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Electronic Wave Functions in One-Dimensional Disordered Systems[*]

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The nature of wave functions in a one-dimensional disordered system is examined in terms of a model system in which the central portion of a cell is represented by the same potential in all cells and only the lengths of the flat arms vary randomly from cell to cell. It has been shown previously that although most wave functions are localized, states corresponding to the resonances states of the central potential have extended wave functions. Here we show that states close to these resonances also have fairly extended wave functions throughout the physical sample. Numerical calculations on a model system formed from symmetric square wells indicate that even in a highly disordered system there are wide energy ranges close to the resonances which have fairly extended wave functions. Wave functions having energies in the allowed bands of the corresponding periodic lattice are also weakly localized, but their degree of localization is raised as a whole with an increase in disorder, whereas an increase in disorder only narrows the energy range of these fairly extended states.

I. INTRODUCTION

Extensive reviews on the electronic properties of one-dimensional disordered systems are available.[1-9] Owing to the complexity of the solutions and their interpretation, and because of the recent indications of the experimentally measurable physical systems,[10,11] the one-dimensional disordered systems are still being actively studied.[12-47] The two key questions studied in the electronic properties of such systems are (a) the existence of energy gaps and the density of states,[12-25,41-44] and (b) the localization of electronic wave functions.[26-40,46]

We studied the problems using the phase-transfer method.[2,41-48] A wave function connecting through a cell of a potential shown in Fig. 1 is represented by a phase-transfer matrix M:

$$\psi_{\text{left}} = A(x)e^{ikx} + B(x)e^{-ikx} , \qquad (1)$$

$$\psi_{\text{right}} = A'(x)e^{ikx} + B'(x)e^{-ikx} , \qquad (2)$$

$$\begin{pmatrix} A \\ B \end{pmatrix} = M \begin{pmatrix} A' \\ B' \end{pmatrix} ,$$

where

$$M = \begin{pmatrix} u^* & v \\ v^* & u \end{pmatrix} \tag{3}$$

and $\det|M| = 1$. The matrix M is like a black box which contains all the characteristics of the potential in the cell, and in many occasions we do not need to know the details of this black box in order to get some definite answers. Unlike most other methods which involve a perturbation-series expansion, or averaging over certain statistical distributions, in our approach we seek exact answers from algebraic relations. This matrix M is also related to the scattering matrix and the phase-shift analysis, which are standard approaches in the three-dimensional problems. Still another way of expressing M, when the wave function is chosen to be of the form in Eq. (1), is to write it in terms of the transmission coefficient t and the reflection coefficient r. This representation of M is simple and is clear in physical interpretation.

In order to answer the above questions, we first set up a model to represent the one-dimensional amorphous material or liquid. We do not arbitrarily draw a random curve (usually restricted by some statistical properties for the potentials[49]), and we do not represent such a system by an array of square-well potentials of arbitrary sizes and depths. A crystalline material and its amorphous-or liquid-state counterpart differ only in the geometric arrangement of the sites of the constituent atoms. The potentials representing the constituent atoms should not change much from those in the crystalline state. In the disordered system, only the geometrical locations, or the site separations, are at random. Our model is therefore the following.[44-46,48]

A one-dimensional liquid or amorphous material is represented by a linear chain of potential cells. Each cell consists of a central potential with two flat arms. The central potentials are assumed to be the same in all cells representing the same atoms (see Fig. 1). The lengths of flat arms vary at random from cell to cell within certain natural limits. In this model the transfer matrix in each cell can be written as

$$M = \begin{pmatrix} e^{-ikh_l} & 0 \\ 0 & e^{ikh_l} \end{pmatrix} M_c \begin{pmatrix} e^{-ikh_r} & 0 \\ 0 & e^{ikh_r} \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i2kh}/t & (r/t)^* \\ r/t & e^{i2kh}/t^* \end{pmatrix}, \quad 2h = h_l + h_r , \tag{4}$$

where h_l and h_r are the lengths of the flat arms.

This model is consistent with the following basic concept that we put forth,[45-47] and has been mentioned by Ziman[50] and Weaire.[51] A one-dimensional system is characterized by the constituent potentials and the specific geometrical arrangement of their sites. These characteristics show up in the electronic spectrum of the particular system. By rearranging the same constituents in a different way, the electronic spectrum will certainly change. It would be most interesting to sort out parts of the spectrum which are completely characterized by the properties of the constituent potentials and are independent of the geometrical arrangements. In other words, these are the sample-independent properties of the amorphous material.

Following this trend of thought, we were able to give a definite answer to the first question.[43-44] We proved, using the phase-transfer method, that energy gaps do exist in such model systems. They depend solely on the property of the central potential. This result is a generalization of the δ-potential study of Borland,[52] and is in agreement with the general theorem established by Hori[3,12] and others.[18,22]

As regards the second question, the prevailing view is that all wave functions in one-dimensional disordered systems are localized. The statement was originated by Mott[5] and subsequently several proofs[26-36] have been given including several recent studies of Economou *et al.*[8,24,39,40] On the other hand, it has also been stated that no state is localized for a system of finite number of scattering sites.[36,37]

The Mott definition[5,6] of a localized wave function is the following: a wave-function whose envelope decays exponentically from a central position x_0; $\psi \sim e^{-|x-x_0|/L}$. By an extended wave function we mean a wave function whose amplitude keeps more or less the same magnitude throughout the whole system. Notice that the Mott definition, when it is applied to one-dimensional systems, does not exclude the extended states which are the limiting case of the localization length $L \to \infty$. Thus to study whether *all* wave functions in one-dimensional disordered systems are localized or not, we should not just show that all wave functions have the exponentially decaying envelopes. It is more meaningful to examine whether extended states exist or not.

In our previous study[45,46] we have shown that such extended states do exist in the model systems. They are the resonance states of the scattering potentials characterized by transmission coeffi-

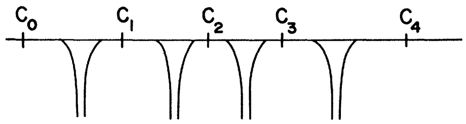

FIG. 1. Model of one-dimensional liquid.

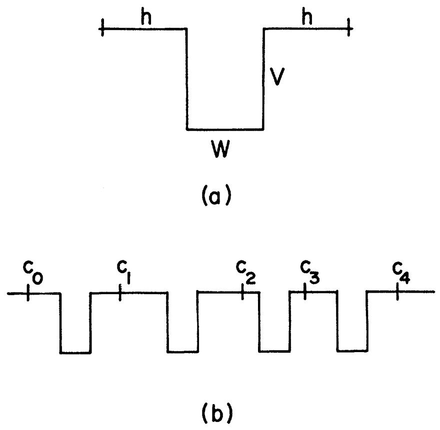

FIG. 2. One-dimensional disordered systems built up from symmetric square wells of the same well width W and depth V but variable arm lengths h.

cient $|t| = 1$ in the transfer matrices [Eq. (4)]. This is related to the Ramsauer–Townsend effect in the three-dimensional-scattering problem.[53] Since the central potentials in the cells represent the same constituent atoms, a resonance state of one central potential is also the resonance state of all other central potentials along the linear chain. A plane wave at the resonance energy coming in from one end will be transmitted through the potential as if the potential is not there. Such a wave will therefore be perfectly transmitted from one end of the one-dimensional disordered system to the other. The disorder in the chain will not affect the transmission and it is a sample-independent property. In all arbitrary one-dimensional potentials other than the δ potentials (see comments in Sec. III) such states exist. They are discrete energy levels. They are observed only in our model systems because we insisted that all constituent potentials are exactly alike. In a more realistic model the potentials in different cells differ slightly. One may ask whether such small deviations in the central potentials will erase all such extended states or not. In Ref. 46, we conjectured that states close to $|t| = 1$ resonance states are also highly extended. If this is the case, such small perturbutions will not affect the localization too much. Perhaps there are wide ranges in the energy spectrum which have wave functions quite extended, say of the size of the sample. The existence of these also opens the possibility of a nonhopping type of conductivity in one-dimensional disordered systems even in the presence of impurities or in alloys.

It is the purpose of this article to study this conjecture and examine the properties of wave functions at energies close to the resonance states. In Sec. II we shall examine the behavior of wave functions in going through a series of the same square-well potentials located at random on the linear chain. We shall examine the growth of wave functions by numerical computation in Sec. II. In Sec. III we shall prove the conjecture analytically and obtain further insights into the problem of one-dimensional disordered systems.

II. COMPUTER CALCULATION OF WAVE FUNCTIONS

To examine the behavior of wave functions at energies close to the resonance energies, we calculate each wave function numerically as it passes through each cell. For simplicity we have chosen the central potentials as square-well potentials of width W (in eV) and depth V (in eV) located symmetrically in the cell having two equal flat arms each of length h (in Å) (Fig. 2). The lengths of the flat arms vary at random from cell to cell within limits (in Å): $1-d \leq h \leq 1+d$, where d is an arbitrarily assigned number designating the degree of disorder. At C_0 of the first cell [Fig. 2(b)], we take a wave function with $A_0 = B_0^* = 1$ [Eq. (1)]. The transfer matrix for such a square well is given by Eq. (4) with

$$\frac{e^{-i2kh}}{t} = \cos(k'w)\cos(2kh) - \frac{k'^2+k^2}{2kk'}\sin(k'w)\sin(2kh) - i\frac{k'^2+k^2}{2kk'}\sin(k'w)\cos(2kh) + \cos(k'w)\sin(2kh) \;, \tag{5}$$

$$\frac{r}{t} = i\frac{(k'^2-k^2)}{2kk'}\sin(k'w) \;, \tag{6}$$

where $k = E^{1/2}$ and $k' = (E+V)^{1/2}$. It can be easily shown[46] that with this choice of A_0 and B_0, $B_j = A_j^*$ at any site C_j. By multiplying the transfer matrices together we can find the amplitude $|A_n|$ at the nth site C_n. For a given energy, this can be calculated numerically on the computer. We also calculate the final change in amplitude $|A_f| \equiv |A_N|$, where N is the last cell in the chain. The quantity $\log_{10}|A_f|$ is closely related to the degree of localization introduced by others.[26,27,31,32]

In Fig. 3, we have plotted $\log_{10}|A_f|$ for a wide range of energy values integrated through 4000 cells. The vertical straight lines indicate boundaries of allowed and forbidden bands in the periodic lattice (i.e., $d = 0$). The wave functions grow to a large magnitude very rapidly at energies lying in the forbidden bands of the corresponding periodic lattice. (A clear explanation why a wave function usually grows in a disordered system is given by Mott[6] and Readig and Sigel.[36]) At energies lying in the allowed bands of the periodic lattice, the wave functions of the disordered system grow less rapidly. $\text{Log}_{10}|A_f|$ is usually small near the middle portions of the corresponding allowed bands of the periodic lattice. They are weakly localized

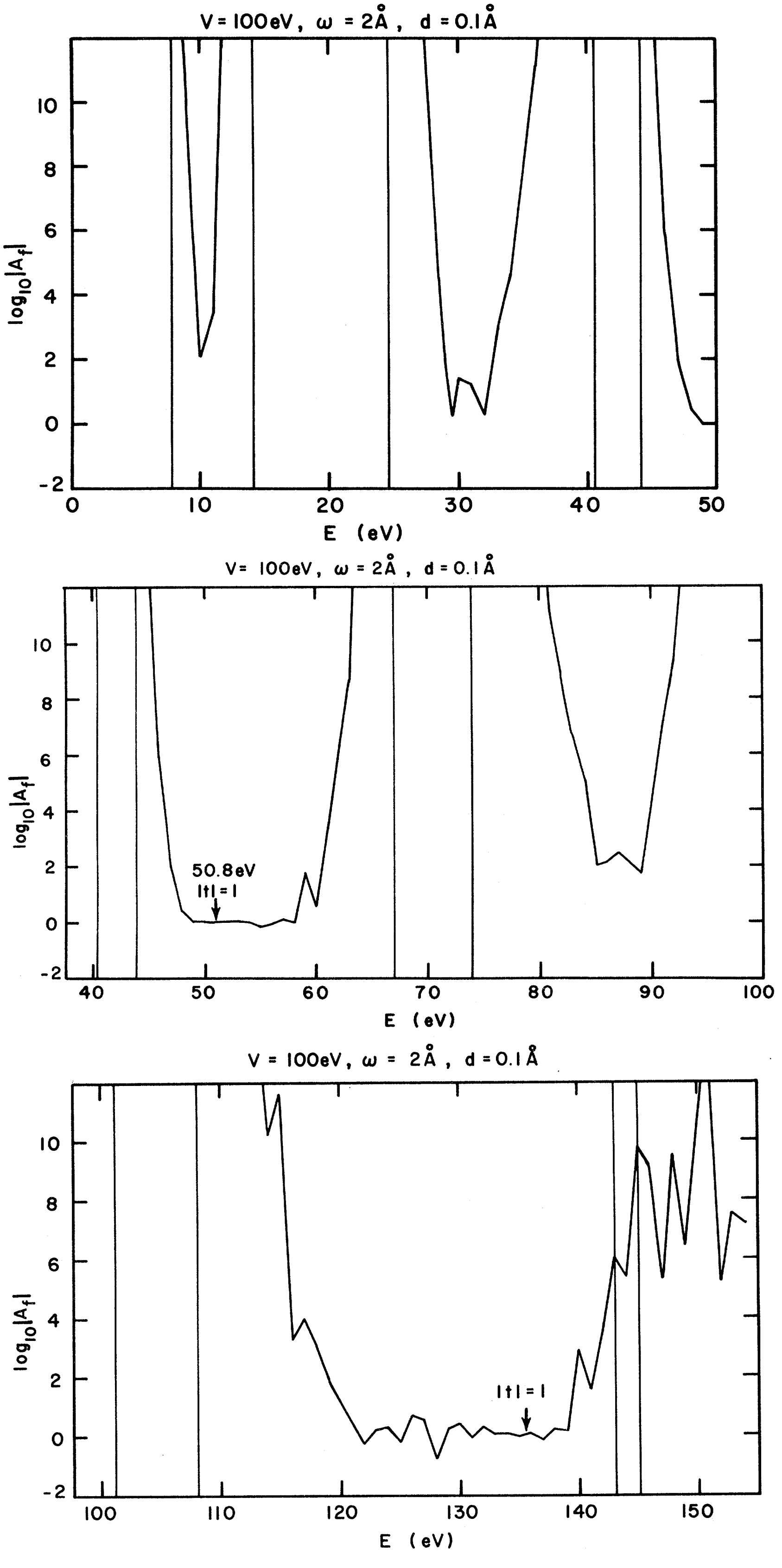

FIG. 3. Localization of a wave function at different energies for the square-well liquid model with $V = 100$ eV, $W = 2$ Å, and variable h: $|1-h| \leq d = 0.1$ Å. The degree of localization is represented by $\log_{10} |A_f|$, where A_f is the amplitude of the wave-function at the last cell. $|A_0|$ is chosen to be 1 and N is taken to be 4000. The vertical straight lines represent the boundaries of the allowed and forbidden bands of a periodic lattice formed from the same square wells (i.e., when the disorder $d = 0$). $|t| = 1$ are the perfectly transmitting resonance states.

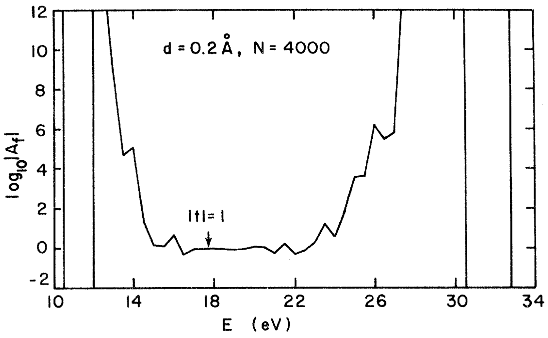

FIG. 4. $\log_{10}|A_f|$ vs energy for square wells having $V = 20$ eV, $W = 1$ Å, $d = 0.2$ Å, and $N = 4000$.

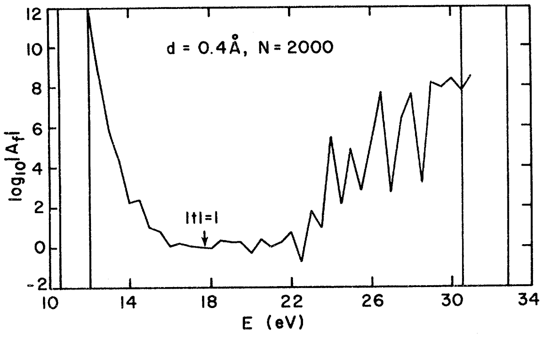

FIG. 6. $\log_{10}|A_f|$ vs energy for square wells having $V = 20$ eV, $W = 1$ Å, $d = 0.4$ Å, and $N = 2000$.

states, and have been reported previously.[27,39,49] The arrows indicate the resonance energies of the central square well. At these points $\log_{10}|A_f| = 0$. The wave functions are extended. There are wide ranges of energies close to these resonance states which also have $\log_{10}|A_f|$ fluctuating close to zero. They are the fairly extended states conjectured by us. (Notice that even in the periodic case the calculated value of $\log_{10}|A_f|$ fluctuates about zero and is usually not exactly zero except at the resonance points. This is related to the choice of the form of ψ and the definition of t and r.) The weakly localized states near the centers of the allowed bands are less extended than these regions close to $|t| = 1$.

We also see that a $|t| = 1$ state always lies in the allowed band of the periodic lattice. This is obvious from Eqs. (5) and (6). At a resonance energy $k'w = n\pi$, the half-trace of the transfer matrix M is $\cos(2kh)$ which is always less than or equal to 1, and therefore it lies in the allowed band.[41-42]

Figures 4-7 give more detailed features of the wave functions with energies close to a resonance state $|t| = 1$. Comparing Figs. 4 and 5, and 6 and 7 we see that an increase in the disorder ($d = 0.2$ Å as compared to $d = 0.4$ Å with h lying between $1 \pm d$ Å) narrows the width of the extended region close to $|t| = 1$.

If instead of integrating through 4000 cells we examine the behavior of a random system of 2000 cells formed from the same square-well potentials we see from Figs. 5 and 6 that the width of the $\log_{10}|A_f| \simeq 0$ region close to $|t| = 1$ does not change much. An increase in N tends to smooth the fluctuation in the $\log_{10}|A_f|$ curve.

Figure 8 shows that in a weakly localized region which *does not* contain $|t| = 1$, an increase in disorder changes the degree of localization quite a bit. Although the $d = 0.2$-Å curve shows a similar shape as the $d = 0.1$-Å curve with a small over-all increase in $\log_{10}|A_f|$, it no longer contains a large region fluctuating about the $\log_{10}|A_f| = 0$ line in this region. On the other hand, in regions *close to* $|t| = 1$, an increase in disorder does not raise the whole curve of $\log_{10}|A_f|$ away from zero. It only narrows the range of the fluctuating $\log_{10}|A_f|$ about zero.

To give us a feeling how extended a wave function is at energies close to a resonance line, Fig. 9 gives a plot of the amplitude against the cell number. The amplitude $|A_n|$ is the accumulated

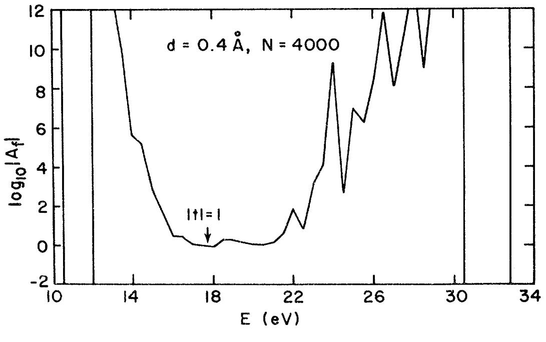

FIG. 5. $\log_{10}|A_f|$ vs energy for square wells having $V = 20$ eV, $W = 1$ Å, $d = 0.4$ Å, and $N = 4000$.

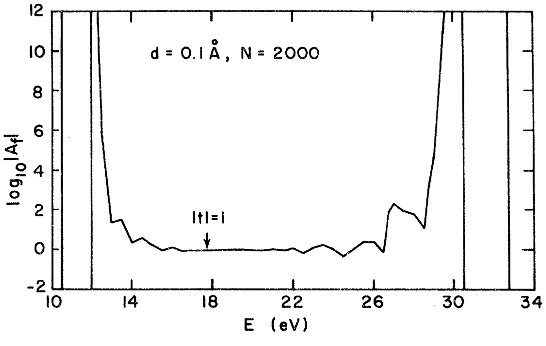

FIG. 7. $\log|A_f|$ vs energy for square wells having $V = 20$ eV, $W = 1$ Å, $d = 0.1$ Å, and $N = 2000$.

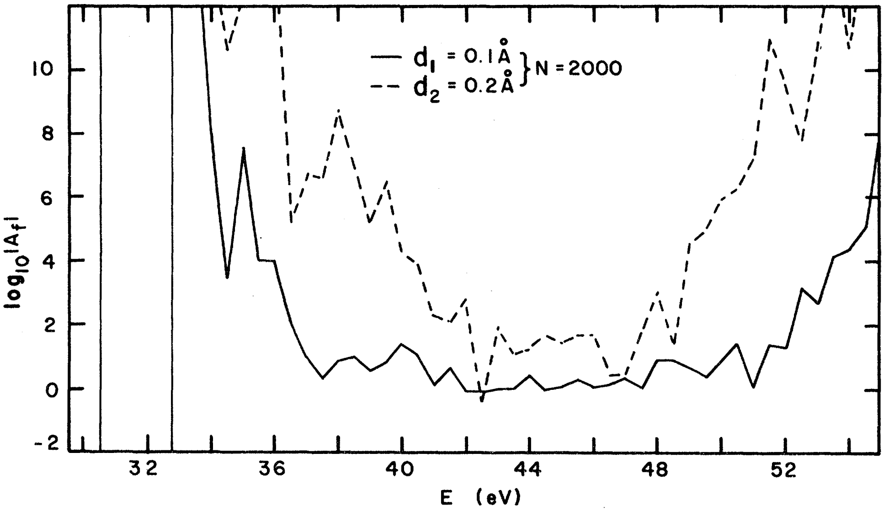

FIG. 8. $\log|A_f|$ vs energy curves for two different disordered systems formed from square wells having V = 20 eV, W = 1 Å, N = 2000, and d_1 = 0.1 Å and d_2 = 0.2 Å.

growth from C_0 to the nth cell. The change in amplitude after 2000 cells is less than 7% at E = 17.5 eV. In the strong-scattering region (i.e., when $|r|$ is large) the wave functions grow rapidly with an exponential envelope indicating that the wave functions are localized (Fig. 10). This has been repeatedly pointed out by authors who studied the question of localization of wave functions in one-dimensional disordered systems.[26–40] The regions close to $|t| = 1$ belong to the weak-scattering regions. A weak scatterer is defined to be one which has a small reflective coefficient $|r|$ in Ref. 46. The amplitudes of the wave functions as shown in Fig. 9 fluctuate about the initial value. The growth, if it is present, is very slow indeed.

III. WEAK-SCATTERING STATES

In this section we shall examine analytically the weak-scattering states having energies close to the resonance states. First of all let us note that such resonance states always exist in an arbitrary central potential. In δ potentials, however, the resonance energy is at $E \rightarrow \infty$. This is perhaps the reason why such resonance states have not been discussed by Borland.[26,27] A typical example of the transmission coefficient $T = |t|^2$-vs-energy curve is represented by that of a square well (Fig. 11). We are interested in the weak-scattering states. $T = 1$ states are discrete points, but $T \simeq 1$ states lie on the approximately parabolic portions of the T-vs-E curve. It is therefore quite likely to have bands of considerable width whose states have wave functions not too different from the extended wave functions of the resonance states.

Another indication that a weakly scattering state has a fluctuating wave function along the linear chain is the following. It has been shown [Eqs. (20)–(22) of Ref. 46] that in going through the jth

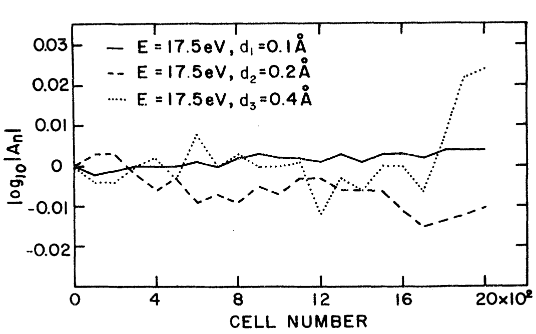

FIG. 9. Growth of a wave function at E = 17.5 eV close to the resonance state at 17.7 eV along the linear chain of three disordered systems formed from square wells having V = 20 eV, W = 1 Å, N = 2000, and d_1 = 0.1 Å, d_2 = 0.2 Å, and d_3 = 0.4 Å, respectively. A_n is the amplitude at the nth cell and $|A_0| = 1$.

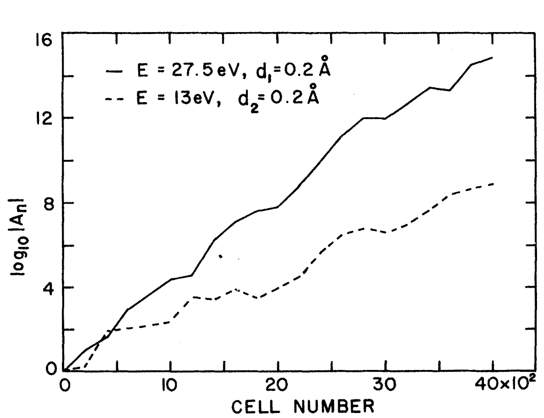

FIG. 10. Growth of wave functions at energies away from the resonance energy at 17.7 eV. A_n is the amplitude at the nth cell and $|A_0| = 1$.

cell, the amplitude is modified by a factor α_j characterizing all the effects of the potential in the jth cell, and that the values of α_j lie between

$$\frac{1-|r|}{1+|r|} \leq \alpha_j \leq \frac{1+|r|}{1-|r|} \quad \text{for all } j. \tag{7}$$

The allowed values of α_j are shown as the shaded area in Fig. 12. For strong scatterers, i.e., for a particular $|r|$ close to 1, it is far more likely for α_j to take up a value greater than one. As a result, a wave function tends to grow exponentially. In the weak-scattering region, i.e., $|r|$ close to zero, α_j has practically equal chance to be greater than or less than one, resulting in a fluctuating amplitude in going through the cells. This is indeed observed in the numerical study of square-well potentials in Fig. 9. Notice that even in a perfectly periodic lattice, $|r|$ is in general nonzero, but the phase relation introduced by the periodicity guarantees equal probability for α_j to be greater than or less than one.

To examine this more closely, let us return to the transfer matrix [Eq. (14)]. It is obvious that a $|t|=1$ state always lies in the allowed band of the periodic lattice, for

$$\tfrac{1}{2}\,\mathrm{Tr}M = \mathrm{Re}(e^{-i2kh}/t)\big|_{t=1} = \cos 2kh \leq 1. \tag{8}$$

In transferring a wave function from C_0 through two cells to C_2 (Fig. 1), we multiply two such matrices together:

$$\begin{pmatrix} \dfrac{e^{-i2kh_1}}{t} & \dfrac{r^*}{t} \\[2ex] \dfrac{r}{t} & \dfrac{e^{i2kh_1}}{t^*} \end{pmatrix} \begin{pmatrix} \dfrac{e^{-i2kh_2}}{t} & \dfrac{r^*}{t} \\[2ex] \dfrac{r}{t} & \dfrac{e^{i2kh_2}}{t^*} \end{pmatrix} = \begin{pmatrix} \dfrac{e^{-i2k(h_1+h_2)}}{tt} + \dfrac{r^2}{t} & \dfrac{r^*}{t}\left(\dfrac{e^{-i2kh_1}}{t} + \dfrac{e^{-i2kh_2}}{t^*}\right) \\[2ex] \dfrac{r}{t}\left(\dfrac{e^{i2kh_1}}{t^*} + \dfrac{e^{-i2kh_2}}{t}\right) & \dfrac{e^{+i2k(h_1+h_2)}}{tt} + \left|\dfrac{r}{t}\right|^2 \end{pmatrix}. \tag{9}$$

If in the weak-scattering region we can neglect $|r/t|^2$ in comparison to $1/tt$, the infinite products of the matrices give diagonal elements of the form

$$M_n = \begin{pmatrix} \dfrac{\exp[-i2k(h_1+h_2+\cdots+h_n)]}{tt\cdots t} & \cdots \\[2ex] \cdots & \dfrac{\exp[i2k(h_1+h_2+\cdots+h_n)]}{tt} \end{pmatrix}, \qquad n\to\infty. \tag{10}$$

We are interested only in the half-trace of M_n or $\mathrm{Re}(\exp[-i2k(h_1+h_2+\cdots)]/tt\cdots)$ in applying Kramer's condition.[41-43] For a perfectly periodic lattice, all the h's are the same. The half-trace of M_n is $\mathrm{Re}(e^{-i2nkh}/t^n)$, $n\to\infty$. In the disordered model, we can certainly impose the condition that the disorder does not change the length as a whole, i.e., $h_1+h_2+\cdots+h_n=nh$. This gives the same half trace of M_n for the disordered system. In other words, if $|r/t|^2$ can be neglected in comparison to $1/tt$ for the central potential in the weak-scattering limit, the state is practically the same as that of a periodic lattice. Since a weak-scattering state in the periodic lattice has an extended wave function (this is obvious from the fact that a $|t|=1$ state lies in the allowed band, and from the property that if $T_1 \leq 1$, $T_n \leq 1$ in Ref. 42), the status of a weak-scattering state in the disordered system is not changed.

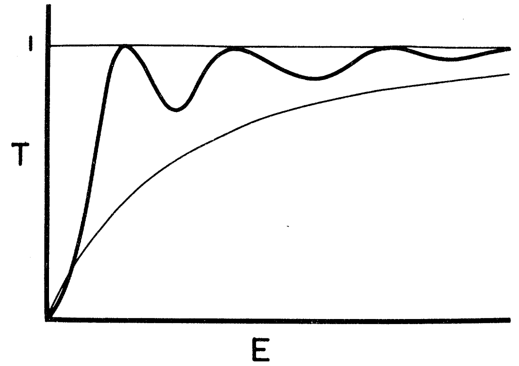

FIG. 11. Schematic sketch of the variation of the transmission $T=|t|^2$ as a function of energy. The heavy oscillating curve represents the T-vs-E curve of a square well, and the thin growing curve is the T-vs-E curve of a δ potential.

We can therefore conclude by saying that a weak-scattering state in a one-dimensional disordered system has a wave function which is extended to the approximation of neglecting $|r/t|^2$ in comparison to $1/tt$. If we do not make such an approximation, the wave function has a very broad localization envelope. The resonance states $|t|=1$ are definitely extended. Unlike the three-dimensional

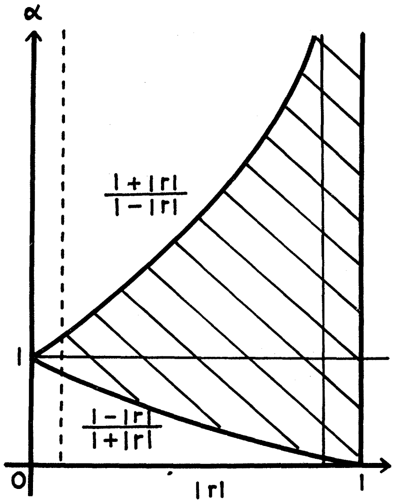

FIG. 12. Allowed values of α (shaded region). The vertical dotted line represents a weak-scattering state and the vertical solid line represents a strong-scattering state.

case, we do not expect a sharp change from an extended to a localized state in the one-dimensional disordered system. There is, however, a physical length parameter to help us in the discussion. This is the size of the physical system. Most amorphous materials are studied in the form of thin films several thousand angstroms thick. If the localization length is greater than the thickness of the sample, we can, for practical reasons, call it an extended state in the one-dimensional problem. Our study here shows that they are most likely to occur at the weak-scattering regions close to the resonance states. These regions are fairly wide. Unlike the weakly localized states in the allowed bands of the corresponding periodic lattice, these regions persist when the disorder is increased. Of course, their widths decrease with increase of disorder.

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Acoustic Geometric and Acoustic Cyclotron Resonances in Gallium

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Acoustic geometric and acoustic cyclotron resonances in high-purity single crystals of gallium were investigated at 1.3 °K and in the normal geometry where the magnetic field is perpendicular to the wave vector of the ultrasonic waves. These waves, polarized longitudinally and of frequencies in the range 60–400 MHz, were propagated along the three principal crystallographic axes a, b, and c of gallium. The extremal dimensions of the Fermi surface in the k_ak_b, k_bk_c, and k_ck_a planes, obtained by measuring the periodicity $\Delta(1/H)$, of the geometric-resonance oscillations, are compared with the predictions of the augmented-plane-wave and pseudopotential models. The results are in good agreement with the values given by the pseudopotential model. A map of effective masses in the *ab*, *bc*, and *ca* planes, obtained from acoustic-cyclotron-resonance experiments, is given. These data are compared to those of Moore, who used the Azbel'-Kaner cyclotron resonance (AKCR). Some branches of effective masses were found which have not been observed by AKCR and, reciprocally, many resonances observed by AKCR were not observed in the present work.

I. INTRODUCTION AND THEORY

Although many experimental studies of the Fermi surface of gallium[1] have already been done, this surface, which appears to be a very complicated one, is still far from well known. The methods which have been used to investigate its properties include de Haas–van Alphen effect, magnetoresistance, magnetoacoustic effect, cyclotron resonance, and others. The comparison of the experimental data with the theoretical models proposed for gallium shows that, whereas the nearly free-electron model[2] is not confirmed, the augmented-plane-wave model (APW)[3] is in better agreement with available data. Recently, Reed[4] made some calculations using the pseudopotential model. The form factor was adjusted in order to give the best fit between the calculated surface and the experimental results.

First ultrasonic measurements on gallium were carried out by Roberts,[5] who was the first to observe acoustic cyclotron resonance (ACR) in single crystals of gallium. Some data were published,[6–9] too, on the shape of the Fermi surface determined by acoustic geometric resonance. ACR was also further investigated[10–12] and led to the knowledge of some effective masses of the carriers.

In the present work we have studied the properties of gallium by propagating longitudinal ultrasonic waves along the three principal crystallographic axes of high-purity single crystals. All the experiments were made in the so-called normal geometry where the magnetic field H is perpendicular to the ultrasonic wave vector $\vec{q}$. The ultrasonic frequencies used ranged from 60 to 400 MHz, which corresponds to $ql \gg 1$, and $\omega\tau \cong 1$ or $\omega\tau > 1$ (l is the mean free path of the electrons; it is related to the collision time τ by $l = \tau v_F$, where v_F is the Fermi velocity).

Before presenting the experimental data, we will review the basic results of the theory of the magnetoacoustic interaction, using the formalism developed by Cohen, Harrison, and Harrison (CHH).[13]

At low temperatures, the attenuation of an ultrasonic wave in a metal is due to mainly the electron-phonon interaction. Instead of a real metal, we consider a gas of free electrons moving through a uniform background of positive charges. The interaction between the sound wave and the electrons takes place via the electromagnetic field associated with the wave. Under such conditions it was shown in Ref. 13 that the attenuation α of a longitudinal wave, propagated perpendicularly to a