low $T_c = 7$ K, which has an almost linear resistivity for a large range of temperatures: $\rho \sim T^\nu$ with $\nu \sim 1.1$.

The above linearity of the resistivity has of course been the central theme for the current theoretical efforts to understand high- T_c systems. The usual framework, however, is the single-band Hubbard model.³ The justification of the one-band model usually starts from a three-band model^{4,5} that is projected down invoking the idea of local singlet formation,^{6,7} whereby the moments of doped oxygen holes and the copper moments lock up to give holes, i.e., spinless charges. The range of validity in hole doping of such a projection is somewhat uncertain on theoretical grounds, particularly for a large concentration of holes. Experimentally, the overdoped materials show low T_c and a more "normal" behavior in transport properties. Also, recent experiments⁸ on the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ family for various x show a fascinating variety of behavior of the resistivity from low to rather high temperatures (~ 1000 K), at various doping levels, with convex temperature dependences ($\sim T^\alpha$ with $\alpha > 1$) at dopings that are greater than the optimum T_c composition. Another impetus to the study comes from the photoemission data in the 2:2:1:2 compound $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$,⁹ which shows that there are two bands at the Fermi surface, at least in this family of compounds.

The above has motivated our interest in the classic problem discussed almost 60 years ago by Baber¹⁰ (following a suggestion of Mott), of a two-band model of carriers: the s and d electrons in the transition metals. It seems useful to obtain a complete picture of the be-

havior of the resistivity in this model problem in two dimensions, as a function of, as we will soon see, a rich set of parameters.

We consider light and heavy electrons of masses m_s, m_d with circular Fermi surfaces of diameter k_s, k_d with the heavy particles acting as momentum sinks. Similar results are expected for typical, noncircular bands. The two sets of carriers are treated as noninteracting fermions, and a Boltzmann equation is used to set up the resistivity. This apparently humble problem possesses some points of interest. There is a basic temperature scale $T_F(d) = \hbar^2 k_d^2 / 2m_d$, the Fermi temperature of the heavy particles. For $T \gg T_F(d)$ we expect a saturation of the resistivity at a value that we expect to be of the order of the maximum metallic resistivity in two dimensions, since we have one "impurity" per lattice constant at high temperatures, thereby satisfying the Ioffe-Regel criterion (unless the scattering mechanism is pathologically small). The resistivity at high temperatures, in a quasi-two-dimensional material with a three-dimensional lattice constant d should therefore be of order $\rho_{\text{Mott}} = dh/e^2$, which for $d = 10 \text{ \AA}$ is $\sim 2.5 \text{ m}\Omega \text{ cm}$. At low temperatures, we find a Fermi liquid like T^2 or, $T^2 \ln(T)$ behavior. We thus have an interesting crossover with the resistivity necessarily going through an inflexion point in between. The question of how low in T we need to get in order to see the Fermi-liquid behavior, and the complete temperature dependence are worked out in this paper. The model has an interesting "commensuration" effect when the Fermi diameters of the two species are equal: in this case the resistivity has an extra logarithmic correction, which we evaluate exactly.

The plan of the paper is as follows: in Sec. II we derive the formula for the resistivity by using the Boltzmann approximation. In Sec. III the low-temperature dependence of the conductivity is computed. In Sec. IV the full temperature dependence is obtained by using a numerical integration technique and the pertinence of such analysis to experiments is discussed.

II. RESISTIVITY

Let us consider a model of two types of fermions of effective masses m_s and m_d and of Fermi wave vectors k_s and k_d , related to particle densities through $k_s = \sqrt{2\pi\rho_s}$ and $k_d = \sqrt{2\pi\rho_d}$. We will assume for simplicity that they can be described by a parabolic band. The Hamiltonian of the system is therefore

$$H_0 = \sum_{k,\sigma} [\epsilon_s(k) c_{k,s,\sigma}^\dagger c_{k,s,\sigma} + \epsilon_d(k) c_{k,d,\sigma}^\dagger c_{k,d,\sigma}], \quad (2.1)$$

where

$$\epsilon_{s,d}(k) = \frac{k^2 - k_{s,d}^2}{2m_{s,d}}. \quad (2.2)$$

Bounds can be imposed on k to simulate a more realistic system: we choose a spherical Brillouin zone with radius $2\sqrt{\pi}$ in a Debye approximation of the zone. We will assume in the following the two species interact through a spin-spin interaction of the Kondo lattice form

$$H_{\text{int}} = \frac{J}{\sqrt{S(S+1)\Omega}} \sum_{k,k',q} \mathbf{S}_{k+q,k}^s \cdot \mathbf{S}_{k'-q,k'}^d, \quad (2.3)$$

where $S = \frac{1}{2}$ is the spin of the species, Ω the volume, and

$$\mathbf{S}_{k+q,k}^\mu = \frac{1}{2} \sum_{\sigma,\sigma'} c_{k+q,\mu,\sigma}^\dagger \boldsymbol{\sigma}_{\sigma,\sigma'} c_{k,\mu,\sigma'}, \quad (2.4)$$

and $\boldsymbol{\sigma}$ stands for the Pauli matrices. At the level of the Boltzmann approximation that we use, the fact that the interaction is spin dependent is of no consequence, and the same results obtain for a pure potential interaction:

$$H'_{\text{int}} = \frac{g}{\sqrt{\Omega}} \sum_{k,k',q} \rho(s)_{k+q,k} \rho(d)_{k'-q,k'} \quad (2.5)$$

with $\rho(s)_{k+q,k} = \sum_{\sigma} c_{k+q,\sigma}^\dagger c_{k,\sigma}$, etc. From (2.1) and (2.3) or (2.5) the resistivity can be computed in a simple Boltzmann approximation. We show in the Appendix

$$\rho_{\text{var}}(T) = \frac{(\beta/2) \sum_{k,p,q} \Gamma_0(k,p;q) [\phi_s(k) + \phi_d(p) - \phi_s(k+q) - \phi_d(p-q)]^2}{\{ \langle (-\partial f_s^0 / \partial \epsilon); \phi_s v_s^x \rangle + \langle (-\partial f_d^0 / \partial \epsilon); \phi_d v_d^x \rangle \}^2}, \quad (2.9)$$

where the notation $\langle a; b \rangle$ stands for

$$\langle a; b \rangle = \int a(k) b(k) \frac{d^2 k}{(2\pi)^2}. \quad (2.10)$$

It can be seen that the first variation of ρ_{var} with respect to $\phi_{s,d}$ treated as variational parameters, leads to the integral equations (2.8). In order to get an estimate of the resistivity one makes the simplest choice for ϕ ,

$$\phi_{s,d} = v_{s,d}^x(k). \quad (2.11)$$

Note that if one were strictly in the continuum, a better choice of variational ϕ would be $\phi_{s,d} = k_{s,d}$. With such a choice, since the momentum is conserved in each colli-

how the same result can be obtained from the memory function formalism. The Boltzmann formulation has the advantage of being a variational one and provides an upper bound for the resistivity of the system.

The Boltzmann equation can be derived as usual.¹¹ Let the scattering operator be defined as

$$\Gamma(k,p;q) = \frac{2\pi J^2}{\Omega} [f_s(k) \tilde{f}_s(k+q) f_d(p) \tilde{f}_d(p-q) \times \delta(\epsilon_s(k) - \epsilon_s(k+q) + \epsilon_d(p) - \epsilon_d(p-q))], \quad (2.6)$$

where f_s and f_d are the Fermi functions for s and d particles and $\tilde{f} = 1 - f$. The linearized Boltzmann equation may be written down as usual by expressing $f_a = f_a^0 - \Phi_a((\partial f_a^0)/(\partial \epsilon))$, where $a = (s,d)$. In the presence of an electric field E_x along for example the x axis, the linearized transport equation is

$$-\frac{\partial f_s^0}{\partial \epsilon} v_s^x(k) e E_x = \beta \sum_{p,q} \Gamma_0(k,p;q) [\Phi_s(k) + \Phi_d(p) - \Phi_s(k+q) - \Phi_d(p-q)] \quad (2.7)$$

and a similar equation for d electrons. Γ_0 in (2.7) is the scattering operator (2.6) with the unperturbed Fermi distributions f^0 and $v_{s,d}^x$ are the velocities of the particles along the x direction $v_{s,d}^x = [\partial \epsilon_{s,d}(k)]/(\partial k_x)$. Writing $\Phi_{s,d} = -e E_x \phi_{s,d}$, the Boltzmann equation reads

$$\frac{-\partial f_a^0}{\partial \epsilon} v_a^x = \beta \sum_{p,q} \Gamma_0(k,p;q) [\phi_a(k) + \phi_{a'}(p) - \phi_a(k+q) - \phi_{a'}(p-q)], \quad (2.8)$$

where a' is the complement of $a = (s,d)$.

A variational calculation of the resistivity can readily be performed. One can write a variational resistivity as

sion, the resistivity would be zero. This occurs because due to momentum conservation the system has no way to relax to equilibrium, and although the current is not conserved it cannot decay to zero. In order to achieve a finite resistivity one has to allow for the momentum to relax as well. In a real solid this can occur through a variety of processes, the most simple one being the umklapp process due to the presence of the lattice. In presence of such momentum nonconserving processes, if one assumes that the dominant scattering mechanism for electrons is the one in (2.3) then the resistivity will be correctly given by the choice (2.11). A similar situation occurs for the usual electron-phonon scattering mechanism, where in the absence of umklapp processes for the

phonons, the resistivity would remain zero due to the phonon-drag effect.¹¹

The resistivity (2.9) is then given by $\rho = N/D$, where $D = (D_s + D_d)^2$. Let us start with the denominator

$$D_a = \int_{W_{-,a}}^{W_{+,a}} \frac{\beta e^{\beta(\epsilon - \mu_a)}}{(e^{\beta(\epsilon - \mu_a)} + 1)^2} n_a(\epsilon) \frac{(2m_a\epsilon + k_a^2)}{m_a^2} d\epsilon, \quad (2.12)$$

where $W_{\pm,a}$ are the band edge, $n(\epsilon)$ the density of state per spin, which for the parabolic band we have chosen is $n(\epsilon) = (\Omega m_a)/(2\pi)$, and μ_a the chemical potential fixed by the condition that the number of particles is constant,

$$\int_{W_{-,a}}^{W_{+,a}} n_a(\epsilon) f(\epsilon) d\epsilon = \int_{W_{-,a}}^0 n_a(\epsilon) d\epsilon. \quad (2.13)$$

The resistivity is therefore given by^{12,13}

$$\rho(T) = \rho'_0(T) \beta \sum_{k,p,q} v_{k,p,q}^2 f(\epsilon_s(k)) \tilde{f}(\epsilon_s(k) + \Delta_s) \times f(\epsilon_d(p)) \tilde{f}(\epsilon_d(p) + \Delta_d) \delta(\Delta_s + \Delta_d), \quad (2.14)$$

where $\rho'_0(T) = J^2\pi/(\Omega D)$. In the above equation, we have defined

$$v_{k,p,q} = [v_s(k+q) - v_s(k) + v_d(p-q) - v_d(p)] = \left(\frac{1}{m_s} - \frac{1}{m_d} \right) q \quad (2.15)$$

and

$$\epsilon_s(k+q) = \epsilon_s(k) + \Delta_s, \quad \epsilon_d(p-q) = \epsilon_d(p) + \Delta_d. \quad (2.16)$$

One can easily see from (2.14) and (2.15) that the resistivity vanishes if the two species have the same mass. This is due to the fact that all collision processes conserve momentum, and if the particles have the same mass, due to Galilean invariance, the current is also conserved.

Using the condition $\Delta_s + \Delta_d = 0$ in (2.14) we find

$$q = 2\mu \left(\frac{p \cos \theta_d}{m_d} - \frac{k \cos \theta_s}{m_s} \right), \quad (2.17)$$

where $\mu = (m_s m_d)/(m_s + m_d)$ is the reduced mass. This allows us to simplify (2.14) which reads

$$\rho(T) = \frac{\mu \beta \Omega^3 \rho'_0(T)}{16\pi^5} \frac{(m_s - m_d)^2}{m_s m_d} \int_{W_{-,s}}^{W_{+,s}} d\epsilon_s \int_{W_{-,d}}^{W_{+,d}} d\epsilon_d \int_0^\pi \int_0^\pi d\theta_s d\theta_d q^2 \theta(q) f(\epsilon_s) \tilde{f}(\epsilon_s + \Delta) f(\epsilon_d) \tilde{f}(\epsilon_d - \Delta), \quad (2.18)$$

where the Δ through $\epsilon_s = \epsilon_s(k)$ and $\epsilon_d = \epsilon_d(p)$, with $k = \sqrt{2m_s\epsilon_s + k_s^2}$, $p = \sqrt{2m_d\epsilon_d + k_d^2}$ as

$$\Delta = \frac{q}{m_s + m_d} (k \cos \theta_s + p \cos \theta_d) \quad (2.19)$$

and q defined in (2.17).

In the following we will define $\rho_0(T)$ by absorbing the prefactor of the integral (2.18) and compute the resistivity

$$\rho(T) = \frac{\rho_0(T)}{(m_s + m_d) T_F^2} \beta \int_{W_{-,s}}^{W_{+,s}} d\epsilon_s \int_{W_{-,d}}^{W_{+,d}} d\epsilon_d \int_0^\pi \int_0^\pi d\theta_s d\theta_d q^2 \theta(q) f(\epsilon_s) \tilde{f}(\epsilon_s + \Delta) f(\epsilon_d) \tilde{f}(\epsilon_d - \Delta), \quad (2.20)$$

where T_F is defined as

$$T_F = \frac{k_s k_d}{2(m_s + m_d)}. \quad (2.21)$$

The temperature dependence of $\rho_0(T)$ solely arises from D defined in (2.12), since $\rho_0(T) \propto 1/D$. The above expression is a resistivity $\rho_0(T)$ times a dimensionless integral, which we proceed to evaluate by a low-temperature expansion in the following section, and by numerical integration in the next.

III. LOW-TEMPERATURE EXPANSION

Although the full temperature dependence of the conductivity requires a numerical integration, which will be discussed in Sec. IV, one can get an analytic expression for low temperatures as discussed below. At low temperatures the chemical potential is independent of the temperature, up to terms exponentially small in temperature. One then gets from (2.12)

$$\sqrt{D} = \frac{\Omega k_s^2}{2\pi m_s} + \frac{\Omega k_d^2}{2\pi m_d} = \frac{N_s}{m_s} + \frac{N_d}{m_d}, \quad (3.1)$$

where N_a is the total number of particles of the species a . The square root of the denominator is the sum of the squares of the two plasma frequencies of the two species. Therefore, $\rho_0(T)$ can be taken as a constant ρ_0 in (2.20), to get the leading temperature dependence.

If one wants only the lowest order in T one can make in (2.20) the substitution

$$\epsilon_a \pm \Delta_a(\epsilon_a, \epsilon_b) \rightarrow \epsilon_a \pm \Delta_a(0, 0), \quad (3.2)$$

since one can make an expansion of Δ in $\epsilon_{a,b}$ and, due to the Fermi factors in (2.14), $\epsilon_{a,b} \sim T$. Up to terms exponentially small in T one can also extend the limits of integration for $\epsilon_{s,d}$ to infinity. The integration over $\epsilon_{s,d}$ can then be performed to give

$$\int_{-\infty}^{\infty} \frac{d\epsilon_s}{(1 + e^{\beta\epsilon_s})(1 + e^{-\beta(\epsilon_s + \Delta_s)})} = \frac{\Delta_s}{1 - e^{-\beta\Delta_s}}. \quad (3.3)$$

The result for the integration over ϵ_d is obtained from (3.3) by changing $\Delta_s \rightarrow -\Delta_d$ in the denominator of the left-hand expression. One therefore gets for the resistivity

$$\rho(T) = \frac{\rho_0}{(m_s + m_d)T_F^2} T \times \int_0^\pi \int_0^\pi d\theta_s d\theta_d q^2 \theta(q) \frac{(\Delta\beta/2)^2}{\sinh^2(\Delta\beta/2)}, \quad (3.4)$$

where q and Δ are given by (2.17) and (2.19) with $k = k_s$ and $p = k_d$.

The low-temperature behavior of (3.4) will be different depending whether the two species have the same Fermi wave vector or not. The main results of this section are the low-temperature expansions in (3.17) and in (3.19), which are exact to $O(T^2)$. The details may be skipped in a first reading.

A. $k_s = k_d = k_f$

To exponentially small terms we have $\Delta \sim T$. Because of the factor q^2 in the integral (3.4), the lowest order in

$$\rho = \frac{\rho_0}{(m_s + m_d)T_F^2} 2k_f^2 T \int_0^1 \int_0^1 d\mu_s d\mu_d \frac{1}{\sqrt{1-\mu_s^2}} \frac{1}{\sqrt{1-\mu_d^2}} [2 - \mu_s^2 - \mu_d^2] \frac{(\Delta\beta/2)^2}{\sinh^2(\Delta\beta/2)}. \quad (3.8)$$

By using $\mu_+ = \mu_s + \mu_d$ and $\mu_- = \mu_s - \mu_d$ (3.8) becomes

$$\rho = \frac{\rho_0}{(m_s + m_d)T_F^2} k_f^2 T [I_1 + I_2], \quad (3.9)$$

where

$$I_1 = \int_0^1 d\mu_+ \int_{-\mu_+}^{\mu_+} d\mu_- G(\mu_+, \mu_-), \quad I_2 = \int_1^2 d\mu_+ \int_{-(2-\mu_+)}^{2-\mu_+} d\mu_- G(\mu_+, \mu_-), \quad (3.10)$$

and

$$G(\mu_+, \mu_-) = \frac{2 - (\mu_+^2 + \mu_-^2)/2}{\sqrt{\{1 - [(\mu_+ + \mu_-)/2]^2\} \{1 - [(\mu_+ - \mu_-)/2]^2\}}} \frac{(\beta_f \mu_+ \mu_-)^2}{\sinh^2(\beta_f \mu_+ \mu_-)}, \quad (3.11)$$

where we have introduced the dimensionless quantity $\beta_f = \beta T_F$. To evaluate I_1 one introduces $\phi = \beta_f \mu_+ \mu_-$ and $\chi = \mu_-/\mu_+$. Then I_1 becomes

$$I_1 = \beta_f^{-1} \int_0^{\beta_f} d\phi \frac{\phi^2}{\sinh^2(\phi)} \int_{\phi/\beta_f}^1 \frac{d\chi}{\chi} \frac{2\chi - [\phi/(2\beta_f)](1 + \chi^2)}{\sqrt{\chi^2 - \chi[\phi/(2\beta_f)] + [\phi/(4\beta_f)]^2(1 - \chi^2)^2}}. \quad (3.12)$$

The singularity of (3.12) comes from the terms, where $\chi \sim \phi/\beta_f$. The most singular term of (3.12) is therefore

$$I_1' = \beta_f^{-1} \int_0^{\beta_f} d\phi \frac{\phi^2}{\sinh^2(\phi)} \int_{\phi/\beta_f}^1 \frac{d\chi}{\chi} \frac{2\chi - [\phi/(2\beta_f)](1 + \chi^2)}{\sqrt{\chi^2 - \chi[\phi/(2\beta_f)] + [\phi/(4\beta_f)]^2}} \simeq \beta_f^{-1} \int_0^{+\infty} d\phi \frac{\phi^2}{\sinh^2(\phi)} 2 \ln(\beta_f/\phi). \quad (3.13)$$

The next singular terms are given by $I_1 - I_1'$. In the difference one can let $\beta_f \rightarrow \infty$, this is permissible, since we are interested in the leading T dependence. One has then $I_1 - I_1' \rightarrow 0$, therefore I_1' contains all the contribution up to order T . This is the usual idea of a subtraction integral, and it must be stressed that the corrections to the results here are of $O(T^3)$.

I_2 can be computed in a similar fashion. One can notice that, since $\Delta \sim \beta_f^{-1}$ and $\mu_+ \sim 1$, $d \sim T$. Therefore

T is controlled by the terms for which $\cos \theta_s + \cos \theta_d \sim T$. One can therefore replace in (2.19), $\cos \theta_d$ by $-\cos \theta_s$ up to higher orders in T . This gives

$$\Delta = \frac{2k_f^2}{m_s + m_d} [\cos \theta_s + \cos \theta_d] \cos \theta_s, \quad (3.5)$$

and one can symmetrize the expression using $\cos \theta_d \sim -\cos \theta_s$ as

$$\Delta = \frac{k_f^2}{m_s + m_d} [\cos^2 \theta_s - \cos^2 \theta_d]. \quad (3.6)$$

The resistivity is therefore given by

$$\rho = \frac{\rho_0}{(m_s + m_d)T_F^2} 4k_f^2 T \times \int_0^{\pi/2} \int_0^{\pi/2} d\theta_s d\theta_d \cos^2 \theta_s \frac{(\Delta\beta/2)^2}{\sinh^2(\Delta\beta/2)}. \quad (3.7)$$

Again one can symmetrize (3.7). If one introduces $\mu_{s,d} = \sin \theta_{s,d}$, (3.7) becomes

$\mu_+ + d \sim \mu_+ - d \sim \mu_+$. By making the change of variables $\phi = \beta_f \mu_+ d$, $\chi = d/(2 - \mu_+)$ one gets for I_2

$$I_2 = 2\beta_f^{-1} \int_0^{\beta_f} d\phi \frac{\phi^2}{\sinh^2(\phi)} \int_{\phi/\beta_f}^1 \frac{d\chi}{\chi} \frac{\sqrt{\chi} - \sqrt{\chi - \phi/\beta_f}}{\sqrt{\chi - T_F \phi}} \simeq 2\beta_f^{-1} \int_0^{+\infty} d\phi \frac{\phi^2}{\sinh^2(\phi)} \ln(4). \quad (3.14)$$

Using

$$\int_0^{+\infty} d\phi \frac{\phi^2}{\sinh^2(\phi)} = \frac{\pi^2}{6}, \quad (3.15)$$

$$\int_0^{+\infty} d\phi \frac{\phi^2}{\sinh^2(\phi)} \ln(1/\phi) = \frac{\pi^2}{6} \ln(\sigma), \quad (3.16)$$

where $\sigma \simeq 1.4054$, one gets for the resistivity

$$\rho(T) = \rho_0(T/T_F)^2 \frac{2\pi^2}{3} \ln(4\sigma T_F/T). \quad (3.17)$$

B. $k_s \neq k_d$

We will assume in the following that for example $k_s < k_d$. In the limit where $\beta \rightarrow \infty$ one can approximate $(\beta x)^2 / \sinh^2(\beta x)$ by $(\pi^2)/3T\delta(x)$, since

$$\int dx F(x) \frac{(\beta x)^2}{\sinh^2(\beta x)} = TF(0) \frac{\pi^2}{3} + O(T^2) \quad (3.18)$$

if F is a regular function. Then using the usual properties of the δ function one gets

$$\begin{aligned} \rho(T) &= \rho_0(T/T_F)^2 \frac{4\pi}{3} \frac{k_s}{k_d} \int_0^{\pi/2} d\theta \frac{\cos \theta}{\sqrt{1 - (k_s/k_d)^2 \cos^2 \theta}} \\ &= \rho_0 \frac{2\pi^2}{3} (T/T_F)^2 \ln \left(\frac{k_s + k_d}{k_d - k_s} \right). \end{aligned} \quad (3.19)$$

One therefore sees that the $T^2 \ln(T)$ dependence is obtained only when the Fermi wave vector of the two carriers are the same. This is related to a weak singularity of the forward scattering process in two dimensions.

IV. FULL TEMPERATURE DEPENDENCE

In order to obtain the full temperature dependence of the conductivity one needs to perform a numerical integration of (2.20). The temperature scale will be given by T_F [defined in (2.21)] so we will measure all temperatures in units of T_F defining $\tilde{T} = T/T_F$. T_F is of the order of $T_F(d) = k_d^2/(2m_d)$, but more convenient to scale out in the integrals. The resistivity in (2.20) is given by a dimensionless integral times the prefactor $\rho_0(T)$. In order to get the temperature dependence correctly, particularly for $T \gg T_F$, the temperature dependence of the denominator (2.12) in $\rho_0(T)$ must be taken into account as well. The unknown remaining constant in ρ_0 can be fitted in this model such that at sufficiently high temperatures the resistivity saturates to roughly the Mott value, i.e., dh/e^2 . In fact, the Boltzmann equation approach does not contain the essential physics of the Mott-Ioffe-Regel saturation, and we have to put it in by hand. Within this calculation the resistivity could saturate at a value lower than the Mott value, if the scattering potential is cho-

sen to be very weak. In these units the low-temperature expansions (3.17) and (3.19), respectively, become

$$\rho(T) = \rho_0 \frac{2\pi^2}{3} \tilde{T}^2 \ln(4\sigma/\tilde{T}), \quad k_s = k_d, \quad (4.1)$$

$$\rho(T) = \rho_0 \frac{2\pi^2}{3} \tilde{T}^2 \ln[(k_s + k_d)/(|k_s - k_d|)], \quad k_s \neq k_d. \quad (4.2)$$

For the numerical integration we fix the Fermi wave vectors through the density of the particles by

$$k_{s,d} = \sqrt{2\pi n_{s,d}}. \quad (4.3)$$

The bandwidth is determined by the Debye approximation as $k_{\max} = 2\sqrt{\pi}$:

$$W_{+,s} = \frac{4\pi - k_s^2}{2m_s}, \quad W_{-,s} = \frac{-k_s^2}{2m_s}, \quad (4.4)$$

$$W_{+,d} = \frac{4\pi - k_d^2}{2m_d}, \quad W_{-,d} = \frac{-k_d^2}{2m_d}.$$

This choice is somewhat arbitrary and only imperfectly reproduces the features of a real band structure. But although different and more realistic choices of the band will change the precise numerical values, they are not expected to change the qualitative features of our results. For a given tight-binding set of parameters, say a hopping integral t on a square lattice, we can estimate $m_{\text{eff}} = \hbar^2/(2ta_{\text{lattice}}^2)$. The chemical potentials that enter the Fermi occupation factors in (2.20) are fixed so that the number of particles of each species remains constant and independent of the temperature by (2.13). This constraint is unimportant if $T \ll T_F$, since the chemical potentials are independent, up to exponentially small terms, of the temperature but will be crucial if $T \gg T_F$. If one does not work with a fixed number of particles, as one should in a solid, but with a fixed chemical potential, the temperature dependence of the resistivity will be radically altered, as we will discuss later.

The results of the numerical integration are shown in Fig. 1 together with the asymptotic formula for the case of commensurate density, for two typical mass ratios. Note the rapid departure of the asymptotic curves from the exact values. Around $T/T_F = 0.5$ the resistivity is reasonably linear, and the Fermi-liquid behavior only shows up below $\sim 0.2T_F$. For $T_F \ll T \ll T_s$ the resistivity saturates. Figure 2 shows the same comparison for noncommensurate values of the Fermi diameters. Figures 3 and 4 show similar results for emptier bands, at both commensurate and incommensurate densities. Here also the departure from the asymptotic result occurs at temperatures much lower than T_F . The crossover region is larger but shows no improvement in the linearity, and at high temperature the differences between commensurate and incommensurate densities disappears. Note that in this model the ‘‘linear’’ regime found between the Fermi liquid and the saturation regime is merely a consequence of the existence of an inflection point in the curve and is rather limited in temperature.

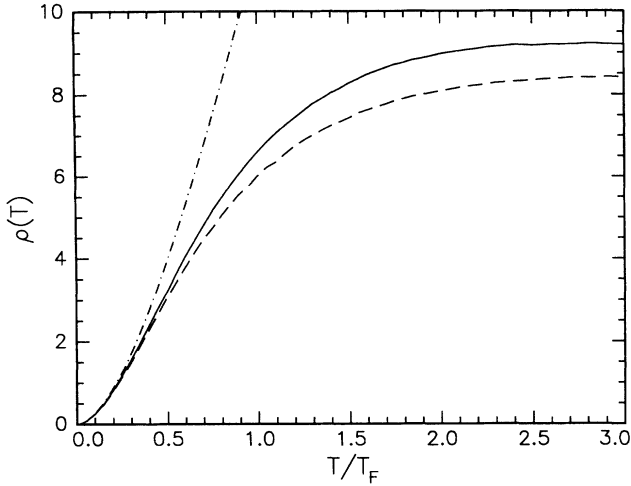


FIG. 1. Dimensionless resistivity $\rho(T)/\rho_0$ as a function of the temperature for $k_s = k_d = \sqrt{\pi}$. The solid line is for $m_s = 1$, $m_d = 5$, the dotted line for $m_s = 1$, $m_d = 10$, and the dashed-dotted line is the asymptotic formula, valid for low temperatures.

It is interesting to note that if the constant number constraint on the d electrons is replaced by a constant chemical potential, then a very large region of linearity results for $T_F \ll T \ll T_s$. This artificial linearity is due to the fact that a large number $[O(T)]$ of scatterers (d electrons) becomes available by the neglect of the number conservation, when $T \gg T_F(d)$.

Some recent data of Takagi and Batlogg⁸ on the family $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, shows a progression of behavior on increasing x . They find three regions: (a) $x \ll 0.15$, where the resistivity increases very rapidly with temperature, and saturates at a value near the Mott resistivity; (b)

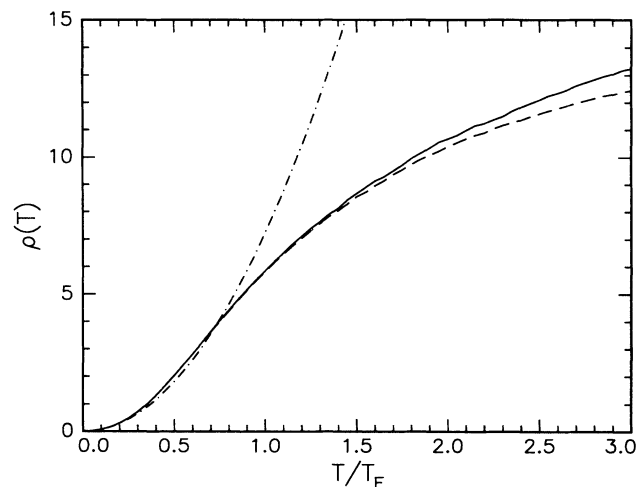


FIG. 2. Dimensionless resistivity $\rho(T)/\rho_0$ as a function of the temperature for $2k_s = k_d = \sqrt{\pi}$. The solid line is for $m_s = 1$, $m_d = 5$, the dotted line for $m_s = 1$, $m_d = 10$, and the dashed-dotted line is the asymptotic formula, valid for low temperatures.

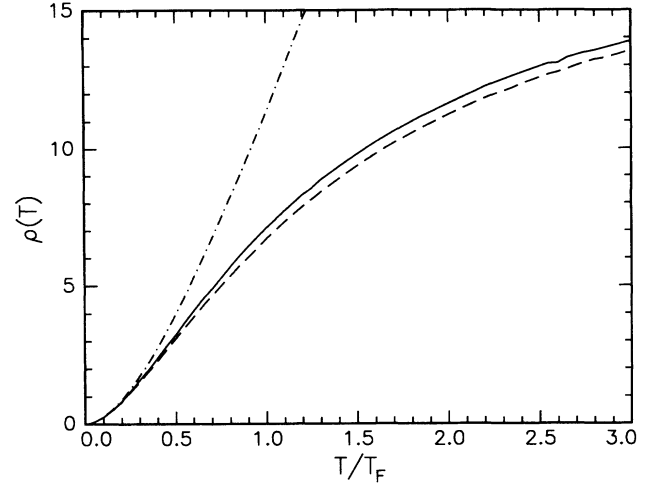


FIG. 3. Dimensionless resistivity $\rho(T)/\rho_0$ as a function of the temperature for $2k_s = 2k_d = \sqrt{\pi}$. The solid line is for $m_s = 1$, $m_d = 5$, the dotted line for $m_s = 1$, $m_d = 10$, and the dashed-dotted line is the asymptotic formula, valid for low temperatures.

$x \sim 0.15$, where the resistivity is linear over a very large range—this is the optimum T_c case, and (c) $x \gg 0.15$, where the resistivity is sublinear and shows no saturation. In view of our results, we feel that the linear and the underdoped cases are not understandable within the framework of a two-band model, but the overdoped case may very roughly be consistent with it.

We also take this opportunity to point out what seems to be an error in a recent series of papers, on the same model in two dimensions, asserting that the resistivity is linear in T in the asymptotic regime.^{12,13} The asymptotic behavior is $O(T^2)$ with possible log corrections as we have

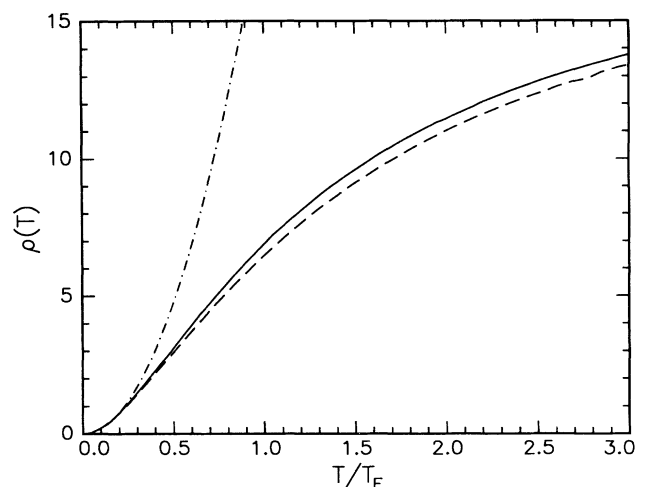


FIG. 4. Dimensionless resistivity $\rho(T)/\rho_0$ as a function of the temperature for $k_s/\sqrt{\pi} = 0.5$, $k_d/\sqrt{\pi} = 0.447$. The solid line is for $m_s = 1$, $m_d = 5$, the dotted line for $m_s = 1$, $m_d = 10$, and the dashed-dotted line is the asymptotic formula, valid for low temperatures.

shown in detail by direct calculation here.

The issue of logarithmic corrections was first pointed out for a one-band model in Ref. 14. In fact, umklapp scattering in a one-band model has much of the character in our "commensurate" case, since the two species are collapsed into one. This case, however, lacks the richness of the two-band model, since there is only one Fermi temperature in that problem, namely, a high-temperature scale, and the entire issue of crossover has a very different character.

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APPENDIX

In this appendix we rederive the resistivity for a two-band system using the memory function formalism.¹⁵ This formalism has the advantage to show in a clearer way that the finite resistivity is related to the noncommutativity of the current operator with the Hamiltonian, and can be straightforwardly extended to the finite frequency response. Conversely the variational principle is

lost. In our case both Boltzmann and memory function give the same answer.

If one assumes that the system is a normal conductor (σ finite) at zero frequency then the conductivity can be expressed in terms of the meromorphic memory function $M(\omega)$ by¹⁵

$$\sigma(\omega) = \frac{-i\chi(0)}{\omega + M(\omega)}, \quad (\text{A1})$$

where

$$M(\omega) = \frac{\omega\chi(\omega)}{\chi(0) - \chi(\omega)}, \quad (\text{A2})$$

and $\chi(\omega)$ is the retarded current-current correlation function. $\chi(0)$ is equal to the plasma frequency of the system if the system has a finite resistivity at $\omega = 0$.¹⁵ One has $\chi(0) = N_s/m_s + N_d/m_d$. The calculation of the memory function can be carried out perturbatively to give at the lowest order¹⁵

$$M(\omega) = \frac{[\langle F; F \rangle_\omega^0 - \langle F; F \rangle_{\omega=0}^0]/\omega}{-\chi(0)}. \quad (\text{A3})$$

The F operators take into account the fact that the current is not a conserved quantity $F = [j, H]$ and $\langle F; F \rangle_\omega^0$ stands for the retarded correlation function of the operator F at frequency ω computed in the *absence* of the scattering potential [(2.3) in our case]. Notice the similitude between (2.9) and (A3). In particular, the denominators are identical in the two formulations as can be seen from (2.12).

The commutator of the current and the Hamiltonian is given by

$$F = [J, H] = \frac{J}{\sqrt{S(S+1)}\Omega} \sum_{k,p,q} [v_s(k+q) - v_s(k) + v_d(p-q) - v_d(p)] \mathbf{S}_{k+q,k}^s \cdot \mathbf{S}_{p-q,p}^d, \quad (\text{A4})$$

where v is the velocity of the particle and is simply, for our parabolic band model, $v_a(k) = k/m_\mu$. It is obvious from (A4) that if the masses of the two species are equal the resistivity vanishes since now the current is a conserved quantity.

One can easily show

$$\langle F; F \rangle = -\frac{J^2}{\Omega} \sum_{k,p,q} v_{k,p,q}^2 \frac{[f(\epsilon_s(k)) - f(\epsilon_s(k) + \Delta_s)][f(\epsilon_d(p)) - f(\epsilon_d(p) + \Delta_d)][f_b(\Delta_d) - f_b(-\Delta_s)]}{\omega - \Delta_d - \Delta_s + i\epsilon}, \quad (\text{A5})$$

where $v_{k,p,q}$ and Δ have been defined in (2.15) and (2.16). f is the Fermi function and f_b the Bose one. By using (A1) and (A5) one can get the temperature and frequency dependence of the conductivity. For $\omega = 0$ the resistivity is simply the imaginary part of M . One gets from (A5) for the imaginary part of the memory function

$$\chi(0)\text{Im}M(\omega) = \frac{1 - e^{\beta\omega}}{\omega} \frac{J^2\pi}{\Omega} \sum_{k,p,q} v_{k,p,q}^2 f(\epsilon_s(k)) \tilde{f}(\epsilon_s(k) + \Delta_s) f(\epsilon_d(p)) \tilde{f}(\epsilon_d(p) + \Delta_d) \delta(\omega - \Delta_s - \Delta_d) \quad (\text{A6})$$

and by taking the limit $\omega \rightarrow 0$ one recovers (2.14).

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