Stochastic resonances and the mobility edge in a three-dimensional tight-binding Anderson model

Indra Dasgupta, Tanusri Saha, and Abhijit Mookerjee
Satyendra Nath Bose National Centre for Basic Sciences, DB17, Sector 1, Salt Lake City, Calcutta 700064, India
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We carry out a numerical study of the transmittance in a three-dimensional disordered Anderson model and study the weakly localized regime in the vicinity of the mobility edge, by the vector-recursion method of Godin and Haydock. This regime is straddled by stochastic resonant states and characterized by negative magnetoresistance. These stochastic resonances are very different in character to the strong fluctuations in the extended regime which arise due to lead-sample mismatch at the boundary.

Since Anderson's[1] suggestion that, unlike crystalline systems, where the electronic states are extended over the system, sufficient disorder can localize electron states within the allowed energy band, the physics of quantum transport in disordered materials has received much interest. The most successful theory to date is the one-parameter scaling theory,[2] the main prediction of which is that in one and two dimensions almost all electronic states of a disordered Hamiltonian are localized. However, for systems with higher dimensions there exist sharp energy barriers between parts of the band which are localized and those that are extended. Though the predictions of the one-parameter scaling theory of localization explains the gross features of quantum transport in disordered media, there are several finer points which are not taken into account by the configuration averaging inherent in that theory. There are indications[3] that although the one-parameter hypothesis is correct, the analytic approximations used for the scaling function may be questioned. Questions have also been raised regarding the correct choice of the scaling variable. Recent analytic work in one dimension based on the invariant embedding method[4] and random matrix theory[5] predicted features which are obviously not captured by the simple one-parameter scaling theory.

Since in two and three dimensions analytic work becomes increasingly difficult, one has to rely on numerical techniques. Recent numerical works[6,7] on two dimensions suggest that though *all* states in two dimensions are localized, there exists a pseudomobility edge separating exponentially or strongly localized states near the band edges and nonexponential or weakly localized states near the band center. This is contrary to the predictions of one-parameter scaling ideas. It has also been observed that the transmittance in two dimensions is dominated at $T=0$ by stochastic resonances,[8] which are probabilistically exceptional transparent states close to this pseudomobility edge. This is a feature which is lost under configuration averaging and therefore absent in one-parameter scaling ideas.

The scenario for three dimensions is quite interesting. Mott,[9] using classical ideas of Ioffe and Regel[10] about the mean free path in disordered materials, argued that at $T=0$ there exists a minimum metallic conductivity $\sigma_{\min}$ which for three-dimensional systems is of the order of the inverse interatomic spacing ($\sim k_f$). The scaling theory calls Mott's prediction into question, and argues that below $\sigma_{\min}$ quantum interference effects will reduce the conductivity even further, so that the conductivity continuously falls to zero at the mobility edge. The metal-insulator Anderson transition in three dimensions is thus a continuous transition with $\sigma(T=0)\simeq(E-E_c)^{-\mu}$, where E_C is the mobility edge and μ the critical exponent $\simeq 1$. The one-parameter hypothesis for the continuous Anderson metal-insulator transition at the Mott mobility edge is consistent with experiments[11] on the temperature-, frequency-, and magnetic-field-dependent resistivity of disordered conductors. The physics at and close to the mobility edge ($0<\sigma<\sigma_{\min}$) in three dimensions appears to be interesting. The narrowness of the critical region and the effect of electron-electron interaction make a comparison of experiments with scaling predictions not clear cut. Tit *et al.*[12] anticipated that in a three-dimensional Anderson model the mobility edge E_C separates exponentially localized states from resonant states which extend from E_C [where $\sigma(E_{C'})=\sigma_{\min}$] to E_C. On the other side of $E_{C'}$ one has extended diffusive states. Recently Karpov[13] employed a modification of the optimum fluctuation method to demonstrate that long-lived resonant electronic states lie above the mobility edge of a disordered system. He further demonstrated that the density of such states decays exponentially with energy above the mobility edge into the extended states, and the tail is almost symmetric to the tail of localized states with respect to the mobility edge. He further argued that the signature of such a state is negative magnetoresistance. He supplemented his arguments with the large negative magnetoresistance recently observed in the amorphous alloy of $Cd_{43}Sb_{57}$ (Ref. 14) near the metal-insulator transition.

The main objective of this work is to study the quantum transmittance of a three-dimensional Anderson tight-binding model of disordered systems, and to detect whether the coherent backscattering really develops into resonances before fully developed localized states are encountered below E_C. We employ the vector-recursion method,[15] which has been found to be stable and accurate in a series of earlier works[6,8,16] for determining the quantum transmittance as a function of the incoming energy. We shall study the fine structure in the transmittance, and determine by a scaling argument whether resonances exist near the mobility edge. Further we will supplement

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our studies with the effect of magnetic field on transport properties in this region.

Our system is a three-dimensional cubic lattice with N sites. The Hamiltonian is taken to be a tight-binding, nearest-neighbor overlap type of model with disorder only in the diagonal terms. To this cubic lattice we attach M semi-infinite perfectly conducting leads. The purpose of these leads is to bear the incoming reflected and transmitted waves into and away from the sample. The Hamiltonian is given by

$$H_{\text{sample}} = \sum_i \varepsilon_i |i\rangle\langle i| + V\sum_i \sum_j |i\rangle\langle j| \; , \qquad H_{\text{leads}} = V_L \sum_i \sum_j |i\rangle\langle j| \; . \tag{1}$$

The nearest-neighbor overlap term V is chosen to be 1. This sets the scale of energy in the system. The site energies are uniformly randomly distributed between $-W/2$ and $W/2$.

The choice of the lead overlap V_L determines the energy window in which electrons can propagate without decay in the system.

The essence of the vector-recursion technique is the block tridiagonalization of the system Hamiltonian *without* changing the lead Hamiltonian. This is achieved by a change of basis. The restriction leaving the lead Hamiltonian unchanged makes the transformation slightly different from the traditional Lanços method. As the method has been described in detail by Godin and Haydock[7] as well as our earlier work, here we shall describe only those salient points which would be relevant to our present work.

A representation of the original basis is a column vector of length N. A representation of our basis are $N\times M$ matrices. The members of our basis are generated in the following way: we give an example of the case where $M=2$, where there is only one incoming and one outgoing lead. The starting state where the leads join the system is chosen to be

$$|\Phi_1\rangle = \begin{bmatrix} |1\rangle \\ |N\rangle \end{bmatrix} \; .$$

The subsequent members of the basis are generated from the recursive relations

$$B_2^\dagger|\Phi_2\rangle = (H-A_1)|\Phi_1\rangle \; , \qquad B_{n+1}^\dagger|\Phi_{n+1}\rangle = -(H-A_n)|\Phi_n\rangle - B_n|\Phi_{n-1}\rangle, \quad n\geq 2 \; . \tag{2}$$

The elements $\{A_n, B_n\}$ are $M\times M$ matrices. The wave function has a representation $|\Psi\rangle = \sum_n \Psi_n|\Phi_n\rangle$, where Ψ_n are the wave-function amplitudes in our basis. They satisfy an equation identical to (2). The solution in the leads are known, since the periodicity of the potential in the leads to wave-function amplitudes proportional to $\exp(in\vartheta)$. The wave function on the nth member of the basis is given by $\Psi_n = X_n\Psi_0 + Y_n\Psi_1$, where X_n and Y_n are $M\times M$ matrices which satisfy the same recursion relations as the basis with EI replacing the Hamiltonian H. They also satisfy the boundary conditions: $X_0=I, Y_0=0; X_1=0, Y_1=I$. Now, originally the rank of the sample basis space since was N, the number of our basis members are $N/M=p$, since our basis is produced by bunching M of the old basis members together. This leads to another boundary condition: $\Psi_{p+1}=0$.

We have shown earlier that this leads to an equation for the scattering S matrix: $S(E) = -[X_{p+1} + Y_{p+1} \times\exp(i\vartheta)]^{-1}[X_{p+1} + Y_{p+1}\exp(-i\vartheta)]$, and the transmittance is given by $T(E) = |S_{12}(E)|^2$.

In the presence of an external magnetic field the Hamiltonian of the sample is modified:

$$H = \sum_i \varepsilon_i|i\rangle\langle i| + V\sum_i\sum_j \exp\left[-\frac{2\pi i}{\phi_0}\int_i^j \mathbf{A}\cdot d\mathbf{s}\right]|i\rangle\langle j| \; ,$$

where ϕ_0 is the unit of quantum flux, $\mathbf{A}$ is the vector potential. The Hamiltonian remains Hermitian, so that the spectrum is still real. However, because the Hamiltonian matrix elements are complex, the vector-recursion equations are trivially generalized.

We have calculated the transmittance as a function of energy for samples ranging in size from 10^3 to 20^3, and disorder ranging between $W/V=1.0$ and 4.0. In each case, there is a steep drop in the transmittance at a particular energy E_C. In practice, to locate the precise position of the mobility edge which separates extended and weakly localized states is numerically very difficult. The sharp drop of transmittance is suggestive of a mobility edge which lies between the band edge of the disordered sample and that of the corresponding ordered one (with $W=0$).

Figures 1(a) and 1(b) show the plot of the logarithm of the transmittance for a cubic sample with 10^3 sites and disorder $W/V=0$ (an ordered sample) and 2.0, respectively. For the ordered sample the band edge is at 6 V. amd for the disordered samples the band edge is given by the Gershgorin theorem and the Lifshitz criterion[17] to be at $6V+W/2$. The energies along the x axes in the two figures are scaled by their respective half- bandwidths. The perfectly conducting linear leads are attached to the corners on opposite faces of the sample at the two ends of the body- diagonal, and the hopping integral in the leads is so chosen that the lead bandwidth is equal to that of the sample bandwidth.

For the crystalline sample, one obtains evanascently decaying states beyond the band edge. This leads to a steep fall in the transmittance. We see this in Fig. 1(a). We also note that within the band the transmittance is high, but not equal to unity. As discussed by Godin and Haydock,[7] this is due to the scattering from the sample boundary and the leads. This lead-sample mismatch results in resonant coupling between the lead and the sample states, producing sharp structure in the transmittance inside the band.

For the disordered sample $W/V=2.0$, shown in Fig. 1(b), the band edge is at 7 V. One observes a sharp decrease of transmittance analogous to the crystalline case, but *well within the band*, suggesting the presence of universally accepted mobility edge in the three-dimensional Anderson model.

Once we have identified the position of the mobility edge approximately, the first step is to determine transmittance, highly resolved in energy, in the neighbor-

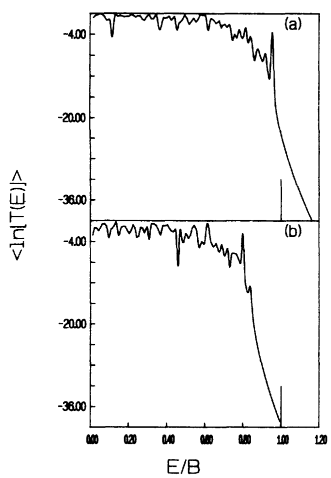

FIG. 1. (a) $\ln_e$ transmittance vs energy for a cubic lattice of size 10^3 without disorder. The energy E is expressed in units of half-bandwidth B. (b) Same as in (a) but with disorder $W/V=2.0$, where V is the nearest-neighbor overlap term in the lead.

hood of this region, and to examine whether it is dominated by stochastic resonances as indicated earlier. We have to carefully distinguish between the resonances near the mobility edge and the fluctuations in the extended regime caused by lead-sample mismatch. Figure 2(a) shows an energy-resolved plot of transmittance vs energy for the extended part of the spectrum ($E/V=1.0-2.0$), and Fig. 2(b) shows the same near the mobility edge ($E/V=4.0-5.0$) for a cube of size 10^3, and $W/V=2$ for a specific configuration. Just within the mobility edge we note dense sharp resonances resembling the stochastic resonances we found in one- and two-dimensional Anderson models. The transmittance fluctuations in the extended regime are denser compared to the transmittance near the mobility edge.

Figures 3(a) and 3(b) show much resolved plots of transmittance vs energy in the two regimes discussed in

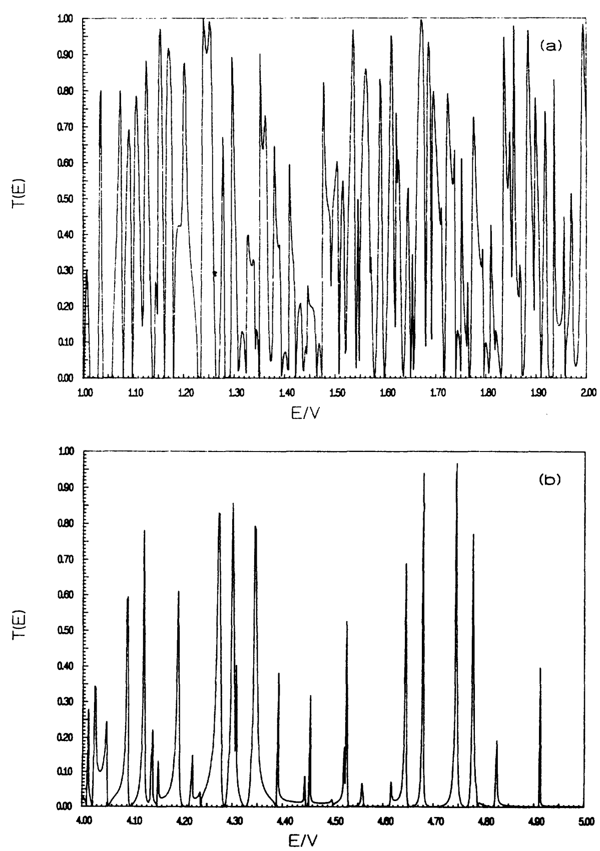

FIG. 2. (a) $\ln_e$ transmittance vs E/V, where V is the nearest-neighbor overlap term in the lead, in an energy window in the extended regime. (b) $\ln_e$ transmittance vs E/V, where V is the nearest-neighbor overlap term in the lead, in an energy window near the mobility edge.

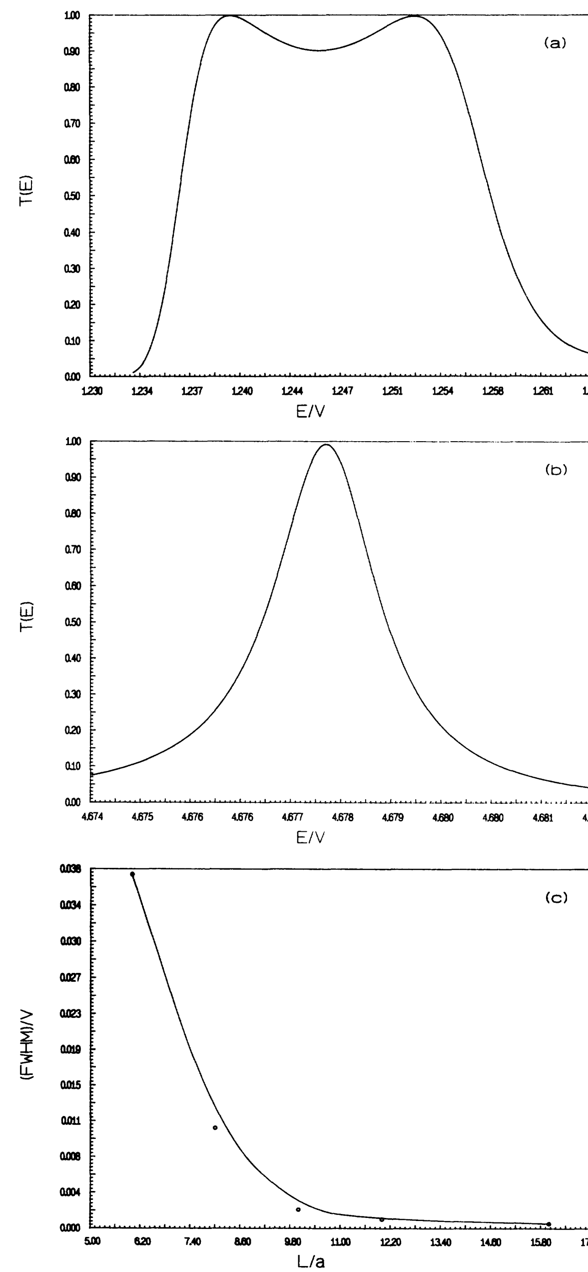

FIG. 3. (a) A *resonance* in the extended regime arising due to lead-sample mismatch, shown in a much resolved energy window. (b) A stochastic resonance with a Lorentzian shape in the weak localized regime in a much resolved energy window. (c) The decrease of resonance width with size for a stochastic resonance. We show the full width at half maximum as a function of L/a, where the system is a cube of sides of length L, and a is the lattice spacing.

the earlier paragraph. In the energy regime $[4<E/V<5]$ we observe the resonance shape be Lorentzian, characteristic of stochastic resonances as described by Pendry[18] and Azbel.[19] This Lorentzian shape of the resonance is easily understood within the model. Since a resonance at a real energy E arises out of a second-order pole of the propagator in the complex energy plane at $E+i\gamma$, the resonance shape, related to the imaginary part of the propagator, is a Lorentzian centered at E and with a half-width γ/π.

The stochastic resonances observed in the weak localized regime are detected for larger sample sizes ranging from 12^3 to 20^3. These resonances are found to be slightly shifted in energy as the size increases and the width rapidly decreases. Figure 3(c) shows the plot of full width at half maximum vs system size for a particular stochastic resonance which we have tracked with increasing size. We find that the width decreases with size in agreement with Azbel and Pendry's idea. However, no such feature is observed for resonances arising due to lead-sample mismatch. The same feature persists for resonances in other configurations.

Our next step is to identify whether the weak localization develops in the region near the mobility edge, which is dominated by the stochastic resonances. An important aspect in which the quantum diffusion differs from the classical transport is the phenomenon of coherent backscattering. As long as the scatterings are elastic and time reversal invariant, the scattered waves in the backward direction are coherent in time and therefore exhibit constructive interference. This introduces a negative correction to the classical diffusion constant. As the scattering strength increases, this correction due to back-scattering effect increases. This results in the reduction of conductivity beyond $\sigma_{\min}$. In the weak-localization region the quantum interference effect should begin to show up. If a magnetic field is now applied, the time-reversal symmetry responsible for producing the backscattering effect is broken, and one expects an increase of conductance (or transmittance). To look at this we have calculated the transmittance with magnetic field applied to the sample. This is displayed in Fig. 4, where we plotted configuration averaged ln (transmittance) vs energy for a cube of size 10^3 with strength of disorder $W/V=2.0$, in the absence and in presence of a magnetic field of strength $H=0.08$ expressed in units of fraction of quantum flux ϕ_0. We have used typically 50 configurations for the averaging procedure. A comparison of the two plots

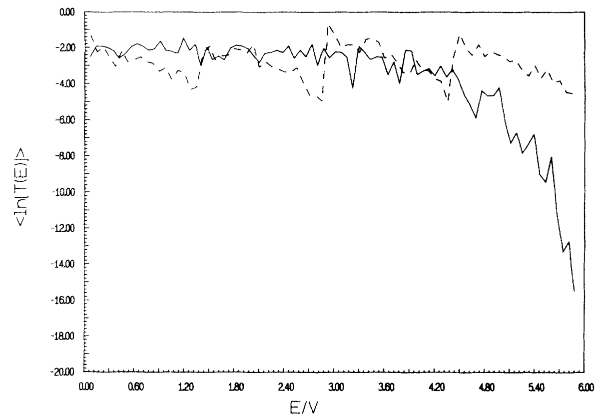

FIG. 4. $\ln_e$ transmittance vs E/V, where V is the nearest-neighbor overlap term in the lead, for a three-dimensional disordered Anderson model of 10^3 sites and disorder $W/V=2.0$, with and without magnetic field.

shows that in the presence of the magnetic field there is no appreciable change in transmittance in the extended region, while transmittance begins to increase in the knee region with E/V between 4 and 5, and is supposed to be the weak-localization regime. One obtains a negative magnetoresistance in this region, as expected by Karpov and also experimentally observed by Gantmakher *et al.*[14] This is clear from Fig. 4.

Our numerical work suggests that the weak-localization regime in the disordered three-dimensional Anderson model is dominated by stochastic resonances. Such resonances, which were anticipated earlier, find confirmation in our numerical work. Furthermore, it appears that sharp resonances arising in the extended region due to lead-sample geometry mismatch are quite distinct in character from those due to probabilistically exceptional stochastic resonant states in the localized regime. This is indicative of the fact that an electron may become localized due to geometry mismatch even in the absence of any disorder, which needs further investigation.

In conclusion, we have studied the transmittance in the weak localized regime of a three-dimensional disordered system, and our work indicates that resonating states dominate the spectrum near the mobility edge before the fully developed localized states appear below in the spectrum.

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