Exchange theory of resistivity saturation

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We suggest that the well-known phenomenon of resistivity saturation in *d*-band metals can be due to the density-of-states anomaly of Altshuler and Aronov. We derive the functional form of the saturation equation and an expression for the saturation resistivity.

It has been known[1,2] for many years that electrical resistivities of strong-scattering metals often equal and rarely exceed a value ρ_{max} given approximately by

$$\rho_{max} \simeq \frac{\hbar}{e^2} a \simeq 150\ \mu\Omega\ \text{cm}\ , \tag{1}$$

where a is a typical interatomic spacing. Three examples of this,[3–5] each associated with a different scattering mechanism, are shown in Fig. 1.

Although its relevance to all of Fig. 1 is commonly assumed, the term "resistivity saturation" refers specifically to the behavior shown in Fig. 1(b): A linear increase of ρ with temperature until ρ_{max} is reached, and then "saturation" at ρ_{max} thereafter. We are persuaded by the arguments of Allen[1] that this behavior has not yet been satisfactorily explained. It has been quantified, however, by Wiesmann *et al.*,[3] who observe that measured resistivities ρ_{meas} of radiation-damaged $A15$'s are accurately given by a law of the form

$$\frac{1}{\rho_{meas}} = \frac{1}{\rho_{ideal}} + \frac{1}{\rho_{max}}\ , \tag{2}$$

where the ideal resistivity takes a form linear in T

$$\rho_{ideal}(T) = \rho_0 + \rho_1 T \tag{3}$$

consistent with most solutions of the Boltzmann equation.[6] Resistivity saturation has been correctly associated by these authors and others[7] with the approach of the mean free path l to a minimum value near a. It is thus vaguely consistent with Mott's[8] ideas about the existence of a minimum metallic conductivity $\sigma_{min} \simeq 0.026 e^2/\hbar a$. However, there are several difficulties with associating ρ_{max} with σ_{min}^{-1} (Ref. 1): Ba attains a resistivity of 213 $\mu\Omega$ cm before melting, with no sign of saturation; in layer materials such as TaS_2 $\rho_{max} \sim 300\ \mu\Omega$ cm; Mott's original estimate of σ_{min} yields $\rho_{max} \sim 3000\ \mu\Omega$ cm. We venture to add that neither resistivity saturation nor σ_{min} has been observed in phosphorous-doped silicon,[9] a system in which the metal-insulator transition has been studied in great detail. Furthermore, neither is consistent with recent scaling theories of the transition.[10,11]

In this paper, we suggest that a law of the form of Eq. (2) can be a consequence of the depression of the density of states at the Fermi surface due to diffusion, recently identified by Altshuler and Aronov[12] as the cause of the giant zero-bias anomaly in tunneling spectroscopy. In our picture, resistivity saturation occurs because increasing disorder, via the exchange interaction, increases the Fermi velocity, and thus causes carriers to scatter less efficiently.

Following Abrahams *et al.*[13] we shall argue using the metal's known neutral density-density correlation function, given at small q and ω by

$$\chi(q,\omega) = -2\nu(0)\left[\frac{(sq)^2}{\omega^2 - (sq)^2 + i\omega/\tau}\right]\ , \tag{4}$$

where $\nu(0)$ is the single-spin density of states at the Fermi surface, s is the sound velocity, given nominally by $v_F/\sqrt{3}$, and τ is the semiclassical elastic collision time. χ is formally related to ψ_j, the eigenstates of the full single-particle Hamiltonian, by

$$\chi(q,\omega) = \sum_{j\ \text{filled}} \sum_{j'\ \text{empty}} \frac{1}{\epsilon_{j'} - \epsilon_j - \hbar\omega + i\delta} \int \langle \psi_{j'}^*(r)\psi_j(r)\psi_{j'}(r')\psi_j^*(r')\rangle \exp[-iq(r-r')]\, d(r-r')\ , \tag{5}$$

where angle brackets denote ensemble average. We emphasize that this is true even near the melting point so long as $kT \ll \hbar/\tau$, which is the case in strong-scattering metals. The single-particle eigenstates of the hot system are those of a disordered cold one, ensemble averaged over configurations sampled by the thermal motion of the nuclei. Equation (4) is commonly obtained from Eq. (5) diagrammatically using a ladder approximation. This is tantamount in most cases to solving the Boltzmann equation for quasiparticle motion, and thus we emphasize that χ takes the form of Eq. (4) for any met-

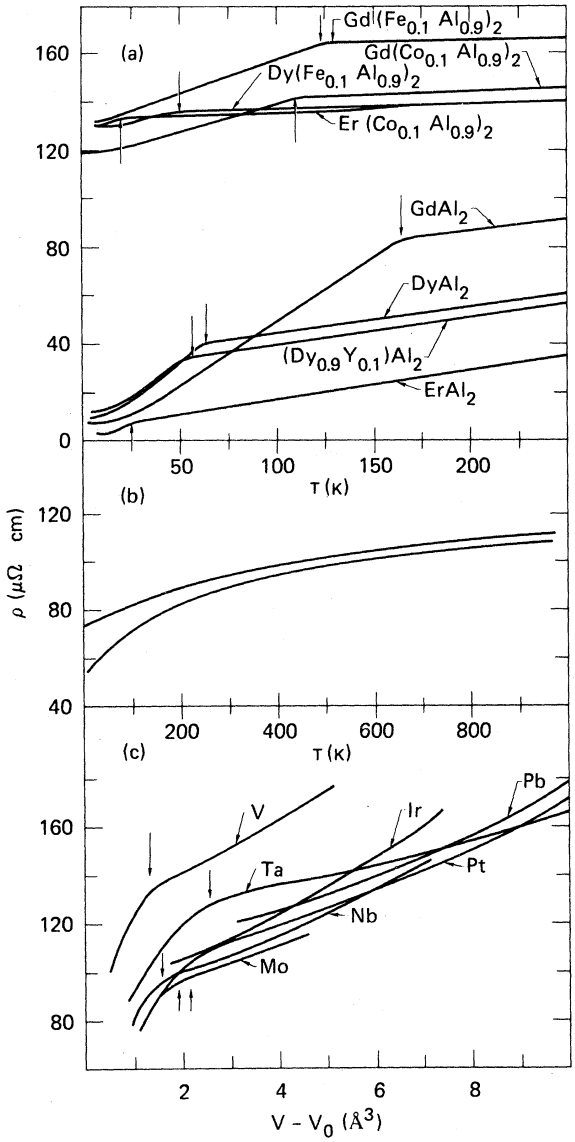

FIG. 1. (a) Resistivity vs temperature for stoichiometric and nonstoichiometric magnetic alloys taken from Ref. 4. Arrows indicate the Curie point. Residual $T=0$ resistivity due to leftover spin-disorder scattering. (b) Resistivity vs temperature for α-damaged films of Nb_3Ge taken from Ref. 3. Results for samples with different annealing histories are shown. Resistivity due to damage and phonons. (c) Resistivity vs volume gain per atom for certain expanded liquid metals taken from Ref. 5. Arrows indicate the melting point. Temperature-independent resistivity due to configurational disorder in the fluid.

al which is a good Fermi liquid. We observe that if the Fermi velocity is dialated in the manner

$$v_F \rightarrow v_F/x \ , \tag{6}$$

and if all other parameters in the system, e.g., the area of the Fermi surface and the scattering potential, remain unchanged, then χ becomes

$$\chi \rightarrow -2\nu(0)(x)\left[\frac{(sq/x)^2}{\omega^2-(sq/x)^2-i(\omega/x\tau)}\right] \ . \tag{7}$$

Following Abrahams *et al.* we assume that the average exchange interaction between two electrons depends only on their separation in energy $\hbar\omega$. We may then write this interaction $V(\omega)$ as

$$V(\omega)=\frac{1}{\pi\hbar\omega[\nu(0)]^2L^3} \times \mathrm{Im}\left[\frac{1}{(2\pi)^3}\int\frac{\chi(q,\omega)}{2}v(q)\,dq\right] \ , \tag{8}$$

where L^3 is the sample volume and $v(q)$ is, again nominally,

$$v(q)=\frac{4\pi e^2}{q^2+\lambda^2} \ . \tag{9}$$

The exchange self-energy felt by an electron ϵ above the Fermi surface is then

$$\Sigma(\epsilon)=\int_{\epsilon}^{\infty}V(\omega)\ \nu(0)L^3 d(\hbar\omega) \ , \tag{10}$$

and thus the exchange contribution to the reciprocal density of states is proportional to

$$\frac{\partial\Sigma}{\partial\epsilon}=\frac{e^2\lambda}{\hbar\pi}\left[\frac{\hbar}{\epsilon}\mathrm{Re}\left(\frac{z\sqrt{z}}{1+z}\right)+\frac{1}{(s\lambda)^2\tau}\frac{1}{|1+z|^2}\right] \ , \tag{11}$$

where

$$z=\frac{\epsilon^2+i\epsilon/\tau}{(\hbar\lambda s)^2} \ . \tag{12}$$

This is plotted for various values of τ in Fig. 2. We observe that the $\tau\rightarrow\infty$ limit agrees poorly with the known value of $V(\omega)$ for the electron gas, in that it goes to zero as $\omega\rightarrow 0$ and increases in magnitude with increasing ω. This is because of the unrepresentative behavior of Eq. (4) at large values of q, which are weighted heavily in Eq. (8). However, as we are interested in the changes in $V(\omega)$ induced by the presence of a nonzero $1/\tau$, this discrepancy is unimportant. Figure 2 shows that electrons nearby in energy exchange more strongly in the presence of scattering than in its absence. This is because scattering causes the eigenstates ψ_j to have inhomogeneities on the scale of l which correlate for states nearby in energy.

The physical significance of the density-of-states suppression described by Eq. (1) is that disorder and exchange together increase the Fermi velocity. In general, the combined effects of Coulomb interactions and disorder are difficult to couch in terms of Fermi-surface parameters; indeed, in the limit $\partial\Sigma/\partial\epsilon \ll 1$, corrections to the electron-hole scatter-

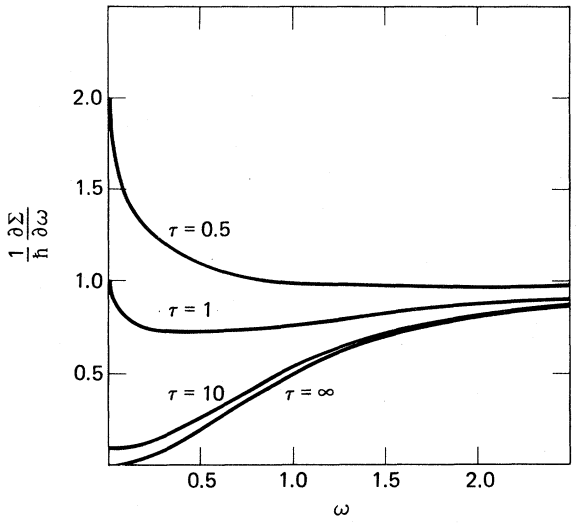

FIG. 2. $\partial\Sigma/\partial\epsilon$ as given by Eq. (11) vs ω for various values of τ. The units of ω and $1/\tau$ are $s\lambda$. $e^2\lambda/\hbar\pi$ is taken to be 1. Note that the cusp at $\omega = 0$ will be smoothed at high temperature by approximately $\Delta\omega = kT$.

ing rate can be shown[12] to overwhelm the Fermi velocity increase and cause the resistivity to rise. However, we are interested in the limit $\partial\Sigma/\partial\epsilon \gtrsim 1$, when the expansion in the strength of the Coulomb interaction leading to this result diverges. As in a disorder-free metal, it is appropriate in this case to sum the Coulomb interaction to all orders via the screened Hartree-Fock approximation. This can be done simply if we make two assumptions: (1) that, as in the disorder-free metal, the Coulomb vertex correction is small, and (2) that the "impurity lines" connecting the particle and hole in the conductivity diagram have a negligible effect. Neither of the assumptions is justified when $\partial\Sigma/\partial\epsilon << 1$.[12] However, they preclude non-Fermi-liquid behavior, which we note has not been observed to be significant in the strongly interacting case. We perform the Hartree-Fock calculation by solving Eqs. (7) and (11) self-consistently. If we denote quantities in the absence of the density-of-states suppression by subscript 0, and let

$$x = \frac{\nu(0)}{\nu_0(0)} \ , \tag{13}$$

we have

$$\frac{1}{x} = 1 + \frac{1}{x}\frac{\partial\Sigma}{\partial\epsilon}\bigg|_{\epsilon=0} = 1 + x^2\left(\frac{T}{\tau_0}\right) \ , \tag{14}$$

where

$$T = e^2/\pi\hbar s_0^2\lambda \ . \tag{15}$$

If we let

$$\rho_{\text{ideal}} = \frac{1}{2\nu_0(0)s_0^2e^2\tau_0} \ , \tag{16}$$

$$\rho_{\max} = \frac{1}{2\nu_0(0)s_0^2e^2T} = \frac{\pi\hbar\lambda}{2\nu_0(0)e^4} \ , \tag{17}$$

and

$$\rho_{\text{meas}} = \frac{1}{2\nu(0)s^2e^2\tau} = x^2\rho_{\text{ideal}} \ , \tag{18}$$

the solution of Eq. (14) yields

$$\rho_{\text{meas}} = \tfrac{4}{3}\rho_{\max}\sinh^2\left\{\tfrac{1}{3}\sinh^{-1}\left[3\left(\frac{3}{4}\frac{\rho_{\text{ideal}}}{\rho_{\max}}\right)^{1/2}\right]\right\} \ . \tag{19}$$

This is plotted, together with Eq. (2), in Fig. 3. The two can be seen to agree closely over the range of interest.

We use Eq. (17) to estimate the size of $\rho_{\max}$ in Nb. From the augmented plane wave (APW) calculation of Mattheiss[14] we obtain a bare single-spin density of states at the Fermi surface of $\nu_0(0) = 0.045$ Å^{-3}eV^{-1}, and a Fermi-Thomas screening parameter of $\lambda_{\text{FT}} = [(8\pi e^2\nu_0(0)]^{1/2} = 4.04$ Å^{-1}. From the electronic susceptibility calculations of Cooke *et al.*[15] we find a disorder-free $\chi(q,w,)$ which varies from its Fermi-Thomas value of $2\nu_0(0)$ at the zone center to 0.36 of this value at the zone edge. Thus, defining

$$\rho_{\max}^{\text{FT}} = \frac{\pi\hbar\lambda_{\text{FT}}}{2\nu_0(0)e^4} = \simeq 400\ \mu\Omega\ \text{cm} \ , \tag{20}$$

we have approximately

$$\rho_{\max}^{\text{FT}} \gtrsim \rho_{\max} \gtrsim \sqrt{0.36}\rho_{\max}^{\text{FT}} \ , \tag{21}$$

which agrees well with the 230 $\mu\Omega$ cm estimated by Wiesmann *et al.*[3]

We remark that the energy scale in Fig. 2 is determined by λs, which equals the plasma frequency in simple metals. Even with the parameters we assume for Nb, the width of the cusp in the saturation regime is several eV, which is sufficient to prevent significant thermal smearing at temperatures comparable

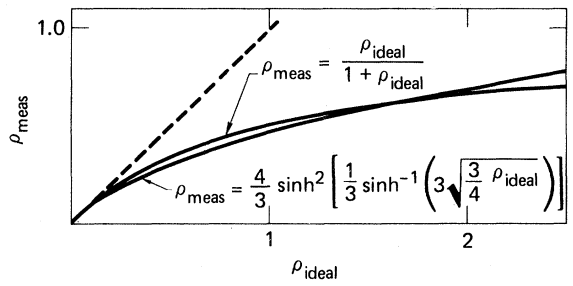

FIG. 3. Resistivity saturation given by Eq. (19) compared to that given by Eq. (2). $\rho_{\max}$ is taken to be 1.

to the melting temperature. Were this not the case, the more complicated high-temperature version of the Altshuler-Aronov theory would need to be invoked. We remark also that the validity of our explanation of resistivity saturation implies a relationship between resistivity and the Fermi-surface density of states involving only the empirically determined parameter $\rho_{\max}$. We have

$$\frac{\nu(0)}{\nu_0(0)} \simeq \left[1 - \frac{\rho}{\rho_{\max}}\right]^{1/2} . \tag{22}$$

This can be tested experimentally either by direct tunneling measurements of the density of states of by correlating impurity resistivities of superconductors with their transition temperatures.

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