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Evidence for a first-order correction to the Boltzmann conductivity of a disordered three-dimensional electron gas

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Analysis of data from several experimental groups on electron mobility in dense neutral gases from 3 to 300 K reveals the existence of a correction to the mobility arising from incoherent multiple scattering that is proportional to $1/k\ell_o$. This correction overwhelms the traditionally used $1/(k\ell_o)^2$ term arising from coherent backscattering and dominates the gas density dependence of the mobility of thermal electrons in helium. We also reanalyze Si:P data above the metal-insulator transition in terms of these incoherent scattering corrections.

The past two decades have seen a varied and richly productive research effort into electron transport in disordered media.[1,2] Many of the ideas and formalisms developed to explain the behavior of disordered conductors have spilled over into other fields such as acoustics,[3] light propagation,[4] and atomic physics.[5] In the simplest picture one considers a noninteracting system with some intrinsic disorder. In 1958 Anderson[6] showed that, for sufficiently strong disorder, electrons become completely localized with exponentially decaying wave functions. Further work by Mott[7] revealed the existence of a mobility edge or finite-energy threshold for conduction in presence of strong disorder. In the moderate disorder regime, much work was devoted to studying the most singular perturbative corrections, commonly known as weak localization. These corrections arise from constructive interference between electron trajectories which are related by time-reversal symmetry and which lead to an enhanced backscattering amplitude. The magnitude of these corrections is determined in part by the dephasing length L_ϕ, which is the distance an electron travels before losing phase coherence. In two dimensions, the weak-localization terms give a conductivity of the form[2,8]

$$\sigma = \sigma_B \left[1 - \frac{1}{\pi k_F \ell_o} \ln\left(\frac{L_\phi}{\ell_o}\right)\right], \tag{1}$$

where k_F is the electron Fermi wave vector, ℓ_o is the elastic mean free path, and σ_B is the Boltzmann conductivity. Equation (1) has been verified in several elegant experiments[9–11] in which the effective electron dephasing length is changed by applying a perpendicular magnetic field, adding magnetic impurities, or changing the temperature. Indeed, the great success of weak-localization theory has been its explanation of the generic nature of the observed scale dependencies of a wide variety of disordered two-dimensional (2D) electron systems in terms of coherent scattering processes. The fact that these corrections can be studied without varying the disorder of the sample has been one reason for the extensive experimental work.

The evidence for weak localization in 3D transport is much less clear than in 2D. In 3D there is known to exist a finite impurity density mobility edge[7] at T=0 implying that perhaps the transport is no longer dominated by the coherent (i.e., time-reversed) multiple-scattering effects. A naive extrapolation of the 2D coherent scattering formalism predicts a first-order correction to the 3D conductivity of the form[8,12]

$$\sigma = \sigma_B \left[1 - \frac{3}{(k_F\ell_o)^2}\left(1 - \frac{\ell_o}{L_\phi}\right)\right]. \tag{2}$$

Unfortunately, there is relatively little experimental data directly measuring the first-order corrections to the 3D conductivity. As a result of this, along with the historical emphasis on 2D transport in the localization community, there has been no rigorous test of Eq. (2) though it has been extensively applied to the analysis of transport in amorphous semiconductors.[1,12,13] In the present paper we present irrevocable experimental evidence extracted from electron-gas atom scattering data in the literature and Si:P data taken by the authors that Eq. (2) is *incorrect.* We show that the data are instead consistent with a first-order quantum correction proportional to $1/k\ell_o$.

In the gas atom scattering experiments we will be considering one measures the drift velocity of thermalized electrons injected into a neutral gas.[14] These systems are simpler to interpret than amorphous semiconductors where there are complications due to spin-orbit scattering and electron-electron interaction effects.[1,15] Furthermore, electron-gas atom scattering is highly elastic, phase coherent, and almost purely s wave even at room temperature. The classical electron mobility is[14]

$$\mu_{cl} = \frac{4e\ell_o}{3\sqrt{2\pi m_e k_B T}}. \tag{3}$$

The electron mean free path is $\ell_o = 1/4\pi a^2\rho$ at all gas densities, where a is the electron-gas atom scattering length and $\rho = n_g k_B T/(\partial P/\partial n_g)$ is the mean-square fluctuation density of a nonideal gas with density n_g. The effective number of scatterers is ρ so all of the data will be a function of ρ and not n_g.

There have been quite a number of experiments measuring the mobility of electrons in H_2 (Ref. 16) and He (Ref. 17–20) in a range of temperatures from 3K to 300K. These gases have a well known, positive scattering length that is a relatively weak function of energy[21] which simplifies the analysis. There have also been recent measurements in Ne,[22] which we will not consider here because Ne exhibits a strong energy dependence in the scattering length which complicates our analysis.

All of the experiments we will be addressing show that at low gas densities there are deviations from Eq. (3) that are linear in ρ. At sufficiently high gas densities precipitous drops in mobility are seen with measured values as low as several orders of magnitude below the classical curve. For this reason we will consider the two density regimes separately though, as we will discuss below, we believe the two limiting behaviors are fundamentally connected.

We show in Fig. 1 low-density helium data of Schwarz[19] in which the classical density dependence of the mobility has been factored out. The data show a deviation from the classical mobility, shown as horizontal curves in this plot. The deviation is linear in the gas density, and disagrees with the predicted $1/(k_T\ell_o)^2 \propto \rho^2$ dependence of Eq. (2). Schwarz suggested that he was seeing a $1/k_T\ell_o$ deviation, where $k_T = \sqrt{2m_e k_B T}/\hbar$ is the electron thermal wave vector, but the implications of his observations were not appreciated by the localization community.

There has been work that interpreted deviations from the classical mobility as arising from the energy dependence of the either the electron self-energy[23] or the scattering cross section without invoking weak localization[24]. Quantum multiple-scattering contributions to the conductivity, or equivalently to the mobility, of thermal electrons in a gas with low polarizability were first calculated by Atrazhev and Iakubov.[25] They predicted a first-order correction proportional to $1/k_T\ell_o$. More recently Kirkpatrick and Belitz,[26] correcting earlier work by Kirkpatrick and Dorfman,[27] have calculated the static, zero-temperature,[17] impurity corrections to the conductivity of a noninteracting 3D electron gas and obtained results similar to those of Atrazhev and Iakubov.[25] In both these calculations the maximally crossed diagrams which yield Eq. (2) are only a subset of the multiple-scattering processes summed in the perturbation expansion. Kirkpatrick and Belitz[26] find that the lowest leading-order corrections are

$$\sigma = \sigma_B\left[1 - \frac{\pi}{3}\left(\frac{2}{k_F\ell_o}\right) - \frac{\pi^2-4}{32}\left(\frac{2}{k_F\ell_o}\right)^2 \ln\left(\frac{k_F\ell_o}{2}\right)\right]. \tag{4}$$

The last term is only a few percent of the $1/k_F\ell_o$ term for all $k_F\ell_o > 2$ and can be neglected in the following analyses. This result is completely different from the T=0 extrapolation of Eq. (2) where one simply neglects the ℓ_o/L_ϕ term. To test the applicability of Eq. (4) to low density gas atom scattering we have digitized the data of several groups and plotted in Fig. 2 the normalized mobility, μ/μ_{cl}, as a function of the dimensionless parameter $\chi = 2/(k_T\ell_o) \propto \rho/\sqrt{T}$ which is proportional to the first order in term in Eq. (4). To properly normalize the data we have included the weak energy dependence of scattering lengths[21] of He and H_2. Note that all of the data, taken over a temperature range of 3K to 300K, fall on a universal *linear* curve. This behavior was discovered by Schwarz[19] in He data but at the time was not understood. Also shown in Fig. 2 are the predicted dependence of Eq. (2) for weak localization and the prediction of Eq. (4). To apply the degenerate expressions to the nondegenerate case we have integrated over all wave vectors weighted by a Boltzmann distribution. For instance, using Eq. (4) we have

$$\frac{\mu}{\mu_{cl}} = \frac{1}{(k_BT)^2}\int_{E_c}^{\infty} dE\, E\, e^{-E/k_BT}\left(1 - \frac{2\pi}{3}\frac{\hbar}{\sqrt{2m_eE}\ell_o}\right), \tag{5}$$

where $E_c = \pi^2\chi^2 k_BT/9 = 2\pi^2\hbar^2/(9m_e\ell_o^2)$ is a mobility edge where the integrand of Eq. (5) vanishes. In the low-density regime E_c is small and the behavior of Eq. (5) is dominated by the density dependence of the second term in the integrand. The data agrees well with Eq. (4) and suggests that the coherent backscattering processes in a 3D system are relatively unimportant. Moreover, Fig. 2 leaves little doubt that Eq. (2) does not describe the dc conductivity and cannot be extrapolated to T=0. We have also observed similar though less direct evidence for incoherent scattering effects in gas atom scattering of 2D electrons on hydrogen.[28] Unfortunately, the static impurity scattering theory breaks down[29] in 2D and we have no perturbative estimate of any terms other than Eq. (1).

In strong disorder, i.e., $\chi > 1$, Eq. (5) falls off as

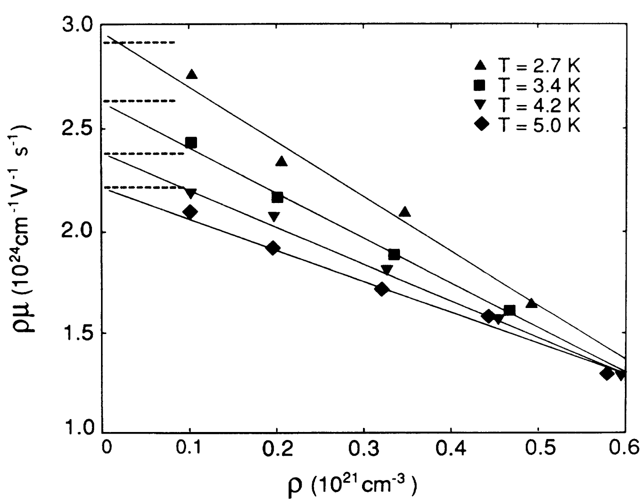

FIG. 1. Deviations from classical transport at low helium gas densities, from Ref. 19. The dashed lines are the classical dependence of Eq. (3). The solid lines are provided as a guide to the eye.

$\exp(-E_c/k_BT) = \exp(-\pi^2\chi^2/9)$. In Fig. 3 we have plotted the normalized mobility of several experiments in the literature as a function of χ^2. The solid line is the prediction of Eq. (5). Note that the data falls on a nearly linear universal curve. The three order-of-magnitude decrease below the classical mobility arises solely from the dependence of the mobility edge on gas density. While we estimated E_c above using Eq. (3) for the mobility, one also finds $E_c \propto \rho^2$ with about the same prefactor when Eq. (2) is used. This is a consequence of the fact that the high-density data is a probe[30] of the behavior of the mobility edge, which is determined by $k\ell_o \approx 1$. In fact, the same dependence of E_c on ρ can be obtained by estimating the maximum binding energy of quantum wells formed out of random fluctuations in the helium gas density.[28]

Early investigators interpreted the strong density dependence in Fig. 3 as evidence for formation of electron bubbles in the gas.[14,31] This interpretation has been criticized,[19] and given the complete collapse of the data onto a universal localization curve, we contend that there is no definitive evidence for bubble formation in these experiments. The saturation of the mobility for $\chi^2 > 5$ is a consequence of the finite mass of the gas atoms which is ignored in the present model. Even the most deeply localized electrons, whether they are trapped in random density fluctuations, in bubbles, or as negative ions, will have a finite mobility owing to gas atom diffusion.

The incoherent corrections seen in electron mobility in dense gases should also be important in transport in degenerate electron systems like doped semiconductors and disordered metals. To demonstrate this we have analyzed the density dependence of the zero-temperature conductivity of phosphorous doped silicon, Si:P. In uncompensated Si:P, the ionized phosphorous donors also act as scattering centers. The density of the scattering centers can be increased over the free-electron density n by compensating Si:P with acceptors such as boron. The metal-insulator transition takes place in these silicon-based systems at a critical carrier density[32] $n_c \approx 4 \times 10^{18}$ cm^{-3}.

We analyze the density dependence of the Si:P data of Thomanschefsky[33] in Fig. 4 using the incoherent terms from Eq. (4). The Boltzmann conductivity in Si:P is

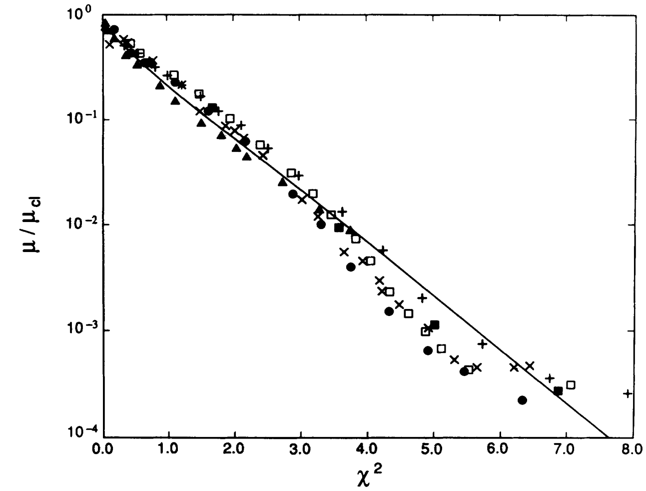

FIG. 3. Normalized mobility as a function of χ^2 at high gas densities from Ref. 19, solid squares, 3.8 K; solid crosses, 4.2 K; solid circles, 5.0 K; Ref. 17, open squares, 7.3K; Ref. 18, ×, 20.3 K; from Ref. 16, solid triangles, 77 K. The solid line is the prediction of Eq. (5) with $E_c = \pi^2\chi^2 k_BT/9$.

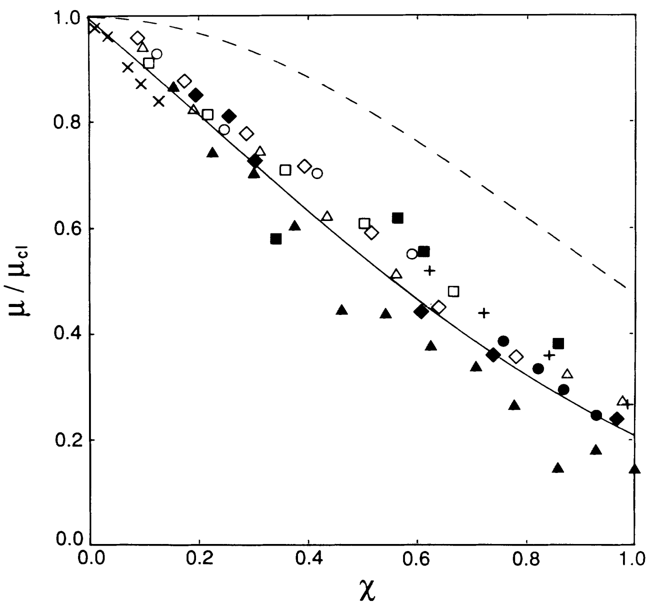

FIG. 2. Normalized mobility as a function of the dimensionless parameter $\chi = 2/k_T\ell_o \propto \rho/\sqrt{T}$ from Ref. 19, open circles, 2.7 K; open squares, 3.4 K; open triangles, 4.2 K; open diamonds, 5.0 K; from Ref. 17, crosses, 7.3 K; solid circles, 18.1 K; from Ref. 18, solid squares, 20.3 K; from Ref.[16], solid triangles, 77 K; solid diamonds, 77 K (H_2); from Ref. 20, × 293 K. The dashed line is the prediction of the weak-localization correction given in Eq. (2). The solid line is the prediction of the static impurity corrections given in Eq. (4).

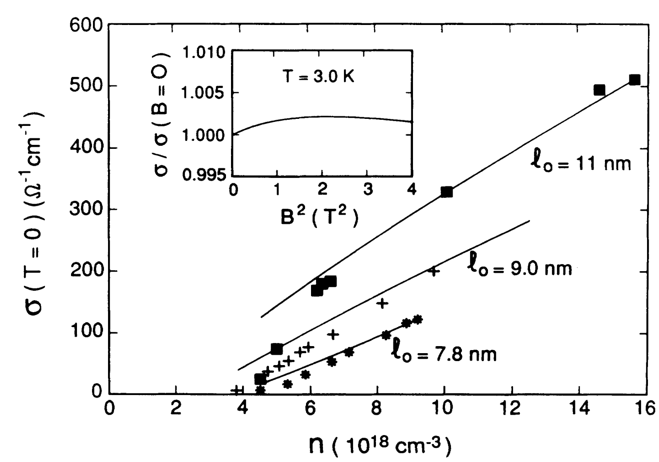

FIG. 4. Low-temperature conductivity of Si:P as a function of carrier density from Ref. 33 for three different compensations K; solid squares, $K = 0$; plusses, $K = 0.4$; asterisks, $K = 0.5$. The dashed lines are the prediction of Eq. (4) where ℓ_o has been varied to fit the highest density data point at each compensation. The inset shows the relative weakness of the field dependence of the conductivity in Si:P.

$\sigma_B = \nu e^2 k_F^2 \ell_o/(3\pi^2\hbar)$, where $k_F^3 = 3\pi^2 n/\nu$, and $\nu = 6$ is the valley degeneracy in Si. We assume as in Ref. 13 that ℓ_o is independent of n and treat it as a fitting parameter for the data taken at different compensation levels in Fig. 4. Our analysis ignores important electron-electron interaction effects but is nevertheless useful in estimating both the electron mean free path and the width of the critical region of the metal-insulator transition. The resulting curves are similar to those found by Bhatt and Ramakrishnan[13] and Thomanschefsky[33] using Eq. (2), but their fitted values of ℓ_o are 30% smaller than ours. Our analysis indicates that the compensated samples do not have a well-defined critical regime.

In the inset of Fig. 4 we have plotted the magnetoconductance at T=3K of a Si:P sample with $n = 1.25n_c$. The Si:P system is complex and unexpectedly small positive magnetoconductances are often thought to be the result of weak-localization effects being offset by significant electron-electron interaction effects which yield negative magnetoconductances of the same order of magnitude. However, given our analysis, an alternative interpretation of the data in the inset is that the backscattering terms are very small when set against the overall suppression of the conductivity by incoherent multiple-scattering processes.

The results presented here conclusively show that the leading-order corrections to the mobility in disordered 3D systems vary as $1/k\ell_o$ and arise from incoherent multiple-scattering processes rather than coherent backscattering. The weak-localization terms only describe the variation in mobility with magnetic field or temperature, while the incoherent scattering processes set the overall conductivity scale. We suggest that magnetoconductance measurements on electrons in moderately dense gases will confirm the small role played by coherent backscattering in 3D disordered transport.

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