SIMPLE MODEL FOR DENSITY OF STATES AND MOBILITY OF AN ELECTRON IN A GAS OF HARD-CORE SCATTERERS*

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We give a semiquantitative model for the density of states and transport properties of an electron in a system of randomly located hard-core scatterers. Our main results are these: (a) The density of states has the usual square-root behavior for high energies and a tail of localized states at the low-energy end; the energy at which the transition occurs is computed from percolation theory. (b) For a fixed temperature the fraction of electrons in localized states increases drastically with the density of scatterers above a critical density. Thus, our model provides a physical explanation for the mobility transition found by Neustadter and Coopersmith.

The theory of the electronic structure and transport properties in disordered materials is presently under active discussion.[1] Neustadter and Coopersmith,[2] in particular, have produced a theory of the mobility of an electron interacting with a random, low-density distribution of hard-core scatterers. They find a rapid decrease in mobility with density far beyond that expected from the usual semiclassical theory at about 10^{20} scatterers per cm^3 for a scattering length of 0.62 Å and a temperature of 3.96°K. The significance of their result is twofold: (1) It is accurate provided only that the two expansion parameters in the problem, ρa^3 and a/λ_T, are small, where ρ is the scatterer density, a is the scattering length, and λ_T is the thermal wavelength.[3] (2) It appears to confirm the current models[4] of the electronic structure of disordered materials pioneered by Mott and Lifshitz which have thus far received support primarily from plausibility arguments. These models have, as their most essential feature, bands of extended states with tails of localized states. The mobility is supposed to drop abruptly at the energy of transition from localized to extended states. The localized states are associated with potential fluctuations within the disordered material. In the present paper we propose a very simple semiquantitative model which exhibits all the above features, and which illuminates the results of Neustadter and Coopersmith and their relation to the more general models.

It is well known that a gas of repulsive scatterers acts as a potential barrier for an electron. The height of the barrier for a dilute gas is given by the optical potential[5,6]

$$V_0 = (\hbar^2/2m)4\pi\rho a, \tag{1}$$

where ρ = density of scatterers and a = scattering length. In order to find the density of electronic states we adapt to the present situation a method due to Kane.[7] We imagine the whole system divided into cells C_i of volume $\omega = L^3$ and treat the number N_i of scatterers (and therefore the optical potential) in each cell as a random quantity. Furthermore we assume that the density of states $n(E)$ is a sum of contributions from the individual cells,

$$n(E) = \sum_i n_i(E), \tag{2}$$

and that each $n_i(E)$ is the density of states corresponding to a box in which there is a constant potential $V_i = 4\pi\hbar^2 N_i a/2m\omega$:

$$n_i(E) = 2\omega \frac{(2m)^{3/2}}{4\pi^2\hbar^3}(E-V_i)^{1/2}. \tag{3}$$

As the cell side L we use the spatial extent of a typical wave packet, $L \sim \Delta x \sim \hbar/p_x \sim \hbar(3/2mE)^{1/2}$. The energies of interest lie around V_0;

$$L \sim \hbar\left(\frac{3}{2mV_0}\right)^{1/2} = \left(\frac{3}{4\pi\rho a}\right)^{1/2}, \tag{4}$$

from which we obtain the average number of scatterers per cell,

$$\langle N\rangle = L^3\rho \sim \left[\left(\frac{3}{4\pi a}\right)^3 \frac{1}{\rho}\right]^{1/2}. \tag{5}$$

The optical potential is valid for $\rho a^3 \ll 1$ (dilute gas),[8] which implies $\langle N\rangle \gg 1$. The probability distribution for the random variables N_i is therefore Gaussian with a mean value $\langle N\rangle$ and a standard deviation $\langle N\rangle^{1/2}$. Using this fact and Eqs. (2) and (3), the density of states for a system of total volume Ω can be written as

$$n(E) = 2\Omega \frac{(2m)^{3/2}}{4\pi^2\hbar^3} \frac{V_0^{1/2}}{\langle N\rangle^{1/4}} F\left(\frac{E-V_0}{V_0}\langle N\rangle^{1/2}\right), \tag{6}$$

where

$$F(\epsilon) \equiv (2\pi)^{-1/2} \int_0^\infty Z^{1/2} \exp[-(\epsilon - Z)^2/2] dZ, \qquad (7)$$

$$\epsilon \equiv \frac{E - V_0}{V_0} \langle N \rangle^{1/2}. \qquad (8)$$

Equations (1), (5), (6), and (7) completely determine the density of states. A plot of $F(\epsilon)$ is given in Fig. 1. The dashed line is $\epsilon^{1/2}$ to which $F(\epsilon)$ tends asymptotically for large ϵ. From the way in which $n(E)$ was obtained, it is easily seen that it has the following properties:

(a) For $\epsilon \gg 1$ (or $E \gg V_0 + V_0/\langle N \rangle^{1/2}$) almost every cell contributes to $n(E)$. An electron with this energy can be anywhere in the system, i.e., is essentially free.

(b) The tail of states with large negative ϵ comes from those few cells in which the density of scatterers is extremely small. If an electron with such a low energy is in cell C_i, the surrounding cells will act as impenetrable potential barriers, thus keeping the electron trapped. The asymptotic form $F(\epsilon) = e^{-\epsilon^2/2}/2\sqrt{2}|\epsilon|^{3/2}$ gives a Gaussian tail, as found by Halperin and Lax in their Gaussian approximation.[9,10]

(c) The band edge is smeared over a region of order $\Delta E \sim V_0/\langle N \rangle^{1/2}$, which is significantly smaller than the shift V_0 in the position of the band edge and goes as $\rho a (\rho a^3)^{1/4}$ in contrast to the ρa dependence of V_0.

These ideas permit a simple interpretation of the mobility transition found by Neustadter and Coopersmith.[2] For a first rough argument we assume that all states with $\epsilon < 0$ (or $E < V_0$) are localized, while all states with $\epsilon > 0$ describe a free electron. According to (6) and (c), the tail of localized states extends over a range $\Delta E \sim V_0/\langle N \rangle^{1/2}$. For $kT \ll \Delta E$ the electron will be trapped most of the time, so $\mu \simeq 0$. For $kT \gg E$, on the contrary, the existence of localized states should not limit the mobility significantly. The transition must occur when ΔE and kT are of the same order, that is, $kT \sim V_0/\langle N \rangle^{1/2}$ which, using (1) and (5), gives

$$\rho \sim \left(\frac{2mkT}{\hbar^2}\right)^{4/5} \frac{3^{3/5}}{(4\pi a)^{7/5}}.$$

Putting in the values $T = 3.96$°K and $a = 0.62$ Å used by Neustadter and Coopersmith we find $\rho = 6.4 \times 10^{19}$ scatterers/cm^3, in excellent agreement with their calculations. We also have the temperature dependence $\rho \sim T^{4/5}$, a result that could be used to check our model.

The idea that low-energy states are localized was crucial for this discussion. To develop it further we use some results from percolation theory.[11,12] For each energy we divide our cells into two classes: Class A, which we call allowed cells, contains all those with

$$V_i = V_0 N_i / \langle N \rangle < E; \qquad (9)$$

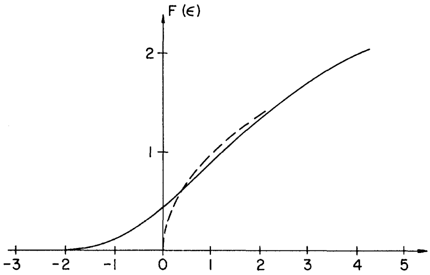

FIG. 1. Function $F(\epsilon)$ obtained by numerical integration of Eq. (7). The dashed line is $\epsilon^{1/2}$.

class B, called prohibited, contains all others. From now on we call a state localized if it is surrounded by some closed surface lying entirely within prohibited cells. A classical electron in such a state cannot "percolate" away, in the sense given by Broadbent and Hammersley[11] to this word, as first pointed out in the present context by Ziman.[12] We make the assumption that states which are localized in this sense give no contribution to the mobility. Let $p(E)$ be the probability that a state of energy E chosen at random is nonlocalized. This quantity, called percolation probability, depends only on the concentration $C(E)$ of allowed cells and was computed by Frisch, Hammersley, and Welsh[13] using Monte Carlo methods. The result of interest to us (three-dimensional cubic lattice) is given in Fig. 6 of their paper, and we approximate their curve with the function

$$p(E) = \begin{cases} 0, & C(E) < 0.3, \\ 1 - \exp\{-25[C(E) - 0.3]\}, & C(E) > 0.3. \end{cases} \qquad (10)$$

On the other hand, the condition (9) for a cell to be allowed is equivalent to $(N_i - \langle N \rangle)/\langle N \rangle^{1/2} < (E - V_0)\langle N \rangle^{1/2}/V_0 \equiv \epsilon$. The left-hand side is a normalized centered Gaussian variable; therefore

$$C(E) = (2\pi)^{-1/2} \int_{-\infty}^{\epsilon} \exp(-x^2/2) dx. \qquad (11)$$

There exists a critical energy E_c which makes $C(E_c) = 0.3$ and below which all states are localized according to (10). The corresponding value of ϵ in (11) is -0.52. This cutoff energy corresponds to the mobility edge in the Mott-CFO model, and

$$E_c = V_0 - 0.52 V_0/\langle N\rangle^{1/2}. \tag{12}$$

In this semiclassical theory, there is a coexistence of localized and extended states at given energy $E > E_c$ because $p(E) < 1$, $\epsilon > -0.52$. However for $\epsilon > -0.52$ each localized state will have in its vicinity some allowed cell to which it can tunnel and from which percolation is then possible. Therefore, when quantum mechanical effects are included, the classically localized states above E_c become extended resonant states which still contribute negligibly to the mobility.

For the mobility at temperature T we use the expression

$$\mu(\rho, T) = \frac{\int e^{-\beta E} n(E)\mu(E)dE}{\int e^{-\beta E} n(E)dE}. \tag{13}$$

According to naive semiclassical ideas we put

$$\mu(E) = \tfrac{2}{3}(e/m)p(E)\tau, \tag{14}$$

where τ is the mean collision time. This differs from the semiclassical result[14] only by the factor $p(E)$ in (14), which we put in in order to ensure that localized states are not counted in (13). To compute τ we notice that a free path can be interrupted by either one of two processes: (I) The electron is scattered by a simple atom, or (II) the electron encounters a prohibited cell. The mean free path associated with each of these processes is easily estimated. For (I) we have the well-known semiclassical result

$$\lambda_{\mathrm{I}} = (\sigma\rho)^{-1} = (4\pi a^2\rho)^{-1}. \tag{15}$$

For process (II) the probability that the electron finds k consecutive allowed cells in its way, the $(k+1)$th cell being prohibited, is

$$p_k = C(\epsilon)^k[1 - C(\epsilon)], \tag{16}$$

which leads to a free path

$$\lambda_{\mathrm{II}} \sim p_1 L + p_2 2L + p_3 3L + \cdots = LC(\epsilon)/[1 - C(\epsilon)]. \tag{17}$$

Combining (15) and (17) we get the mean free path when both processes (I) and (II) are present,

$$\lambda(\epsilon) = \frac{\lambda_{\mathrm{I}}\lambda_{\mathrm{II}}}{\lambda_{\mathrm{I}} + \lambda_{\mathrm{II}}} = \frac{LC(\epsilon)}{1 - C(\epsilon) + L\sigma\rho C(\epsilon)}. \tag{18}$$

The collision time τ can now be written as

$$\tau = \lambda(\epsilon)\langle 1/v\rangle_\epsilon, \tag{19}$$

where $\langle 1/v\rangle_\epsilon$ is a conditional average, taken only over allowed cells. The computation of this quantity is straightforward but rather lengthy; no further details are given on this point. The mobility $\mu(\epsilon)$ as a function of energy, as defined by Eqs. (14), (18), and (19), is plotted in Fig. 2 for the typical density $\rho = 10^{20}$ scatterers/cm^3. We note that it increases linearly with energy from zero away from the mobility edge as a consequence of (10).

Finally we have computed the mobility as a function of density for $T = 3.96$°K and $a = 0.62$ Å by numerical integration of Eq. (13). The result is shown in Fig. 3 and fits the data of Neustadter and Coopersmith (dashed line) surprisingly well for an order-of-magnitude calculation like the present one.

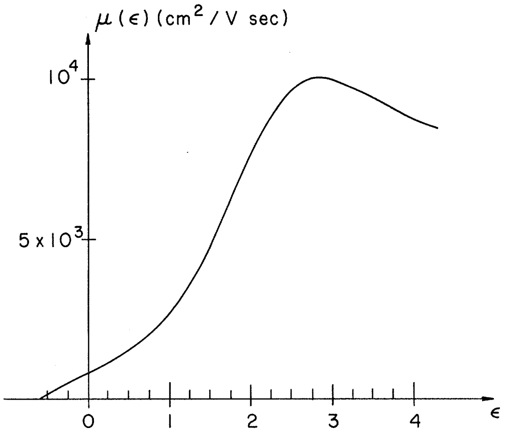

FIG. 2. Mobility versus energy as obtained from Eqs. (14), (18), and (19) for a typical density $\rho = 10^{20}$ scatterers per cm^3.

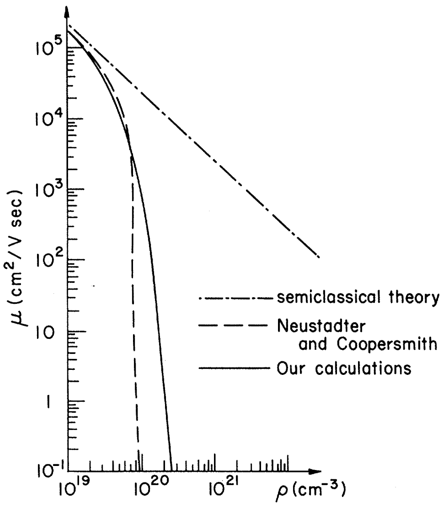

FIG. 3. Electron mobility as a function of scatterer density as obtained by numerical integration of Eq. (13) for $T = 3.96$°K and $a = 0.62$ Å. The dashed line is the result of a more refined calculation by Neustadter and Coopersmith.

We conclude that the rapid drop in mobility with increasing density is mainly the result of the formation of bound and resonant states associated with density fluctuations in the hard-core gas. This is precisely the picture which would have emerged from the current models of the electronic structure of disordered materials. Moreover, our theory yields a transition from bound states to extended states at E_c, Eq. (12). The extended states are of two types above E_c; resonant, which contribute little to the mobility, and nonresonant, with the percentage of the latter continuously increasing with energy away from E_c.

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SPIN SPLITTING, FERMI ENERGY CHANGES, AND ANOMALOUS g SHIFTS IN SINGLE-CRYSTAL AND PYROLYTIC GRAPHITE

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This Letter reports the first observation of spin-split Landau levels in graphite. These are observed in both natural single crystals and in pyrolytic samples. Experimental splittings are compared with the theory of McClure and Yafet. Discrepancy between theory and experiment is partially accounted for by large shifts in the Fermi energy with field.

Spin splitting of Landau levels in graphite is observed for the first time. In natural single crystals we find splittings for the $n=1$ and $n=2$ electron levels, and for the $n=1$ hole level. (The signs of the carriers have recently been determined.[1,2]) In pyrolytic samples only the $n=1$ electron splitting is observable. Splittings are observed as double extrema in several transport coefficients as a function of field, and these are a measure of the conduction-electron g shifts when shifts in the Fermi energy with field are accounted for.

Wagoner[3] observed conduction-electron g shifts from electron spin-resonance studies. Spin resonance, however, measures the g shifts averaged over the Fermi surface for particular magnetic field directions. Splittings of extrema in transport oscillations due to spin-split Landau levels measure the spin-orbit splitting for particular points in the Brillouin zone.[4,5] McClure and Yafet[6] have calculated the g shift for particular locations in the Brillouin zone. However, to compare with the spin-resonance experiment, they had to average over the electron and hole Fermi surfaces. In this Letter we present results which can be compared directly with the McClure and Yafet theory.

Figure 1 shows the magnetoresistance of a natural single crystal as a function of magnetic field to 10 T at 1.1 K for the magnetic field parallel to the [0001] axis. Adams and Holstein[7] have shown that conductivity maxima occur at coincidence of Landau levels and E_F. In graphite we find experimentally[1] that this implies resis-