Conductivity scale in disordered systems

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(Received 3 June 1983)

A reanalysis of the correction to the Boltzmann conductivity due to maximally crossed graphs for degenerate bands explains why the conductivity scale in many-valley semiconductors is an order of magnitude higher than Mott's "minimum metallic conductivity." With the use of a reasonable assumption for the Boltzmann mean free path, the lowest-order perturbation theory is seen to give a remarkably good, semiquantitative, description of the conductivity variation in both uncompensated doped semiconductors and amorphous alloys.

The traditional scale of conductivity in three-dimensional disordered systems undergoing a metal-insulator transition has been the "minimum metallic conductivity" due to Mott[1]:

$$\sigma_M = C_M e^2/\hbar a \ , \tag{1}$$

where a is an average distance between the scattering centers ($a \equiv n^{-1/3}$, where n is the density of scatterers) and C_M is a numerical factor which Mott has estimated[2] to be in the range $C_M \sim 0.025$–0.1. According to Mott, the conductivity drops suddenly from σ_M to zero as the insulating phase is approached. This point of view had been taken in the analysis of many earlier experiments.[3] Recent low-temperature conductivity measurements on a variety of systems[4–8] [the most convincing of which are in Si:P (Ref. 4) and Nb-Si (Ref. 8)], however, have indicated a continuous, critical onset $\sigma = \sigma_0(n/n_c - 1)^{\nu}$, as per the picture put forth by scaling theories for localization induced by disorder,[9] or by disorder with interaction effects.[10,11] The exponent ν in the various cases is found to be different—the metal-semiconductor alloys,[6,8] as well as compensated doped semiconductors,[7] yield $\nu \sim 0.8$–1.0, the upper end coinciding with predictions for the noninteracting case,[9] while uncompensated Si:P exhibits a near square-root onset ($\nu \approx 0.5$), in fair accord with that predicted recently[11] for the interacting case. Another point of difference is the conductivity scale σ_0, estimated on the basis of weak scattering perturbation theory[9] to be $\sim \sigma_M$ within a factor of 2 or so. While this seems to work for the amorphous alloy systems, there is a discrepancy of over an order of magnitude in Si:P as emphasized in a number of papers.[4,7,12] In this paper we present a simple resolution of this apparent discrepancy in the conductivity scale without introducing major changes in the conductivity scale for the amorphous alloy systems. In addition, with the help of one further assumption regarding the Boltzmann mean free path (based on results using Thomas-Fermi screened impurity scattering formulas for doped semiconductors), we investigate to what extent the weak scattering perturbation theory is able to account for the conductivity reduction in these systems.

Consider the set of maximally crossed diagrams[9] which lead to a correction of the Boltzmann conductivity: In an f-fold–degenerate case [$f = v(2s+1)$, where v is the degeneracy of the band extrema and $(2s+1)$ the spin degeneracy], without interband (intervalley) scattering, one has

$$\delta\sigma_L = f\frac{\hbar e^2}{2\pi\Omega}\sum_{\vec{p}}\frac{p_\gamma/m}{(\epsilon_{\vec{p}}-\epsilon_F)^2+(\hbar/2\tau)^2}\sum_{\vec{p}'}W(\vec{p},\vec{p}')\frac{p'_\gamma/m}{(\epsilon_{\vec{p}'}-\epsilon_F)^2+(\hbar/2\tau)^2} \tag{2}$$

as the sum of crossed graphs, where

$$W(\vec{p},\vec{p}') = \frac{n_i V^2 d}{(\vec{p}+\vec{p}')^2 v_F^2 \tau^2} \ , \tag{3}$$

n_i is the impurity density, V the scattering potential, and $\tau(l)$ the elastic scattering time (length) given by

$$\tau = \frac{l}{v_F} = \frac{\hbar}{2\pi n_i V^2 N_0} \ , \tag{4}$$

where N_0 is the Fermi surface density of states for a single spin and single valley.

Performing the integral over $\vec{p}$ and $\vec{p}'$, up to an upper cutoff π/l, one obtains the degenerate band version of the familiar result

$$\delta\sigma_L = -\frac{fe^2}{2\pi^2\hbar}\left(\frac{1}{l}-\frac{1}{L}\right) \ . \tag{5}$$

In the $L \to \infty$ limit, thus for $s = \frac{1}{2}$ electrons,

$$\sigma = \sigma_B - \frac{ve^2}{\pi^2\hbar l} = \sigma_B\left(1-\frac{3}{(k_F l)^2}\right) \ . \tag{6}$$

In this form, derived previously by other methods,[13] the band degeneracy factor is included completely in the Boltzmann conductivity:

$$\sigma_B = ve^2\tau/m^* = ve^2 k_F^2 l/3\pi^2\hbar \ . \tag{7}$$

Equation (6), based on lowest-order renormalized perturba-

tion theory, but believed to be good to many more (perhaps all) orders,[14] implies a critical point ($\sigma \to 0$) at a density n_c given by $k_F l = \sqrt{3}$. We claim therefore that the relevant conductivity scale σ_0 for pure localization is the Boltzmann conductivity at the critical point, i.e.,

$$\sigma_0 \simeq \sigma_B(n_c) = \frac{1}{3^{1/6}} \left(\frac{v}{\pi^2} \right)^{2/3} \frac{e^2}{\hbar n_c^{-1/3}} \simeq 0.18 v^{2/3} \frac{e^2}{\hbar n_c^{-1/3}} \ . \tag{8}$$

For doped silicon ($v = 6$), Eq. (8) yields

$$\sigma_B(n_c) \simeq 0.60 e^2/\hbar n_c^{-1/3} \simeq 12 \sigma_M \ ,$$

where

$$\sigma_M(\mathrm{Si}) = 0.05 e^2/\hbar n_c^{-1/3} \simeq 20 \ (\Omega \ \mathrm{cm})^{-1} \ .$$

This is in excellent agreement with the experimental scale[4] for uncompensated Si:P, $\sigma_0 \simeq 13 \sigma_M$. The calculated result for doped Ge ($v = 4$) is

$$\sigma_B(n_c) \simeq 0.46 e^2/\hbar n_c^{-1/3} \simeq 9 \sigma_M \ ,$$

again in agreement with the experimental result[7] for weakly compensated ($< 5\%$) Ge:Sb, $\sigma_0 \simeq 9 \sigma_M$.

For Nb-Si, which is found to have a linear conductivity onset,[8] as does Eq. (8), a more direct comparison can be made by looking at the coefficient of the linear onset. If the variation of the (noncritical) Boltzmann mean free path with n is neglected,[15] the derivative of Eq. (6) gives

$$\left(n \frac{d\sigma}{dn} \right)_{n_c} = \frac{2}{3} \sigma_B(n_c) \simeq 0.12 \frac{e^2}{\hbar n_c^{-1/3}} \ , \tag{9}$$

which compares quite favorably with the experimental result

$$\left(n \frac{d\sigma}{dn} \right)_{n_c} \simeq 3.4 \sigma_M \simeq 0.09 \frac{e^2}{\hbar n_c^{-1/3}} \tag{10}$$

[$\sigma_M = 0.026 e^2/\hbar n_c^{-1/3}$ for Nb-Si (Ref. 8)]. The difference may be due in part to electron interaction effects and in part to the fact that the real system is compensated; thus the concentration of carriers that enters Eq. (9) is lower than the Nb concentration that enters Eq. (10). The same approximation (constant l) allows rewriting Eq. (6) in the form

$$\sigma_B(n) = \sigma_B(n_c) \left[\left(\frac{n}{n_c} \right)^{2/3} - 1 \right] \ . \tag{11}$$

A plot of Eq. (11) along with data in amorphous alloys[5,6,8] is shown in Fig. 1, using $\sigma_M = 100 \ (\Omega \ \mathrm{cm})^{-1}$.

Next we explore the extent to which weak scattering perturbation theory modifies the Boltzmann conductivity and compare the deviations predicted with those actually seen in disordered systems undergoing a metal-insulator transition. To implement this, it is necessary to include, in addition to the localization term ($\delta\sigma_L$), the corresponding term due to electron interaction effects ($\delta\sigma_I$). As shown by Altshuler and co-workers,[16] electron interactions in a disordered system lead to a temperature dependence of the conductivity of the form

$$\sigma(T) - \sigma(0) = m T^{1/2} \ , \tag{12}$$

where, for the nondegenerate free-electron case,

$$m = \frac{0.4 e^2}{\pi^2 \hbar} \left(\frac{4}{3} - 2F \right) \left(\frac{k_B}{\hbar v_F l} \right)^{1/2} \ . \tag{13}$$

(The equation for m is the many-valley case depends on mass anisotropy as well as intervalley scattering; the reader is referred to Ref. 17 for details.) In Eq. (13), F is the Hartree contribution, which varies depending on the screening length λ between $0 (\lambda \to 0)$ and $1 (\lambda \to \infty)$.

The same processes which give these anomalous, non-Fermi-liquid-like contributions give rise to a correction to the zero-temperature conductivity (from the upper energy cutoff $\hbar/\tau$), given by

$$\delta\sigma_I = -m (\hbar/\tau)^{1/2} \ , \tag{14}$$

which must be added to Eq. (6) to give the net conductivity in this order of perturbation theory.[18] Note that m can be of either sign, depending on whether $F > \frac{2}{3}$ or $F < \frac{2}{3}$, so the correction of Eq. (14) can be positive or negative. [However, its sign is opposite to that of the T dependence, Eq. (12).]

Besides interaction effects, one needs the Boltzmann mean free path l, as well as a wide range of density over which accurate measurements are available, including far from the transition (outside the critical region), where perturbation theory may be expected to work. Of the two systems on which precision measurements are available,[4,8] unfortunately the Nb-Si data are mostly in the critical region where perturbation theory is not likely to be quantitative.[19]

Further, accurate first-principles calculations of the Boltzmann mean free path are not available for either system. For doped semiconductors calculations based on simple screening approximations do exist,[20,21] but, as pointed out in these papers, are reliable only on a scale $\sim 30\%$ or so. However, one remarkable result which comes out is the relative insensitivity of the Boltzmann mean free path on impurity density in the entire range $10 n_c \gtrsim n \gtrsim n_c$ (this is displayed for Si:P in Fig. 2 of Ref. 12 which depicts the

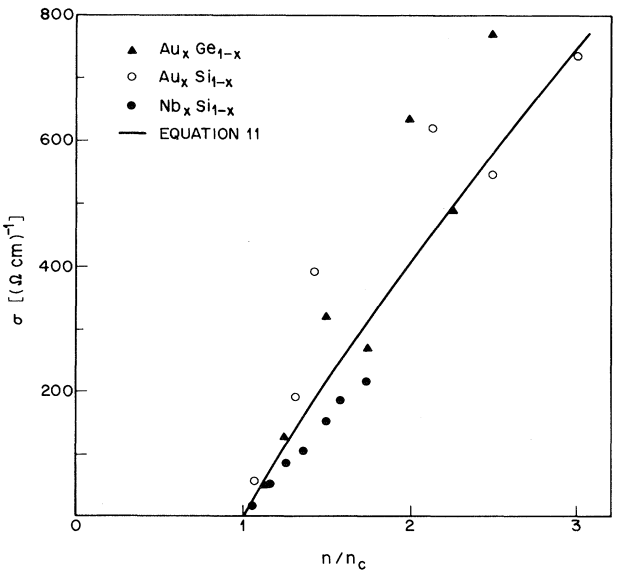

FIG. 1. Conductivity data (points) for amorphous alloys (Refs. 5, 6, and 8) along with Eq. (11) (solid line) with $\sigma_M = 100 \ (\Omega \ \mathrm{cm})^{-1}$.

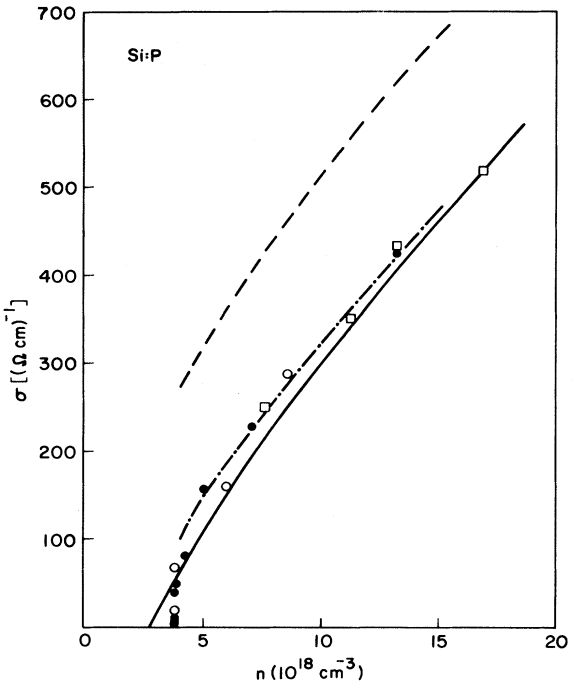

FIG. 2. Boltzmann conductivity σ_B (dashed line), perturbation result without interactions (solid line) fitted at $n = 17 \times 10^{18}$ cm^{-3}, and with interactions (dot-dashed line) along with experimental results (Refs. 4 and 7) as a function of donor concentration in Si:P.

mean free path calculated from the treatment described in Ref. 21). This comes about as a result of a cancellation of two effects: As the impurity concentration is increased, the reduction in scattering resulting from better screening of the impurities is offset by the increase in the number of scattering centers. If we assume this constancy of l,[22] then we can determine the magnitude of l and hence the full n dependence of the conductivity of Si:P as given by Eqs. (6) and (14), by fitting it at one concentration $n >> n_c$, where the weak scattering approximation should be valid. In Si:P, the procedure is simplified by the fact that the interaction correction is small[23] except near n_c, because of a cancellation[17] between the Hartree and exchange terms [Eq. (13)]. Thus l can be determined by fitting the conductivity at the highest density to Eq. (6). With no further adjustable parameters left in Eq. (6) [k_F is determined from the electron density n (Ref. 24)], the resultant curve, shown as the solid line in Fig. 2, represents the perturbation theory result without interaction effects. The dashed line is the Boltzmann result with this value of l (73 Å). We then add the interaction term, Eq. (14), using the *experimentally determined* value[23] of m (since theoretical estimates have uncertainty owing to the cancellation alluded to earlier) to obtain the dot-dashed curve. As can be seen, the perturbation theory result with one adjustable parameter agrees remarkably well with the experiment, right down to $\sigma \sim 100-150$ $(\Omega\,\mathrm{cm})^{-1}$. Further, it has the attractive feature that the critical density predicted by Eq. (6) is below the experimental value, i.e., electron correlations stabilize the insulating phase, and Fig. 2 gives an idea of by how much.

We wish to add one final speculative remark: If we take the perturbative result literally close to the transition, with additive corrections due to interaction and localization effects,

$$\sigma(0) = \sigma_B + \delta\sigma_L + \delta\sigma_I = (\sigma_B + \delta\sigma_L) - m(\hbar/\tau)^{1/2} , \qquad (15)$$

and assume that near n_c the (slow) variation of σ_B, $\delta\sigma_L$, and τ can be neglected, then Eq. (15) suggests a linear relationship between the zero-temperature conductivity and the coefficient of the $\sqrt{T}$ correction. Such a linear relationship *is* seen in stress tuning experiments[12] on Si:P, very close to the transition at temperatures below 100 mK, with the constant term $(\sigma_B + \delta\sigma_L) \sim \sigma_M$, the Mott value [Eq. (1)]. A possible explanation is that at low enough temperatures or large enough length scales one crosses over into a regime where intervalley scattering becomes important.[25] In this coupled many-channel limit localization effects are small.[26] The dependence of $\sigma(0)$ only on the interaction parameter (m) and the small conductivity scale $[(\sigma_B + \delta\sigma_L) \sim \sigma_M \sim \sigma_B/v]$ at which this occurs are both consistent with this explanation. However, the values of m obtained are larger than the theoretical maximum for weak scattering [Eq. (13)]. Thus at present the above scenario can, at best, be described as conjectural.

In conclusion, we have shown, using weak scattering perturbation theory, that the simple estimate for the conductivity scale within the scaling theory of localization for many-valley semiconductors is an order of magnitude larger than Mott's minimum metallic conductivity, and in agreement with experimental findings. Further, the perturbation approach is seen to give a rather clear, quantitative picture of the conductivity far from the transition and identification of the critical region. A similar picture in other disordered systems is clearly desirable.

ACKNOWLEDGMENTS

We thank D. Bishop and G. A. Thomas for helpful discussions and for providing data prior to publication. One of us (R.N.B.) would like to acknowledge a travel grant by the National Science Foundation, and the hospitality of the Indian Institute of Science, Bangalore, where this work was done.

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