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¹⁸The scattering lengths quoted in Ref. 10 are slightly too large owing to the lack of a correction for the long-range potential. If we take this into account, the singlet e^- -H scattering lengths given by Temkin and Lamkin become $6.3a_0$ (exchange adiabatic) and $5.6a_0$ (their polarized orbital), respectively. The exact value is $5.965a_0$, due to Schwartz (Ref. 11). However, the polarization potential used by Temkin and Lamkin in their adiabatic-exchange approximation is not the same as the Bethe potential used here in the AED. Our value for the corrected scattering length in the AED is $6.15a_0$, which is closer to the exact value than the corrected result of the Temkin-Lamkin method.

Localization of Electronic States in One-Dimensional Disordered Systems*

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The localization of electronic states in one-dimensional disordered systems is examined in terms of the reflection and transmission coefficients. The transfer-matrix method is used. The main body of the work deals with a one-dimensional liquid model in which the central part of the potential remains the same in all cells, and only the lengths of the flat arms vary from cell to cell. It is found that the contribution of the initial phase of a wave at the zeroth cell to the phase at the n th cell is reduced by a factor $(1 - |r|)/(1 + |r|)$ every time in passing through a cell. When the phase memory is completely lost, $\Phi_j \sim \phi_j$, where the reflection coefficient of the j th cell is $r_j = |r|e^{i\phi_j}$. If Φ_j obeys a uniform or nearly uniform probability distribution, the wave function always grows exponentially. It is shown that in most cases, especially when cell size distribution has a wide spread, $P(\Phi)$ is nearly always uniform. All wave functions are localized in a completely disordered system, but in the one-dimensional liquid model nonlocalized states do exist.

I. INTRODUCTION

The existence of localized states in disordered systems is of fundamental importance in the understanding of the electronic properties of systems like random impurities and alloys, amorphous substances, and liquids.¹ As an example, when the wave functions are localized, the electrons can move only by activated hopping. The transport properties are therefore quite different from those of the usual propagating solutions. An exact discussion of the general problem in three dimensions

is difficult even in the independent one-electron approximation.

In one-dimensional disordered systems, it has been conjectured by Mott and Twose² that all solutions of the Schrödinger equations are localized. A wave function in one-dimensional space is said to be localized if, starting from a point x_0 , the envelope of its amplitude decays or grows exponentially with the distance $|x - x_0|$ (see Mott, Ref. 1, p. 52). Proofs have been provided by Borland, Hori, and Minami.³ These have been reviewed and commented on by Mott¹ and Halperin.⁴ Here we

shall use the method developed in the previous works,⁵ and study the Mott conjecture in terms of the reflection coefficient r and the transmission coefficient t of the individual potential cells. This provides a clearer understanding of the problem. For this reason, the main body of this report deals with a simplified case – the “one-dimensional liquid.” The discussion can easily be extended to the general one-dimensional cases. A formulation of the latter is sketched in the Appendix.

Let us consider a strongly localized potential symmetric about the center of the cell C_0C_1 [see Fig. 1(a)]. It has two flat arms C_0X and YC_1 of equal lengths d , and a central part XY which varies rapidly with position. A homogeneous real liquid may be looked upon as a collection of the same atoms arranged at random separation from one another. An infinite chain of the one-dimensional cells, $C_0C_1, C_1C_2, \dots, C_{n-1}C_n, n \rightarrow \infty$, with the same central parts XY but varying arm lengths d , is regarded as the model of a one-dimensional liquid [Fig. 1 (b)]. The quantity d is taken to be a random variable obeying certain distribution probability.

It is shown in the following sections that almost all the wave functions are localized in this disordered system. The effect of the probability distribution of d on localization is discussed. Peculiar to this one-dimensional liquid model, non-localized solutions do exist. This is not contrary to the original conjecture; for in a completely disordered system in which the central parts XY of the potentials also differ from cell to cell, these states no longer exist.

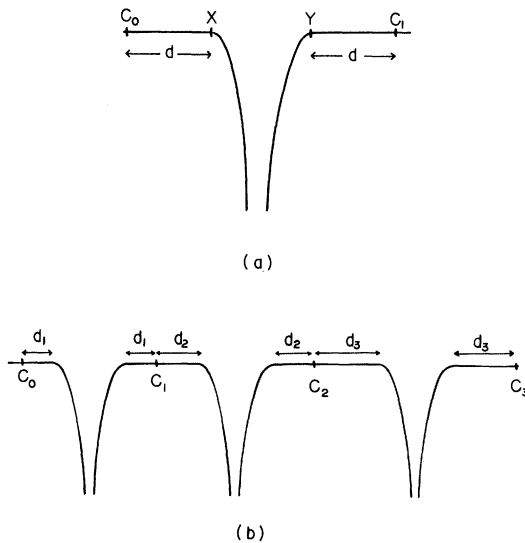


FIG. 1. (a) A central localized potential; (b) Model of one-dimensional liquid.

II. REFLECTION AND TRANSMISSION COEFFICIENTS

For a strongly localized symmetric potential [Fig. 1(a)], it is easily seen that the transfer matrix M defined by⁵

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = M \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad (1)$$

is a product of three matrices describing the regions C_0X, XY , and YC_1 :

$$M = \begin{pmatrix} e^{-ikd} & 0 \\ 0 & e^{ikd} \end{pmatrix} M_c \begin{pmatrix} e^{-ikd} & 0 \\ 0 & e^{ikd} \end{pmatrix}. \quad (2)$$

A and B are coefficients of the wave function at C ; $\Psi = Ae^{ikx} + Be^{-ikx}$ and $k = \sqrt{E}$. M_c is the transfer matrix of the central part XY of the potential and is of the form [Eqs. (6) and (10) of I]

$$M_c = \begin{pmatrix} u_c^* & v_c \\ v_c^* & u_c \end{pmatrix}, \quad v_c^* + v_c = 0. \quad (3)$$

M_c is the same for all cells in the one-dimensional liquid model. It is also shown in I that for localized symmetric potentials the matrix elements of M are expressible in terms of the reflection coefficient r and the transmission coefficient t :

$$M = \begin{pmatrix} 1/t & (r/t)^* \\ r/t & (1/t)^* \end{pmatrix}. \quad (4)$$

Also, r and t have the following properties (see Sec. III of I):

$$|t|^2 + |r|^2 = 1, \quad r^*t + rt^* = 0. \quad (5)$$

Equating (2) and (4), we immediately obtain the following results in the one-dimensional liquid model: (i) $|t| = 1/|u_c|$ is independent of the cell. If we have $|t| = 1$ for certain energy values in one of the cells, $|t| = 1$ for all cells. This leads to the nonlocalized states mentioned in the Introduction. (ii) $|r| = 1 - |t|$ is also independent of the cell. (iii) We can define the reflection coefficient r of the j th cell as

$$r_j = |r| e^{i\phi_j}. \quad (6)$$

ϕ_j can be found from

$$r_j = v_c^* / \left(u_c^* e^{-ikd_j} \right).$$

Call $u_c = \omega + i\xi$, $v_c = i\eta$. We have

$$\tan\phi_j = \frac{\xi \sin(2kd_j) - \omega \cos(2kd_j)}{\xi \cos(2kd_j) + \omega \sin(2kd_j)}. \quad (7)$$

Since d is a random variable obeying certain probability distribution $P(d)$, ϕ is also a random quantity. (iv) From Eq. (5) we see that

$$t_j/t_j^* = -(r_j/r_j^*) = -e^{2i\phi_j}. \quad (8)$$

In fact, if we define

$$t_j = |t| e^{i\psi_j}, \quad \psi_j = \phi_j + \frac{1}{2}(2n+1)\pi,$$

where $n = 0, \pm 1, \dots, \pm \infty$.

III. LOCALIZATION OF WAVE FUNCTIONS

Following Borland,³ we shall consider a real wave function of the form of a cosine at C_0 : $A_0 = |A_0| e^{i\delta_0}$, $B_0 = |A_0| e^{-i\delta_0}$, and examine what are the coefficients A_n, B_n at C_n .⁶ From direct multiplication of (1) at C_1 , we have

$$\begin{aligned} A_1 &= |A_0| (e^{i\delta_0}/t_1^*) + (r_1/t_1) e^{-i\delta_0}, \\ B_1 &= |A_0| (e^{-i\delta_0}/t_1) + (r_1^*/t_1^*) e^{i\delta_0}. \end{aligned} \quad (9)$$

We see that $B_1 = A_1^*$. It is obvious from the properties of the transfer matrix M that when we choose $B_0 = A_0^*$, $B_j = A_j^*$ for all j .

Let us call $A_1 = |A_1| e^{i\delta_1}$ and $B_1 = |A_1| e^{-i\delta_1}$; Eq. (9) becomes

$$|A_1| e^{i\delta_1} = \frac{|A_0|}{|t|^2} (t_1 e^{i\delta_0} + r_1 t_1^* e^{-i\delta_0}). \quad (9')$$

Here, we have dropped the index 1 from $|t|$, since $|t|$ is the same for all cells in the one-dimensional liquid model. In the following we shall only consider this model unless it is mentioned otherwise. Let us study the amplitude A and the phase δ separately:

$$|A_1|^2/|A_0|^2 = (1 + \theta^2)[1 - \tau \cos(2\delta_0 + \phi_1)], \quad (10)$$

where

$$\theta^2 = 2(|r|^2/|t|^2) \quad \text{and} \quad \tau = 2|r|/(1+|r|^2); \quad (11)$$

$$\delta_1 = \tan^{-1}(\tan\{\delta_0 + \frac{1}{2}[\phi_1 + (2n+1)\pi]\}R) + \frac{1}{2}\phi_1, \quad (12)$$

$$\text{where} \quad R = (1 - |r|)/(1 + |r|) \leq 1. \quad (13)$$

These expressions can be extended formally to the n th cell. At C_n , we have

$$|A_n|^2/|A_0|^2 = (1 + \theta^2)^n P_n, \quad (14)$$

where

$$P_n = \prod_{j=1}^n (1 - \tau \cos\phi_j),$$

$$\Phi_j = 2\delta_{j-1} + \phi_j; \quad (15)$$

$$\delta_n = \tan^{-1}(\tan\{\delta_{n-1} + \frac{1}{2}[\phi_n + (2n+1)\pi]\}R) + \frac{1}{2}\phi_n. \quad (16)$$

Let us first examine the phase δ_n . It is related to the previous δ_{n-1} with the addition of a random quantity $\frac{1}{2}\phi_n$. The contribution of δ_{n-1} to δ_n is further reduced by the factor R which is always less than 1. It is this reduction factor that makes δ_n practically forget about the initial δ_0 . This loss of memory of the initial phase has been discussed in detail by Borland³ and by Mott.¹ For the convenience of discussion, we shall call the case $|r| > |t|$, a strong scatterer, and $|r| < |t|$, a weak scatterer. (Of course, this classification depends on the specified energy under consideration.) The stronger the scatterer, the smaller the reduction factor. Memory of δ_0 is nearly completely lost in a chain of very strong scatterers after a few cells. Even when the scatterers are weak, memory is lost if n is large enough. The values of the variable ϕ will cover up the contribution of δ_0 to δ_n .

Let us now look at the amplitude function. Suppose the average spacing of the cells is a . We define

$$L = a/\theta^2. \quad (17)$$

Calling $x = na$, we can put Eq. (14) in the following form:

$$\begin{aligned} \lim_{n \rightarrow \infty} (|A_n|^2/|A_0|^2) &= \lim_{n \rightarrow \infty} (1 + x/nL)^n P_n \\ &= e^{x/L} \lim_{n \rightarrow \infty} P_n. \end{aligned} \quad (18)$$

The ratio of the square of the amplitude at the n th cell to that at the zeroth cell is a product of two factors: one increases exponentially with x independent of the variation of the arm lengths d_j , and the other factor $\lim_{n \rightarrow \infty} P_n$ which depends on ϕ_j and is correlated to the initial phase δ_0 through the "phase memory." A wave function is localized if this ratio either increases or decreases exponentially with distance. The cases for the ratio to be 1 as $n \rightarrow \infty$ are extremely rare, but its probability is nonzero as we have indicated in Sec. II.

As a side note, we see that L defined in (17) is

not the mean free path. $L \leq \frac{1}{2}a$ for strong scatterers, and $L \geq \frac{1}{2}a$ for weak scatterers. It approaches the mean-free-path definition of Mott for weak scatterers.

Let us get a rough idea of the contribution of the factor $\lim_{n \rightarrow \infty} P_n$ on the product in terms of the strength of the scatterer. For very strong scatterers, even when all the ϕ_j are biased to give the same positive $\cos(\phi_j)$ so that we can take $\tau \cos \phi_j \approx 1$ for all j (this gives an estimate of the smallest $\lim_{n \rightarrow \infty} P_n$), we have

$$\begin{aligned} \lim_{n \rightarrow \infty} P_n &= \lim_{n \rightarrow \infty} \prod_{j=1}^n \left(1 - \frac{x\tau \cos \phi_j}{na} \right) \\ &\sim \lim_{n \rightarrow \infty} (1 - x/na)^n = e^{-x/a}. \end{aligned} \quad (19)$$

This is not small enough to overpower the first factor $e^{x/L}$, since $L = a/\theta^2 \ll a$ for very strong scatterers. Therefore, a wave function nearly always increases exponentially with distance when the scatterers are strong. In weak scatterers, the factor $\lim_{n \rightarrow \infty} P_n$ may overpower the first factor and make the ratio decrease exponentially.

To study the problem more precisely, let us return to the expression (10) and write

$$|A_n|^2/|A_0|^2 = \prod_{j=1}^n \alpha_j, \quad (20)$$

where [see Eq. (15)],

$$\alpha_j = (1 - |\tau|^2)^{-1} [1 + |\tau|^2 - 2|\tau| \cos \phi_j]. \quad (21)$$

First, we note that α_j lies between

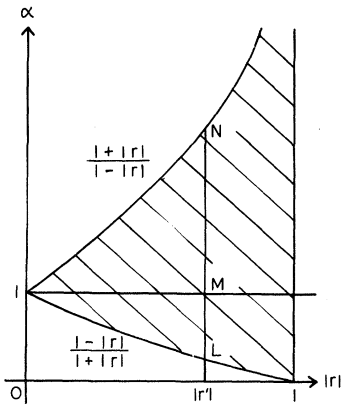


FIG. 2. Allowed values of α (shaded region). For a given value of $|r'|$, α_j can take up any value along the line LN . NM is always longer than ML , except when $|r'| = 0$.

$$\frac{1 - |\tau|}{1 + |\tau|} \leq \alpha_j \leq \frac{1 + |\tau|}{1 - |\tau|}, \quad \text{for all } j. \quad (22)$$

For a given value of $|r'|$, the allowed region of α_j greater than 1 is always larger than that of α_j less than 1, except at $|r'| = 0$ (see Fig. 2). If all $\alpha_j > 1$ the wave function grows approximately exponentially, and if all $\alpha_j < 1$ the wave function decays exponentially. In both cases the electronic state is localized.

Consider the case when the memory of the phase ϕ_j is completely lost so that we can treat ϕ_j as a random variable uncorrelated to the other ϕ_k , $k \neq j$. We shall show that the wave function always grows exponentially in this case. Let us further assume that the random variable Φ which lies between $\pm \pi$ obeys a uniform distribution $P(\Phi) = (2\pi)^{-1}$. This ansatz will be discussed later. A transformation of the variable Φ to $y = \cos \Phi$ gives the probability density distribution of y :

$$P(y) = (\pi)^{-1} \cdot (\sqrt{1 - y^2})^{-1}$$

[see Figs. 3(a) and 3(b)]. It is more probable for y to have values near the two ends, i. e., ± 1 , than the values near zero. This means that the values of α are more probable to be near the two limits $(1 + |\tau|)/(1 - |\tau|)$ and $(1 - |\tau|)/(1 + |\tau|)$. We also note that the distribution of y is symmetric about $y = 0$. This means that the occurrence probability of $+|y|$ is the same as that of $-|y|$. When ϕ_j are uncorrelated, α_j are also uncorrelated [Eq. (21)]. We can, therefore, rearrange the products of α so that we pair the $\alpha(+|y|)\alpha(-|y|)$ together for a given value of $|y|$. In other words, when $n \rightarrow \infty$, we take the product of the right-hand side of Eq. (20) not according to the natural order of the potentials in the chain, but according to the absolute magnitudes of $\cos \Phi$. For any value $|y|$, each pair gives

$$\begin{aligned} \alpha(|y|)\alpha(-|y|) &= [1/(1 - |\tau|^2)^2] [(1 + |\tau|^2)^2 \\ &\quad - 4|\tau|^2|y|^2] = 1 + 4(1 - |y|^2)(|\tau|^2/|t|^2) \geq 1, \end{aligned} \quad (23)$$

since $|y| = |\cos \Phi|$ is never greater than 1. This inequality immediately implies that

$$\begin{aligned} \lim_{n \rightarrow \infty} (|A_n|^2/|A_0|^2) &= \prod_{\text{all values of } |y|} \frac{P(y)}{2} \\ &\times [1 + 4(1 - |y|^2)(|\tau|^2/|t|^2)] \sim e^{\epsilon x/a}, \end{aligned} \quad (24)$$

where ϵ is the average value of $4(1 - |y|^2)(|\tau|^2/|t|^2)$ of the whole chain [see Eq. (18)]. This shows that the wave function always grows exponentially. The growth rate increases with the ratio $|r|/|t|$, i. e., the strength of the scatterer.

The above argument is valid as long as the dis-

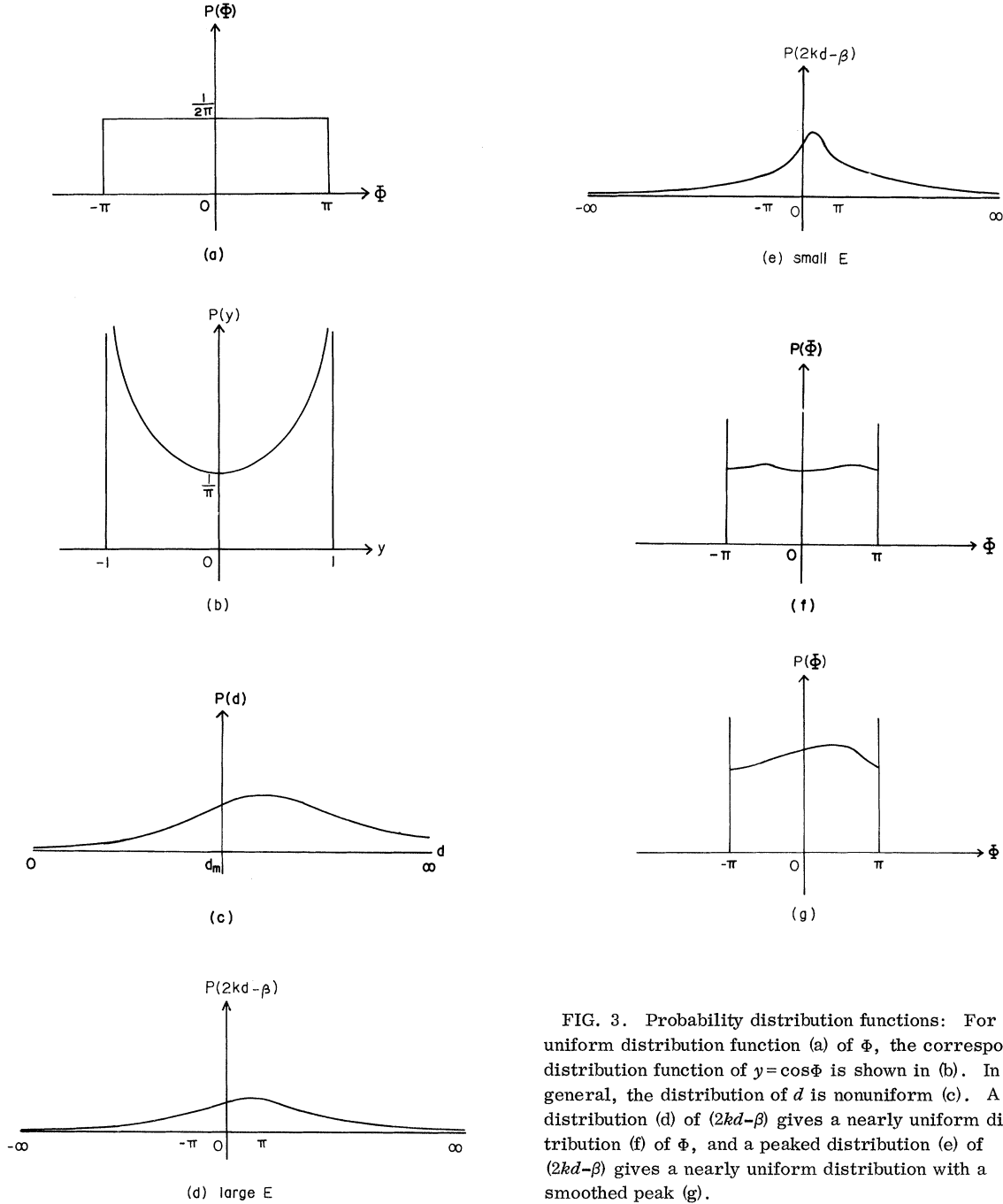


FIG. 3. Probability distribution functions: For a uniform distribution function (a) of Φ , the corresponding distribution function of $y = \cos \Phi$ is shown in (b). In general, the distribution of d is nonuniform (c). A flat distribution (d) of $(2kd - \beta)$ gives a nearly uniform distribution (f) of Φ , and a peaked distribution (e) of $(2kd - \beta)$ gives a nearly uniform distribution with a smoothed peak (g).

tribution $P(y)$ is symmetric or nearly symmetric about zero. This condition is very likely to be satisfied as $n \rightarrow \infty$ even when the Φ_j are correlated.

We shall now justify our assumption that Φ has a uniform or nearly uniform distribution. Under the uncorrelated situation, we can take $\Phi_j \sim \phi_j$ [Eq. (15)]. We can explicitly calculate ϕ_j from Eq. (7):

$$y_j = \cos \Phi_j \sim \cos \phi_j = \cos(2kd_j - \beta), \quad (25)$$

where $\cos \beta = \xi / (\omega^2 + \xi^2)^{1/2}$. ω and ξ are the real and the imaginary parts of u_c , and are the same for all cells. It is the separation d that fluctuates. If we assume that all values of d can occur with equal probability, this implies a uniform prob-

ability distribution of Φ_j , i. e., $P(\Phi) = 2\pi^{-1}$. A more realistic picture is that d fluctuates about some mean value with a certain distribution $P(d)$ [Fig. 3(c)]. The distribution $P(2kd - \beta)$ follows immediately. Note that the elements of M_C of the central part XY of the potentials contribute only to β . This does not change the shape of the probability curve in the transformation from $P(d)$ to $P(2kd - \beta)$, but only shifts the curve as a whole. The multiplication of $k = \sqrt{E}$ does change the flatness or the spread of the curve. For large energies, the curves become flatter [Fig. 3(d)] and, for very small energies, the curve has a smaller spread [Fig. 3(e)]. The range of $2kd - \beta$ runs from $-\infty$ to ∞ , but the range of Φ is taken to be within $-\pi$ and π . The probability distribution $P(\Phi)$ is, therefore, obtained by folding the distribution $P(2kd - \beta)$ into the region $-\pi$ to π . This folding action tends to make the distribution function of Φ more or less uniform. (i) When the distribution $P(2kd - \beta)$ is flat and spreads over regions of several 2π , the assumption that Φ has a uniform distribution is a good one [Fig. 2(f)]. (ii) When the curve $P(2kd - \beta)$ is very narrow and strongly peaked at certain value, the folding process will still smoothen the distribution somewhat, but the peak may remain significant [Fig. 2(g)]. This gives a distribution curve for γ similar to Fig. 2(b) but with a bump somewhere within ± 1 . In turn it will cause the occurrence of α to be biased. It may occur that α values are biased to cause the wave function to decay. In most cases, especially when energies are large enough, we have only to consider situation (i).

Finally, we return to the discussion of the states which are not localized. When $|t| = 1$ at one of the cells, it is perfectly transmitted through the cells. That is,

$$|A_0|^2 = |A_1|^2 = \dots = |A_n|^2, \quad \text{when } |t| = 1 \quad (26)$$

All other nonlocal states, if they exist, must have energies close to these $|t| = 1$ values [Fig. (4)].

In a completely disordered system, i. e., when all the central parts XY of the potentials are different from each other, it is unlikely that energies for which $|t| = 1$ for one cell also give $|t| = 1$ for all the other cells. Since $|t| \leq 1$, an infinite arrangement of different potentials is certainly a perfect reflector of any wave. Nonlocal states cannot exist.

IV. CONCLUSIONS

Using the reflection and the transmission coefficients and relating them to the transfer-matrix technique developed previously,⁵ we have obtained some further understanding of the localization of electronic states in one-dimensional disordered

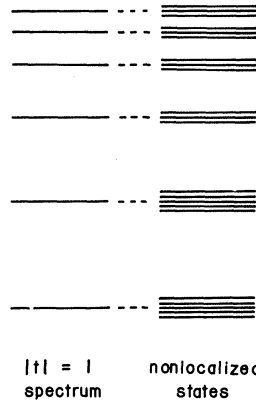


FIG. 4. Nonlocalized states.

systems. We see that (i) the correlation of the phase δ between sites is weakened by a factor $(1 - |r|)/(1 + |r|)$ [Eq. (16)] every time in passing through a cell. The memory of the initial phase δ_0 is easily lost in very strong scatterers, and in weak scatterers the memory is lost if we take n large enough. (ii) When the phase memory is weak, Φ_j are uncorrelated. If Φ has a uniform or nearly uniform distribution, the wave function always grows exponentially with the distance. The growth rate increases with the strength of the scatterers: $|r|/|t|$. These statements are true even if the Φ_j are correlated so long as the occurrence probability of $+\cos\Phi$ is the same as that of $-\cos\Phi$ when $n \rightarrow \infty$. (iii) The uniform probability distribution of Φ is a good one for large energies and large fluctuations of the cell size d , so that $\sqrt{E}d$ extends over several 2π regions and the distribution curve is flat. A sharp bump in the curve $P(\Phi)$ may cause the wave function to grow or decay exponentially. (iv) In the one-dimensional liquid model, nonlocalized states, defined as $\lim_{n \rightarrow \infty} |A_n|/|A_0| = 1$, do exist. The $|t| = 1$ states are quantized states of the well, and are independent of the position of the well. The three-dimensional analog of this certainly exists. (v) Nonlocalized states are unlikely to exist in a completely disordered one-dimensional system. Perhaps the Mott conjecture should be reformulated to state: "If there is any scattering by a noncrystalline array of center, the states are localized."⁷

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APPENDIX

In a general one-dimensional disordered system, we can use the formulation of I to obtain an expres-

sion for the amplitude of the wave function at the n th cell:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M_n^{-1} M_{n-1}^{-1} \dots M_1^{-1} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad (\text{A1})$$

where M_j^{-1} is the inverse of M_j , the transfer matrix referring to the j th cell:

$$M_j = \begin{pmatrix} u_j^* & v_j \\ v_j^* & u_j \end{pmatrix}. \quad (\text{A2})$$

It can be shown that

$$\begin{aligned} & (M_1^{-1})^+ \dots (M_n^{-1})^+ (M_n^{-1}) \dots (M_1^{-1}) \\ &= \prod_{j=1}^n (1 + \theta_j^2) (1 + \beta_{j,j+1,\dots,n}) \\ & \quad \times \begin{pmatrix} 1 & & & \alpha_{1,2,\dots,n} \\ \alpha_{1,2,\dots,n}^* & & & 1 \end{pmatrix}, \end{aligned}$$

where $\theta_j^2 = 2|v_j|^2$,

$$\alpha_j = 2u_j v_j / (1 + \theta_j^2),$$

$$\alpha_{j,j+1,\dots,n} = (1 + \beta_{j,j+1,\dots,n})^{-1} \alpha_j$$

$$\begin{aligned} & + (1 + \theta_j^2)^{-1} (\alpha_{j+1}, \dots, n u_j u_j \\ & + \alpha_{j+1}^*, \dots, n v_j v_j), \end{aligned}$$

$$\beta_j = 0,$$

$$\beta_j = 0,$$

$$\beta_{j,j+1,\dots,n} = (1 + \theta_j^2)^{-2}$$

$$\times \text{Re}(\alpha_{j,j+1,\dots,n} u_j v_j^*). \quad (\text{A3})$$

Hence, the ratio of the amplitudes becomes

$$\begin{aligned} & \frac{|A_n|^2 + |B_n|^2}{|A_0|^2 + |B_0|^2} = \prod_{j=1}^n (1 + \theta_j^2) \\ & \quad \times (1 + \beta_{j,j+1,\dots,n}) [1 + 2\text{Re}\Xi_{n0}], \end{aligned}$$

$$\text{where } \Xi_{n0} = \frac{\alpha_{1,2,\dots,n} A_0^* B_0}{|A_0|^2 + |B_0|^2}. \quad (\text{A4})$$

If all the potentials are symmetric, we can use the reflection coefficient r_j and transmission coefficient t_j of the j th cell in place of the u_j, v_j in the matrix M_j .

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⁶It is more convenient here to use the inverse of M :

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M_1^{-1} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix},$$

$$\text{where } M_1^{-1} = \begin{pmatrix} 1/t^* & r/t \\ (r/t)^* & 1/t \end{pmatrix}.$$

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