Polaron Formation near a Mobility Edge

Morrel H. Cohen, E. N. Economou, [a] and C. M. Soukoulis
Corporate Research Science Laboratories, Exxon Research and Engineering Company, Linden, New Jersey 07036
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By combining the Emin-Holstein scaling theory of polaron formation with the scaling theory of localization in disordered systems, the authors show that the nonuniform extended eigenstates above the mobility edge (responsible for the continuous drop of the mobility to zero) collapse to localized polarons as the electron-phonon interaction is turned on.

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The concept of a mobility edge has played a central role in our attempts to understand the behavior of disordered materials.[1] Recently great progress has been made in analyzing properties near the mobility edge in the absence of interactions.[2-4] Despite these recent developments, many basic issues such as the nature of the carriers in amorphous semiconductors,[5] the Mayer-Neldel correlation,[6] and the peculiar behavior of the Hall effect in p-type materials[7] remain unresolved.

It seems that the main obstacle in achieving a sound understanding of the experimental situation is the presence of interactions. In quasi one-dimensional and quasi two-dimensional systems the important role of electron-electron interaction has been elucidated.[8] Furthermore it is suspected[9] that electron-electron interaction is responsible for the unexplained experimental facts in impurity bands in crystalline semiconductors.

The question of electron-phonon interaction has been addressed by Anderson,[10] who called attention to its importance in the region of localized eigenstates. Emin[11,12] has developed an extensive phenomenology for amorphous semiconductors based on the notion that electrons form small polarons. In this Letter we examine systematically the influence of the electron-phonon interaction on one-electron extended states just above the mobility edge. We show that the character of these states changes qualitatively, and, hence, close enough to the mobility edge the electron-phonon interaction is very important.

Emin and Holstein (EH) have introduced a beautifully simple scaling theory of polaron formation[13] which works in the presence of a Coulombic impurity potential and even for finite-range potentials.[14] The EH theory proceeds by examining the total energy change introduced by constraining a previously extended state to lie within a region of linear dimension L. Thus size scaling is at the heart of the EH theory.

Over the last five years, a considerable body of work on the size scaling of the properties[4] of disordered systems has been built up. The basic scaling parameters of a disordered system without electron-electron or electron-phonon interactions are the dimensionless conductance[5] $g(L)$ and its logarithmic derivative[2] β. The existence of a correlation length ξ characterizing the spatial extent of the amplitude fluctuations of extended states above the mobility edge is now well established.[15,16] For $L \gg \xi$, β approaches unity, the value expected for a uniform state in three dimensions.[2,16] For $L \ll \xi$, on the other hand, β approaches zero, the value expected for a uniform state in two dimensions. Thus, on scales $L < \xi$ the extended eigenfunction appears highly nonuniform occupying only a small fraction of the available volume. A possible way to describe such a behavior of the wave function is by introducing an effective dimensionality $\bar{d}$ which varies continuously[17] from 3 to 2 as L passes from above to below ξ. More explicitly we make the plausible assumption that

$$\bar{d} = \beta + 2. \tag{1}$$

Clearly, a value of $\beta < 1$ cannot persist down to atomic scales. Some distance η of the order of, but larger than, the interatomic separation a, where a^3 is the volume per atom, must be exceeded before the fractal dimensionality can manifest itself.

We have found it possible to combine these two theories into a single $T=0$ scaling theory containing both disorder and the electron-phonon interaction in the adiabatic approximation. Consider an extended state above the mobility edge of a disordered material in the absence of the electron-phonon interaction. Suppose that we confine it to a finite region of linear dimension L by continuously reducing its infinite extent through the imposition of suitable boundary conditions. Following EH, the sum of the electron-phonon interac-

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tion and the polarization energy of the phonon is given by

$$V_I = -\lambda' \sum_l |c_l|^4, \tag{2}$$

where c_l is the amplitude of the wave function on site l and λ' is an effective coupling constant. The sum in (2) is the inverse of the number of sites on which the state has appreciable amplitude, N'. The significance of the fractal dimensionality introduced above is that

$$N' = \gamma L^{\bar{d}}, \tag{3}$$

where lengths are measured in units of the interatomic distance a. From extensive studies of N' already carried out, we know that the prefactor γ has the form

$$\gamma_\infty(\xi) = \xi_0/\xi, \tag{4}$$

for $L \gg \xi$[18] and must be of the order of unity for $L \lesssim \eta$. In (4) ξ_0 is of the order of unity. A simple interpolation formula carrying us between these limits is

$$\gamma(\xi, L/\eta) = \gamma_\infty + (1-\gamma_\infty)(1+L/\eta)^{-1}. \tag{5}$$

It must be pointed out that Eqs. (1), (3), and (5) are definitely valid for $L > \xi$, while for $L \ll \xi$ they represent only plausible interpolations.

To obtain the single-particle energy change E_1 (due to constraining the state into a volume of linear dimension L), we observe that E_1 equals (within a numerical factor) the shift of the eigenenergy due to changing the boundary conditions from periodic to antiperiodic. Thouless[19] has shown that this shift can be expressed in terms of the density of states per volume ρ and the dimensionless conductance $g(L)$. Thus we obtain

$$E_1 = Bg(L)/L^3\rho, \tag{6}$$

where B is a constant. For $L \gg \eta$ we can use the Vollhardt and Wolfe[16] expression for $g(L)$; for $L < \eta$, $g(L)$ must once again be linear in L. A suitable interpolation formula is

$$g(L) = \frac{1}{\pi^3}\left(\frac{1}{1+\eta/L} + \frac{\pi}{2}\frac{L}{\xi}\right). \tag{7}$$

Equations (6) and (7) are valid for $\xi \gtrsim 1$; for $\xi \sim 1$ (corresponding to states of uniform amplitude) and $L \gtrsim \eta$, they reduce to the simple kinetic energy expression $3\pi^2\hbar^2/2m^*L^2$, as they should. This allows us to estimate B: $B \sim 100$. For $\xi \gg 1$ and $L \gg \eta$, E_1 is lower than $3\pi^2\hbar^2/2m^*L^2$ by a factor ξ/a reflecting the simple fact that it costs much less energy to compress a highly fluctuating eigenfunction than a uniform one. This fluctuation-induced reduction of the repulsive contribution combined with the fluctuation-induced enhancement of the attraction [see Eqs. (3) and (4)] accounts for the instability of the states with large enough ξ.

By minimizing the total energy $\Delta E = E_1 + V_I$ with respect to L, we can find the size L_0 of a given eigenstate as a function of the two parameters in our theory: the dimensionless correlation length ξ/a, and the dimensionless coupling constant $\lambda = (100/B)\lambda' a^3\rho \sim \lambda' a^3\rho$, where $a^3\rho$ is the density of states per atom. By employing the EH expression for λ' we can estimate λ roughly as follows:

$$\lambda \sim (\rho/\bar{\rho})(E_s{}^2/Sa^3W), \tag{8}$$

where $\bar{\rho}$ is the band-average density of states per volume, E_s is the deformation potential coefficient, S is the bulk modulus, and W is the bandwidth. Using EH, we estimate the value of λ required for small-polaron formation in a crystal to be between 1 to 10. For crystalline semiconductors λ is roughly equal to or less than 1. On the other hand, because W, $E_s \sim a^{-2}$ and therefore $\lambda \sim a^{-5}$, the value of λ for *impurity bands* in semiconductors is extremely small ($\sim 10^{-8}$ for Si), and one can neglect the electron-phonon interaction in studies[9] of the metal-nonmetal transition there.

Our explicit results, based on the choice $\xi_0 = 0.5$ and $\eta = 3$, are presented in Figs. 1 and 2. The dependence of the total energy on length for fixed λ and several values of ξ is as follows. For small ξ, that is, well above the mobility edge, E has a minimum only for infinite L, implying no polaron formation. In this case, the wave function and all the properties of the state, including *inter alia* the mobility, are unaffected by the electron-phonon interaction (in the adiabatic approximation). As we approach the $\lambda = 0$ mobility edge and ξ increases, a minimum develops in ΔE at finite L, L_0. When this minimum crosses the energy axis, an intermediate polaron, i.e., one of $L_0/a \sim 10$ to 10^2, becomes stabler than the extended state. Further increase of ξ compresses the polaron size, increases its stability, and greatly weakens the barrier against polaron formation. The ξ dependence of $L_0{}^{-1}$ is shown in Fig. 1 for various λ. The value of ξ, ξ_c, at which the transition occurs is plotted in Fig. 2 together with the initial value of L_0, $L_0{}^c$. Both quantities show a power-law dependence on λ,

$$\xi_c = 10\lambda^{-2/3}, \quad L_0{}^c = 10\lambda^{-1/2}, \tag{9}$$

up to a value of λ of about 1, above which the in-

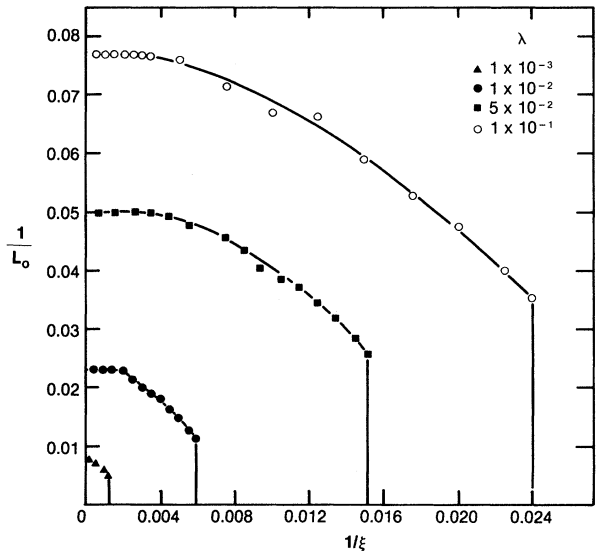

FIG. 1. Dependence of the polaron size L_0 on $1/\xi$ for various λ.

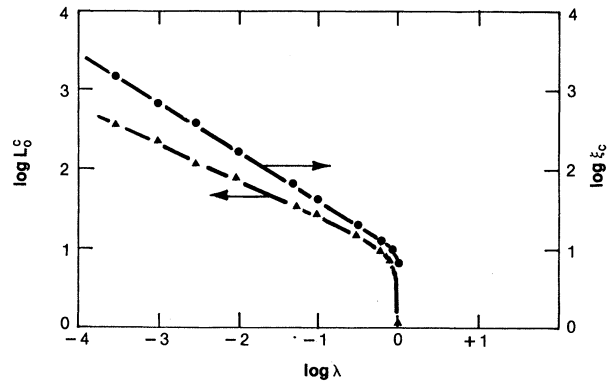

FIG. 2. The critical value ξ_c below which no polaron is formed as a function of λ. The polaron size L_0^c corresponding to λ and $\xi_c(\lambda)$ is also plotted vs log λ.

termediate polaron collapses into a small polaron.

This behavior is in sharp contrast to the behavior of the ordered material, for which the collapse occurs directly from extended states to small polaron at λ values from 1 to 10. We note that for $L > \xi$, the L dependences of E_1 and V_I are essentially the same as for the ordered case so that no polaron with $L_0 > \xi$ can occur. The formation of a polaron with $L_0 < \xi$, for large enough ξ, does not depend on the explicit form of our functions in the regime $L < \xi$. However, the detailed results we presented depend rather strongly on the interpolation formula for N'.

To summarize, the lattice-induced interaction tends to compress the electronic eigenfunctions, while the uncertainty principle favors their expansion. For the extended eigenstates just above the mobility edge E_c the first tendency is enhanced and the second is reduced as a result of their inhomogeneity. Hence polarons are always formed up to an energy E_0 at which they become unstable. As E_0 is crossed from above we switch from an extended state unaffected by the electron-phonon interaction (in the adiabatic approximation) to a localized polaron of finite extent L_0^c. The corresponding discontinuity $\Delta\sigma$ of the conductivity at E_0 was found to follow the scaling relation

$$\Delta\sigma = A\lambda^s$$

with $s = \frac{2}{3}$ and $A \approx 0.05e^2/\pi^2 a\hbar$. In the strong-coupling case ($\lambda \sim 1$) the transition is from uniform extended states as envisioned by Mott to small polarons as proposed by Emin.[11,12] For amorphous tetrahedral semiconductors λ is probably close to 1 and consequently the polarons are expected to be intermediate to small ($L_0^c \sim 10$ to 1).

Several subtle issues must be clarified before one attempts to analyze real materials in the framework of the present results. Even the atypical case of a $T=0$ heavily doped degenerate semiconductor, where the Fermi level may be made to pass through E_0, presents additional complications arising from the electron-electron interactions or the possibility of bipolaron formation. If these complications are ignored, E_0 will appear experimentally as the true mobility edge and $\Delta\sigma$ will be a minimum metallic conductivity, as proposed by Mott although its value for small λ may be substantially lower than Mott's value. In the typical case of a nondegenerate α semiconductor the situation is complicated again because of the possibility of thermal occupation of either the stable or the metastable states. The latter are the extended ($L = \infty$) states for $E < E_0$ and the polaron state for $E > E_0$. The energy range of coexistence of the two branches is determined by lifetime effects arising when the adiabatic approximation is relaxed.[20] Finally, finite-temperature effects[21] will be very important in analyzing experimental data.

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[a]Permanent address: Department of Physics, University of Crete, Crete, Greece, and Research Center of Crete, Heraklio, Crete, Greece.

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