ac conductivity of a one-dimensional site-disordered lattice

R. C. Albers and J. E. Gubernatis

Theoretical Division, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87545

(Received 17 January 1978)

We report the results of a numerical study of the ac conductivity for the Anderson model of a one-dimensional, site-disordered system of 400 atoms. For different degrees of disorder, we directly diagonalized the Anderson Hamiltonian, used the Kubo-Greenwood formula to evaluate the conductivity, and then averaged the conductivity over 12 configurations. We found that the dominant frequency dependence of the conductivity consisted of a single peak which shifted to higher frequency and decreased in overall magnitude as the disorder was increased. The joint density of states and the eigenstate localization were also computed and are discussed in connection with our results.

I. INTRODUCTION

In recent years, much attention has been focused on understanding the properties of strongly disordered systems, principally the density of states and eigenstate localization.[1-3] In contrast, less effort has been devoted to understanding transport properties. With respect to electrical transport, most of the work has been directed towards calculating the dc conductivity,[4] often within the coherent-potential and other single-site approximation schemes.[5]

In this paper we present results of a computer experiment designed to study the ac conductivity of disordered metals and thereby provide calibration standards for approximate theories. We did not attempt to describe any realistic system, but instead chose a model restricted to one dimension and to noninteracting electrons, whose dynamics are described by the site-disordered Anderson Hamiltonian. We chose the Anderson Hamiltonian because of its widespread use in modelling disordered systems and one dimension because of inherent simplifications to the numerical analysis.

In principle, this model was solved exactly by Halperin,[6] who developed a formalism for the ensemble-averaged ac conductivity, related to Schmidt's formalism[7] for the integrated density of states. In practice, Halperin's equations await solution, although steps in this direction have been taken by Hirsch and Eggarter.[8]

In our approach we examined the zero-temperature ac conductivity of many noninteracting electrons in a partially filled band for several different values of the chemical potential. We explicitly diagonalized the Hamiltonian to find the exact eigenvalues and eigenstates for a given random configuration and calculated the ac conductivity by using these eigenvalues and eigenstates in the Kubo-Greenwood formula.[3] We then averaged over 12 configurations to obtain an average conductivity $\langle \sigma(\omega) \rangle$.

This approach is similar to one used by Penchina and Mitchell[9] who studied a single electron in a lattice of randomly positioned δ-function potentials. They concluded that the conductivity was not a well-defined quantity since it varied drastically from configuration to configuration. Using a different model and different numerical techniques, we found the conductivity was well defined with less drastic, but still significant, variations whose source appears to be the matrix elements of the position operator.

II. ac CONDUCTIVITY

In this section we define our model, write the general linear response expression for the ac conductivity of a one-dimensional system, and discuss a number of points relevant to the application of this expression to our model.

This model is described by the Anderson Hamiltonian for N atoms with fixed boundary conditions.

$$H = \sum_{i=1}^{N} \epsilon_i |i\rangle\langle i| + V \sum_{i=1}^{N-1} (|i+1\rangle\langle i| + |i\rangle\langle i+1|). \quad (1)$$

The nearest-neighbor hopping matrix element V is constant, the disorder is in the site energies ϵ_i which are randomly and uniformly distributed between $-\frac{1}{2}W$ and $+\frac{1}{2}W$, and the states $|i\rangle$ are orthonormal and localized at the ith lattice site.

If we assume that linear response theory is valid, then the real part of the ac conductivity of a one-dimensional system can be expressed as either[3]

$$\sigma(\omega) = \frac{2\pi e^2}{L} \omega \sum_{\alpha, \beta} (f_\alpha - f_\beta) |\langle \alpha | x | \beta \rangle|^2$$

$$\times \delta(\hbar\omega + E_\alpha - E_\beta) \quad (2a)$$

or

$$\sigma(\omega) = \frac{2\pi e^2}{\omega L} \sum_{\alpha, \beta} (f_\alpha - f_\beta) |\langle \alpha | v | \beta \rangle|^2$$

$$\times \delta(\hbar\omega + E_\alpha - E_\beta), \qquad (2b)$$

where E_α and $|\alpha\rangle$ are the eigenvalues and eigenstates of H,

$$H|\alpha\rangle = E_\alpha |\alpha\rangle; \qquad (3)$$

f is the Fermi function

$$f_\alpha = [1 + \exp(E_\alpha - \mu)/k_B T]^{-1};$$

μ is the chemical potential; L is the length of the system; x is the position operator; and $v = \dot{x} = (i\hbar)^{-1}[x, H]$ is the velocity operator.

From (1) and (2), the path of analysis appears straightforward: find the eigenvalues and eigenstates of (1), determine $|\langle \alpha | x | \beta \rangle|^2$ (or $|\langle \alpha | v | \beta \rangle|^2$), perform the summations indicated in (2), and then average $\sigma(\omega)$ over a number of configurations. The eigenvalues and eigenstates are easily found by diagonalizing H in the site representation, i.e., in a space spanned by the $|i\rangle$. In this representation for a one-dimensional system, $\langle i | H | j \rangle$ is a tridiagonal matrix

$$\langle i | H | j \rangle = \epsilon_i \delta_{ij} + V(\delta_{i, j+1} + \delta_{i+1, j}), \qquad (4)$$

which is particularly convenient for numerical analysis.

When found, the eigenstates of (4) are linear combinations of the $|i\rangle$, namely,

$$|\alpha\rangle = \sum_i |i\rangle\langle i | \alpha\rangle \equiv \sum_i a_i(E_\alpha) |i\rangle.$$

Consequently, the evaluation of the matrix elements in (2) occurs most naturally in the site representation as one writes, for example,

$$\langle \alpha | x | \beta \rangle = \sum_{i, j} \langle \alpha | i \rangle \langle i | x | j \rangle \langle j | \beta \rangle$$

$$= \sum_{ij} a_i^*(E_\alpha) a_j(E_\beta) \langle i | x | j \rangle,$$

and reduces the problem to finding $\langle i | x | j \rangle$. To determine $\langle i | x | j \rangle$, we first note that in the site representation the only positions are lattice sites so x makes sense only if its action on $|i\rangle$ produces the lattice position of i. Accordingly, we *define* x as

$$x \equiv a \sum_i i |i\rangle\langle i|, \qquad (5)$$

where a is the lattice spacing and as a result

$$\langle i | x | j \rangle = ja \delta_{ij}.$$

Using Eq. (5), we can rewrite the ac conductivity, Eq. (2a), at zero temperature as

$$\sigma(\omega) = \left(\frac{2\pi e^2 a}{\hbar}\right) \left(\frac{\hbar\omega}{N-1}\right)$$

$$\times \sum_{\alpha, \beta} [\Theta(\mu - E_\alpha) - \Theta(\mu - E_\beta)]$$

$$\times \delta(\hbar\omega + E_\alpha - E_\beta)$$

$$\times \left| \sum_{i=1}^N a_i^*(E_\beta) i a_i(E_\alpha) \right|^2, \qquad (6)$$

where the Fermi functions are replaced by the unit step function $[\Theta(x) = 1$ for $x > 0$ and zero otherwise].

If we next attempt to perform the summations in (6), we see that for a finite system $\sigma(\omega)$ is a sum of δ functions, the weight of each determined by an appropriate squared matrix element. This discreteness imposes some difficulties in averaging $\sigma(\omega)$ and in obtaining a result representative of an infinite system: since the frequencies in the arguments of the δ functions are just differences in the eigenvalues for a given configuration and since different configurations have different distributions of these differences, an average of the conductivity would be a sum of δ functions, all with different arguments.

To overcome this difficulty we perform a smoothing operation, which we call frequency averaging, that allows us to define for a given configuration a $\sigma(\omega)$ at a regularly spaced frequency interval $\Delta\omega$, i.e., for a given configuration we define a frequency-averaged conductivity as

$$\langle \sigma(I\Delta\omega) \rangle_{\text{frequency}} = \frac{1}{\Delta\omega} \int_{(I-1)\Delta\omega}^{I\Delta\omega} \sigma(\omega) \, d\omega. \qquad (7)$$

Our $\langle \sigma(\omega) \rangle$ is the average of the above over a number of configurations.

The results of the frequency averaging depend on $\Delta\omega$. On one hand, if $\Delta\omega$ is chosen too small, for instance, smaller than the average spacing between eigenvalues, a very large and impractical number of configurations are needed for $\langle \sigma(\omega) \rangle$ to converge to a well-defined value. On the other hand, if $\Delta\omega$ is chosen too large, meaningful structure in the real $\langle \sigma(\omega) \rangle$ is lost. Our choice of $\Delta\omega$ is discussed in Sec. III.

To assess further the effects of a finite system, we examined the exact analytical solution for $\sigma(\omega)$ in the perfectly ordered case (see the Appendix). This examination indicated that for a finite system $\sigma(\omega)$ has a frequency dependence dominated by a strong peak at a frequency of the order of the bandwidth divided by N and for an infinite system the conductivity is proportional to $\delta(\omega)$. Thus, other than the discreteness in $\sigma(\omega)$, the boundary effects are relatively insignificant for an ordered system

of moderate size even though the eigenstates are very extended and expected to be sensitive to the boundary. For the disordered case we expect the boundary effects to become negligible as the disorder is increased and the eigenstates become more localized (see Sec. III).

III. RESULTS

The ac conductivity was directly calculated from Eq. (2) by explicitly diagonalizing the $N \times N$ symmetric tridiagonal Hamiltonian, Eq. (4), to find the exact eigenvalues and eigenstates for a given configuration of random diagonal elements in the Hamiltonian. The final results were obtained by an average over 12 different configurations.

The eigenvalues were generated through the QR algorithm[10] with implicit shift for symmetric tridiagonal matrices. Once the eigenvalues were determined, the eigenstates were then determined by the inverse iteration technique.[11,12] For a 400-atom chain, those calculations together took about one minute of computing time on a CDC 6600 computer. The subsequent evaluation of Eq. (2) took about 2 min of computing time on the same machine for the chemical potential set in the middle of the band. The accuracy of the eigenvalues, eigenstates, and the degree to which orthonormality and the boundary conditions were satisfied was at least to six significant figures and often to machine accuracy (14 significant figures).

As we discussed in Sec. II, it was necessary to average the conductivity over a small frequency interval $\Delta\omega$ to eliminate effects of the finite size of the system and to average sensibly over different configurations. The frequency averaging has several important effects: one, the averaging smooths out any rapid variations of $\sigma(\omega)$ as a function of frequency. A larger $\Delta\omega$ of course leads to greater smoothing. Two, as we increase the size of $\Delta\omega$, we need fewer configurations to obtain a true ensemble average of the frequency-averaged $\langle\sigma(I\,\Delta\omega)\rangle_{\text{frequency}}$, since we will improve the statistics on the number of transitions contributing to $\langle\sigma(I\,\Delta\omega)\rangle_{\text{frequency}}$, i.e., more δ functions $\delta(\hbar\omega + E_\alpha - E_\beta)$ will fall in the range $\omega_0 - \frac{1}{2}\Delta\omega \leq \omega \leq \omega_0 + \frac{1}{2}\Delta\omega$.

The $\Delta\omega$ we used is $\hbar\Delta\omega = 3B/N$, where B, the theoretical bandwidth, is $W + 4V$. This choice appeared large enough to give reasonable confidence that the statistics are sufficiently good, that is, the averaging over 12 ensembles is approaching the true ensemble average, while at the same time not changing the qualitative shape of $\langle\sigma(\omega)\rangle$.

We found that the fluctuations in $\sigma(\omega)$ from configuration to configuration result from fluctuations in the effective-energy-dependent matrix element of the position operator. To explain what we mean

by this, we rewrite our equation for $\sigma(\omega)$ [Eq. (2a)] in the form

$$\sigma(\omega) = \frac{2\pi e^2}{L}\,\omega \int dE[\,f(E) - f(E + \hbar\omega)]$$

$$\times R(E, E + \hbar\omega), \qquad (8)$$

where

$$R(E, E') \equiv \sum_{\alpha,\beta} |\langle\alpha|x|\beta\rangle|^2 \delta(E_\alpha - E)\delta(E_\beta - E')$$

$$\equiv M(E, E')D(E, E'), \qquad (9)$$

and $D(E, E')$, joint density of states per atom squared, is defined to be

$$D(E, E') \equiv \frac{1}{N^2}\sum_{\alpha,\beta}\delta(E_\alpha - E)\delta(E_\beta - E'). \qquad (10)$$

If we could neglect the energy dependence of the matrix elements $\langle\alpha|x|\beta\rangle$, then at zero temperature the ac conductivity would be proportional to $D(\omega)$, where

$$D(\omega) \equiv \int_{\mu-\hbar\omega}^{\mu} dE\,D(E, E + \hbar\omega), \qquad (11)$$

energies are measured from the bottom of the band, and μ is the chemical potential. By dividing $\sigma(\omega)$ by $D(\omega)$, we can therefore determine the effect of the matrix elements, a factor which we call $M^*(\omega)$:

$$\sigma(\omega) \equiv (2\pi e^2/L)\omega M^*(\omega)D(\omega). \qquad (12)$$

In Fig. 1 we show $D(\omega)$ for a 400 atom chain, $W/V = 10$, the chemical potential μ placed in the middle of the conduction band. This result was obtained by diagonalizing the Hamiltonian, using Eq. (11), and then averaging $D(\omega)$ over 12 different configurations. We compared this result with a more exact calculation obtained by applying the negative factor counting method[11,12] to a 10 000-atom lattice and found virtually exact agreement between the results obtained by these two different methods. The triangular shape of the *joint* density of state $D(\omega)$ is a consequence of the approximately rectangular density of states.

From a comparison of $D(\omega)$ in Fig. 1 and $\sigma(\omega)$ in Figs. 2–5, it is clear the "noise" in the spectrum of $\sigma(\omega)$ is not a consequence of the availability of states permitting transitions (the joint density of states), but rather is a consequence of $M^*(\omega)$.

The $\langle\sigma(\omega)\rangle$ shown in Figs. 2–5 are for several different values of W/V. In these plots $\langle\sigma(\omega)\rangle$ is in dimensionless units and should be multiplied by $2\pi e^2 a/\hbar$ to be converted to cgs units. The results are averaged over a frequency width $\Delta\omega = 3B/N$, and all frequencies are measured in units of B.
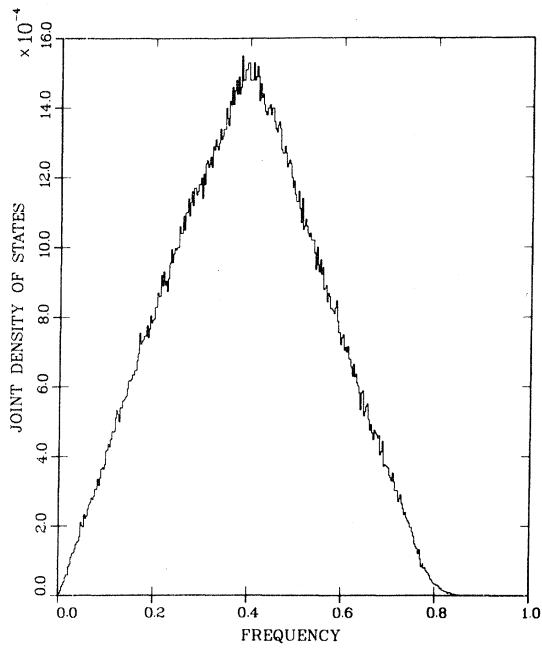
For the ordered case ($W = 0$), only the low-fre-

FIG. 1. Average joint density of states per number of atoms squared. The chemical potential is in the middle of the band ($W/V = 10$), and frequency is in units of the bandwidth.
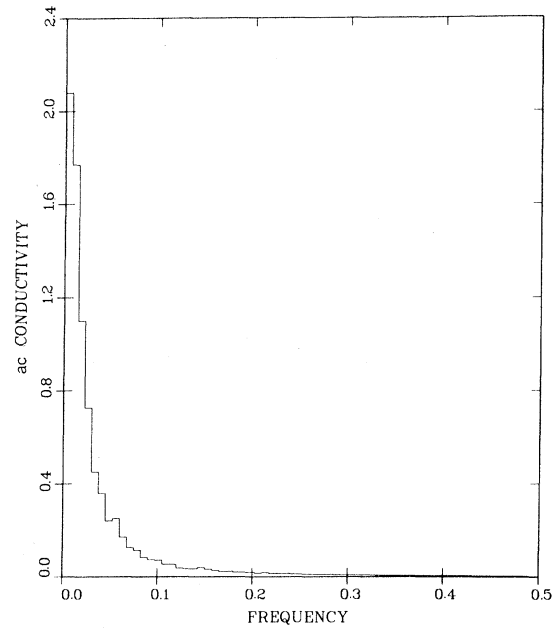

FIG. 3. Average ac conductivity when $W/V = 1$. The units are the same as those in Fig. 2. Note the change in scale. The apparent nonzero conductivity near $\omega = 0$ is a consequence of our frequency averaging procedure. $\Delta \omega = B/3N$.
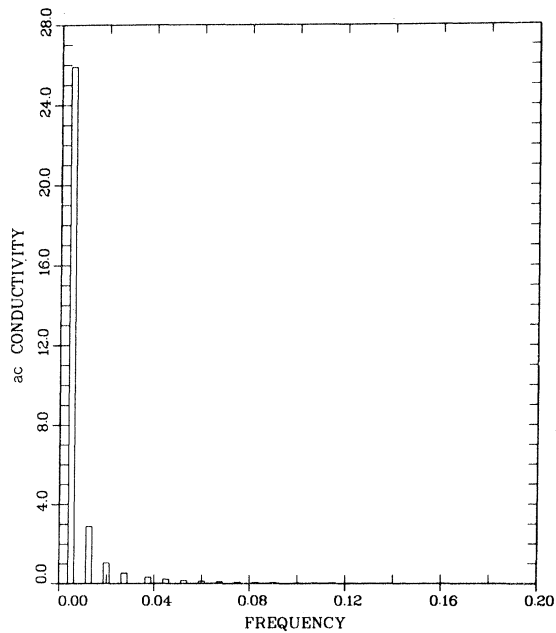

FIG. 2. ac conductivity for an ordered lattice of 400 atoms with fixed boundary conditions. The conductivity is measured in units of $2\pi e^2 a/\hbar$; frequency, in units of the bandwidth. $\Delta\omega = B/N$.
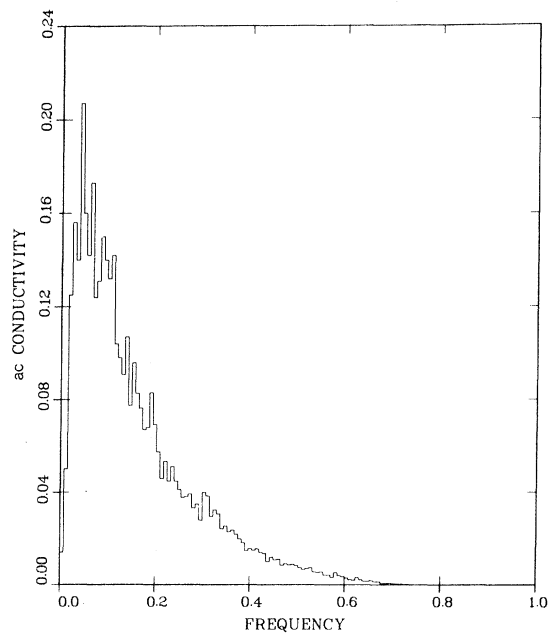

FIG. 4. Average ac conductivity when $W/V = 4$. The units are the same as those in Fig. 2. Note the change in scale; $\Delta\omega = B/3N$.

quency part of $\sigma(\omega)$ is significant enough to be plotted. These results shown in Fig. 2 suggest a δ function near $\omega = 0$. In the Appendix we give an exact expression for $\sigma(\omega)$ for $W = 0$ and show that this conclusion is borne out in the limit $N \to \infty$. For finite N in a lattice with fixed boundary conditions, the δ function becomes broadened as shown in Fig. 2.

In Figs. 3–5 we show the effect of introducing stronger and stronger disorder into the system. As W increases from 0 to 10, the peak at the origin shifts to higher and higher frequencies, broadens and decreases in overall magnitude. The ac conductivity appears to vanish as $\omega \to 0$. However, our resolution and statistics are at their worst for $\omega \sim 0$, and we can make no definitive statement in this regard.

We also studied effects associated with changing μ, i.e., filling up the band to $\frac{1}{4}$ or $\frac{3}{4}$ of its width. For $W/V = 1$, the results were essentially indistinguishable from the half-filled band, even though the eigenstates in the region $E_\alpha \sim \mu$ were slightly more localized than for $\mu = \frac{1}{2}$ (see Fig. 6).

Because of the nature of our numerical procedure, it was possible to calculate eigenvalues and eigenstates in a select limited region of the band. So we concentrated all computational effort on the region of $\sigma(\omega)$ near $\omega = 0$. By doing this, we could increase the number of atoms in the lattice and
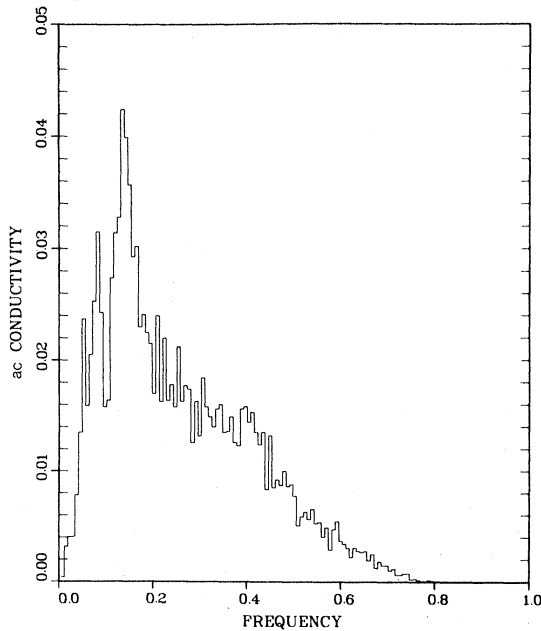

FIG. 6. Localization parameters when $W/V = 4$. Frequency is in units of the bandwidth.

FIG. 5. Average ac conductivity when $W/V = 10$. The units are the same as those in Fig. 2. Note the change in scale; $\Delta\omega = B/3N$.
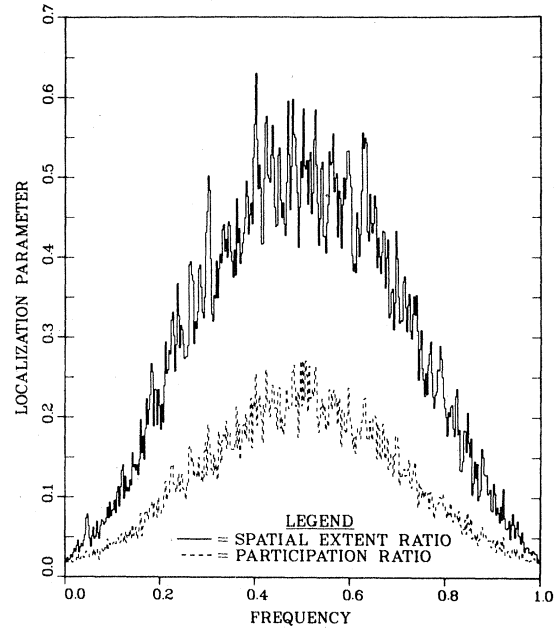
hence hope to look at $\sigma(\omega)$ near $\omega = 0$ on a finer scale of $\Delta\omega$. This analysis was done for a 1000-atom lattice. Unfortunately, near $\omega \sim 0$ the statistics for $\sigma(\omega)$ were very bad, by which we mean that $\sigma(\omega)$ changed drastically from configuration to configuration. When we averaged $\sigma(\omega)$ over 12 configurations, we found that the variances in $\sigma(\omega)$ were of the same size as $\langle\sigma(\omega)\rangle$. In contrast to the results at higher frequency and for larger $\Delta\omega$, here it was evident that the number of configurations needed to obtain the correct ensemble average of $\sigma(\omega)$ was prohibitively large to make this approach an effective one, and we therefore gave up this attempt.

We can understand this difficulty with statistics from an examination of Eq. (2). First, the number of possible transitions that satisfy conservation of energy is given by the joint density of states $D(\omega)$, which from Fig. 1 is seen to be greatly reduced as $\omega \to 0$. Second, for strong disorder the eigenstates $|\alpha\rangle$ and $|\beta\rangle$ are highly localized and hence the overlap matrix element $\langle\alpha|x|\beta\rangle$ is very small unless the centers of localization of $|\alpha\rangle$ and $|\beta\rangle$ are very close to each other. Since this probability is very small, the contributions of the possible transitions are very small, and $\sigma(\omega)$ is dominated by the few transitions where the two states are reasonably close to each other. To average out these effects requires many configurations. These comments probably explain why Penchina and Mitchell[9] had difficulty obtaining a well-defined conduc-

TABLE I. Spatial extent ratio S as a function of energy and disorder W/V. Except for $W/V = 0$, the values of S are averaged over ten eigenstates, centered around the given energy. The energy is in units of the bandwidth B.

| | Energy | | | | |
	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
$W/V = 0$	0.6	1.0	1.0	1.0	0.6
$W/V = 1$	0.03	0.3	0.5	0.3	0.03
$W/V = 4$	0.01	0.03	0.05	0.03	0.01
$W/V = 10$	0.006	0.008	0.01	0.009	0.006

tivity: with only one electron, their statistics were most likely very poor.

To illustrate the localization of the eigenstates, we computed two different localization parameters: the variance of the wave function relative to its mean position (which we call the spatial extent ratio, S)[13] and the participation ratio P.[14,15] They are defined for an eigenstate α by

$$P(E_\alpha) = \left[N \sum_i |a_i(E_\alpha)|^4 \right]^{-1} \tag{13}$$

and

$$S(E_\alpha) = \frac{1}{\sigma} \left[\sum_i |a_i(E_\alpha)|^2 i^2 \right.$$

$$\left. - \left(\sum_j |a_j(E_\alpha)|^2 j \right)^2 \right]^{1/2}, \tag{14}$$

where

$$\sigma = \left[\tfrac{1}{12} (N^2 - 1) \right]^{1/2}, \tag{15}$$

and, of course,

$$\sum_i |a_i(E_\alpha)|^2 = 1. \tag{16}$$

The normalization factor σ is chosen so that $S(E_\alpha)$ is unity when the wave function is completely extended throughout the system (i.e., $a_i = N^{-1/2}$ for all i). The states are more extended for larger values of $P(E_\alpha)$ and $S(E_\alpha)$. As evident in Fig. 6, the two localization parameters agree well with regard to the relative degree of localization between eigenstates and differ, as expected, only in absolute magnitude.

There are two aspects about localization to be considered. The first is the localization properties of the states relative to their position in the band for a given amount of disorder (value of W/V). In Fig. 6 we show results for $W/V = 4$. In agree-

ment with the results of Moore,[13] the states near the middle of the band (frequency = 0.5) are more extended than those at the band edge.

The second aspect is the dependence of the degree of localization in relation to the amount of disorder (ratio of W/V). In Table I we show our results for the two localization parameters S and P for states in various parts of the band as a function of the disorder, as measured by W/V. As expected, states become more and more localized as the disorder increases.

IV. FURTHER REMARKS

We believe the results of our computer experiment accurately represent the overall behavior of the $\langle \sigma(\omega) \rangle$ of the site-disordered one-dimensional Anderson Hamiltonian. In the past, results of computer experiments have been helpful to assess the strengths and weakness of approximate calculations of densities of states and localization lengths of disordered systems.[1-3,12] We hope our results may be useful in similar assessments of approximate calculations of ac conductivities. In this regard, we would like to have also presented results for models of higher dimensions and to have examined the low-frequency behavior of the conductivity in more detail. However, the experience we gained from the present investigation leads us to believe that other techniques may be more appropriate for examining these additional areas.

For example, our ability to diagonalize large (400×400) matrices rapidly and efficiently was largely based on simplifications resulting from its tridiagonal form. In higher dimensions the starting Hamiltonian, depending on the model and boundary conditions, will at best be a real, banded matrix and hence will be more expensive to diagonalize because of increases in computer time and storage. In addition, to insure that the results are indicative of bulk properties, it would be necessary to study much larger systems since in higher dimensions the fraction of atoms on the surface increases dramatically and thereby enhances boundary effects.

An examination of the low-frequency behavior of the conductivity encounters an inherent problem of poor statistics. This problem is exacerbated by the rapid decrease in the joint density of states and is exhibited prominantly as large fluctuations from configuration to configuration that one observes when the conductivity is frequency averaged over a very small $\Delta\omega$. Hence, a detailed study of the region near $\omega \sim 0$ would require a very large number of configurations for the averaged results to converge to the correct average ac conductivity.

ACKNOWLEDGMENTS

This work was performed under the auspices of the Energy Research and Development Administration and the Department of Energy and was motivated by stimulating discussions one of us (J.E.G.) had with P.L. Taylor and S. Y. Wu at the Aspen Center for Physics. We also thank W. M. Visscher for several helpful comments and suggestions.

APPENDIX A. EXACT ac CONDUCTIVITY OF A PERFECTLY ORDERED ONE-DIMENSIONAL LATTICE

Here we give the exact ac conductivity of a perfectly ordered one-dimensional lattice of N atoms with fixed boundary conditions. We found that the model Hamiltonian

$$H = V \sum_{\lambda=1}^{N-1} (|\lambda+1\rangle\langle\lambda| + |\lambda\rangle\langle\lambda+1|) \tag{A1}$$

has the eigenvalues

$$E_m = 2V\cos(k_m a), \tag{A2}$$

where

$$k_m = m\pi/(N+1)a \tag{A3}$$

for $m = 1, 2, \ldots, N$, corresponding to the eigenstates

$$|k_m\rangle = \left(\frac{2}{N+1}\right)^{1/2} \sum_{\lambda=1}^{N} \sin(k_m\lambda a) |\lambda\rangle, \tag{A4}$$

when the boundary conditions are that the amplitudes at sites 0 and $N+1$ are identically zero. (In this Appendix only we use Greek letters for site indices and Latin letters for eigenfunction indices.)

To evaluate the ac conductivity, it was convenient to recast Eq. (2.3) as

$$\sigma(\omega) = \frac{2\pi e^2}{\hbar^2 L} \frac{1}{\omega} \sum_{m,n} (f_n - f_m) |\langle n|[x,H]|m\rangle|^2$$
$$\times \delta(\hbar\omega + E_m - E_n), \tag{A5}$$

since in the present case the commutator matrix element is easier to evaluate than the x matrix element.

After much algebra, we found that

$$\langle n|[x,H]|m\rangle$$

$$= \frac{2Va}{N+1} \frac{\sin^2 \frac{1}{2}(k_m+k_n)a - \sin^2 \frac{1}{2}(k_m-k_n)a}{\sin\frac{1}{2}(k_m+k_n)a \sin\frac{1}{2}(k_m-k_n)a} \tag{A6}$$

for $m \neq n$ and $m-n$ odd and is zero for $m-n$ even.

To establish this result, we used the following identities:

$$\sum_{\lambda=0}^{N} \sin k_m\lambda a = \begin{cases} \cot(\frac{1}{2}k_m a), & m \text{ odd}, \\ 0, & m \text{ even}; \end{cases} \tag{A7}$$

$$\sum_{\lambda=0}^{N} \cos k_m\lambda a = \begin{cases} 1, & m \text{ odd}, \\ 0, & m \text{ even}; \end{cases} \tag{A8}$$

$$\sum_{\lambda=0}^{N} \sin k_m a \sin k_n a = 0, \quad m \neq 0; \tag{A9}$$

$$\sum_{\lambda=0}^{N} \sin\lambda k_m a \cos\lambda k_n a$$

$$= \begin{cases} \dfrac{1}{2} \dfrac{\sin k_m a}{\sin\frac{1}{2}(k_m+k_n)a \sin\frac{1}{2}(k_m-k_n)a}, \\ \qquad\qquad m \neq n, \quad |m-n| \text{ odd}, \\ 0, \quad m \neq n, \quad |m-n| \text{ even}; \end{cases} \tag{A10}$$

$$\sin k_m a \sin k_n a = \sin^2 \frac{1}{2}(k_m+k_n)a$$
$$- \sin^2 \frac{1}{2}(k_m-k_n)a. \tag{A11}$$

When (A6) is substituted into (A5) we find

$$\sigma(\omega) = \frac{2\pi e^2 a}{\hbar} \sum_{m,n} [\Theta(\mu-E_m) - \Theta(\mu-E_n)]\delta\left(\frac{\hbar\omega}{V} + \frac{E_m-E_n}{V}\right) \frac{\sin^2 \frac{1}{2}(k_m+k_n)a - \sin^2 \frac{1}{2}(k_m-k_n)a}{(N-1)(N+1)^2 \sin^3 \frac{1}{2}(k_m+k_n)a \sin^3 \frac{1}{2}(k_m-k_n)a} \tag{A12}$$

for $|m-n|$ odd, zero otherwise. [Note that $L = (N-1)a$]. In the limit $N \to \infty$, $\sigma(\omega)$ resembles a δ function near $\omega = 0$ since for finite ω, $\sigma(\omega) \propto 1/N^3$. The leading contribution to $\sigma(\omega)$ in this limit occurs for $E_m \approx E_n \approx \mu$ and $|m-n| = 1$ so that

$$\sigma(\omega) \sim (2\pi e^2 a/\hbar)\delta(\hbar\omega/V - 2\pi/N \, (2/\pi)^3, \tag{A13}$$

when the chemical potential is in the middle of the band. Note that this leading contribution shrinks to zero frequency as $N \to \infty$.

[1]F. Yonezawa and K. Morigaki, Prog. Theor. Phys. Suppl. 53, 1 (1973).

[2]R. J. Elliot, J. A. Krumhansl, and P. L. Leath, Rev. Mod. Phys. 46, 465 (1974).

[3]D. J. Thouless, Phys. Rep. 13, 93 (1974).

[4]For example, R. Landauer, Philos. Mag. 21, 863 (1970); K. Schönhammer and W. Brenig, Phys. Lett. A 42, 447 (1973); D. C. Licciardello and D. J. Thouless, J. Phys.

C $\underline{3}$, 4157 (1975).

[5]K. Niizeki and K. Hoshino, J. Phys. C $\underline{10}$, 3351 (1977), and references therein.

[6]B. I. Halperin, Adv. Chem. Phys. $\underline{13}$, 123 (1967).

[7]H. Schmidt, Phys. Rev. $\underline{105}$, 425 (1957).

[8]J. E. Hirsch and T. P. Eggarter, Phys. Rev. B $\underline{14}$, 2433 (1976); $\underline{15}$, 779 (1977).

[9]C. M. Penchina and P. L. Mitchell, J. Non-Cryst. Solids $\underline{7}$, 127 (1972).

[10]H. Bowdler, R. S. Marten, C. Reinsch, and J. H. Wilk-inson, Numer. Math. $\underline{11}$, 293 (1968).

[11]P. Dean, Rev. Mod. Phys. $\underline{44}$, 127 (1972).

[12]W. M. Visscher and J. E. Gubernatis, in Dynamical Properties of Solids, edited by G. K. Horton and A. A. Maradudin, (North-Holland, Amsterdam, to be published), Vol. 3.

[13]E. J. Moore, J. Phys. C $\underline{6}$, 1551 (1973).

[14]R. J. Bell, P. Dean, and D. C. Hibbins-Butter, J. Phys. C $\underline{3}$, 2111 (1970).

[15]W. M. Visscher, J. Non-Cryst. Solids $\underline{8-10}$, 477 (1972).