R. B. Cavanagh (private communication).


The fact that the Fermi level is essentially temperature independent likens our insulator model to that of a real amorphous solid in which the Fermi level is also only very slightly temperature dependent (see Ref. 8 for further details).

Effect of blocking contacts at the metal-insulator interface are to be treated elsewhere: J. G. Simmons and G. W. Taylor (unpublished).


J. Frisch, Phys. Rev. 54, 647 (1938).


The DRC flows in the system even in the temperature range $T_0 > T > T_1$ but is very small and is apparent only on a ln$\ln$-vs-$T$ plot. On a linear $I$-vs-$T$ plot the DRC is apparent only for temperatures close to $T_0$

This fact, together with the observation that the DRC curve is observed when the sample is cooled under short-or open-circuit conditions, eliminates the possibility that the effect is due to the filling of the traps by electrons injected from the electrodes.

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**Exact Solution of the One-Dimensional Schrödinger Equation with $\delta$-Function Potentials of Arbitrary Position and Strength**

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The exact solution to the one-dimensional Schrödinger equation which describes the motion of a particle scattering off a finite set of $\delta$-function potentials of arbitrary strengths and positions is found. The behavior of the $T$ matrix both on and off the energy shell is also precisely given. Localization of states is discussed.

---

I. INTRODUCTION

Recently a great deal of work has been done on the problem of understanding the electronic states of a system in which the atomic scattering sites are randomly located. The importance of these studies in the field of semiconductor physics is well known. The mathematical difficulties involved in this problem have made it necessary to look into its one-dimensional version in hopes of getting some insight into the important features, so that extraneous complexities can be avoided in the three-dimensional case.

Even with its simplifications the one-dimensional case has not proven to be trivial in nature and the work in this area has needed to be put on a firmer basis. In this paper we hope we have done this by providing an exact solution to the Schrödinger equation for an electron moving in one dimension in the presence of a set of $\delta$-function potentials of arbitrary strengths and positions. The solution which we present has the feature that a clear delineation is made between terms that are made small due to incoherence effects, in the case of a random distribution of scattering sites, and those that are not. This feature of our solution makes it useful for an understanding of how wave functions grow inside the chain of scattering sites and thus it is applicable to the study of the all-important problem of localization.

In Sec. II we present our solution to the integral form of the Schrödinger equation. In Sec. III we recognize the fact that to obtain the wave function we did not have to completely invert the matrix $M$ [defined by (2.5)]; we complete this task and show that the Fredholm determinant, i.e., $\det M$, has, for positive energy, a magnitude greater than unity. With this inverse of $M$, we obtain, as well, the $T$ matrix both on and off the energy shell and briefly discuss its connection with the evaluation of transport properties and the density of states in a specimen. Section IV is devoted to a discussion of some aspects of the problem of localization. We point out in that section that for positive energies, where $|\det M| = 1$, there can, for a finite chain of scattering sites, be no states which vanish at $\pm \gamma$; thus no precisely localized states exist. For a finite chain, localization at positive energies is always, formally, only approximate.

In Appendix A, we discuss other forms of the solution found in Sec. II, while in Appendix B, we make the connection between our results and the
transfer matrix method.

II. SOLUTION TO SCHRODINGER EQUATION WITH SUM OF $\delta$-FUNCTION POTENTIALS

Our purpose in this section is to obtain an exact solution of the one-dimensional Schrödinger equation

$$-rac{d^2}{dx^2} u(x) + V(x) u(x) = E u(x)$$

(2.1)

when the potential $V(x)$ has the form

$$V(x) = \sum_{j=1}^{N} \beta_j \delta(x - x_j).$$

(2.2)

Here $\beta_j$ and $x_j$ are, respectively, the (arbitrary) strength and position of the $j$th $\delta$-function potential. For simplicity we shall assume $x_1 < x_2 < \cdots < x_N$. In connection with the procedures with which we shall be dealing, it turns out to be more convenient to work with the integral form of (2.1), i.e.,

$$u(x) = -\frac{i}{2k} \int dx' e^{ik(x-x')} V(x') u(x') + A e^{ikx} + B e^{-ikx},$$

(2.3)

where $k = E^{1/2}$ ($k$ is the root lying in the upper half complex plane), $u = u(x_j)$, and $\alpha_j = i\beta_j / 2k$. Note that for $E$ real and positive ($k$ real) $\alpha_j$ is pure imaginary.

In order to solve (2.3), it is clearly necessary to determine $u_j$; this we proceed to do. From (2.3) we obtain

$$\sum_{j'=1}^{N} M_{jj'} u_{j'} = A e^{ikx_j} + B e^{-ikx_j},$$

(2.4)

where

$$M_{jj'} = \delta_{jj'} + \alpha_j e^{ikx_j} \alpha_{j'} e^{-ikx_{j'}}.$$ 

(2.5)

In particular, we have for $j = 1$

$$u_1 = A e^{ikx_1} + [B - S(+) e^{-ikx_1},$$

(2.6)

where

$$S(\pm) = \sum_{j=1}^{N} \alpha_j e^{ikx_j} u_j.$$ 

(2.7)

In terms of $S(\pm)$ and $u_j$, we can also write

$$u_2 = A e^{ikx_2} + [B - S(+)] e^{-ikx_2}.$$

Eliminating explicit reference to $u_j$ [by using (2.6)], we obtain

$$u_2 = A e^{ikx_2} [(1 - \alpha_1) + (1 + \alpha_1) e^{2ikx_2} \phi_j([\alpha], k)]$$

$$+ [B - S(\pm)] e^{ikx_2} [1 + \alpha_1]$$

$$+ (1 - \alpha_1) e^{2ikx_2} \phi_j([\alpha], k),$$

(2.9)

where, in general, we take

$$\phi_j([\alpha], k) = \phi_j(\alpha_1, \alpha_2, \ldots, \alpha_{j-1}, \alpha_j; k)$$

$$= \frac{\alpha_j}{1 - \alpha_j} e^{ikx_j} \prod_{j' < j} \frac{1 - \alpha_j}{1 + \alpha_j},$$

(2.10)

and, in particular, $\phi_j = \phi_j([\alpha_1/(1 + \alpha_1)]) e^{ikx_1}$. In much the same way as we arrived at (2.8), we can find $u_j$ in terms of $S(+)$ and $u_j$, $(j' < j)$; thus we have

$$u_j = A e^{ikx_j} + [B - S(+) e^{-ikx_j}$$

$$+ \sum_{j' = 1}^{j-1} \alpha_j u_{j'} (e^{ik(x_j-x_{j'})} - e^{-ik(x_j-x_{j'})}).$$ 

(2.11)

We now eliminate explicit reference to $u_j$, $(j' < j)$ [as was done to get (2.9)] and write $u_j$ in terms only of $S(\pm)$, $A$, and $B$, i.e., in the form

$$u_j = A e^{ikx_j} \gamma_j(k, {\alpha}; {x})$$

$$+ [B - S(\pm)] e^{-ikx_j} \gamma_j(k, {\alpha}; {x}).$$

(2.12)

For $j = 1, 2$ we have already obtained expressions for $\gamma_j$, i.e.,

$$\gamma_1 = \gamma_1 = 1,$$

$$\gamma_2(k, \alpha_1, x_1, x_2) = \gamma_2(k, \{\alpha\}, \{x\})$$

$$= (1 - \alpha_1) + e^{-2ikx_2}(1 + \alpha_1) \phi_1([\alpha], k),$$

$$\gamma_2(k, \{\alpha\}, \{x\}) = \gamma_2(-k, \{-\alpha\}, \{x\}).$$

(2.13)

We shall now show that, in general, the appropriate forms for $\gamma_j$ and $\tilde{\gamma}_j$ are

$$\gamma_j(k, \{\alpha\}, \{x\}) = \gamma_j(k, \alpha_1 \alpha_2 \cdots \alpha_{j-1}, x_1 x_2 \cdots x_j)$$

$$= \prod_{j'=1}^{j-1} (1 - \alpha_{j'}) \left( 1 + \sum_{m(\text{even}) = 1}^{m_{\text{max}}} \sum_{j'=1}^{j-1} \sum_{l_{m-1} = 0}^{l_{m-1}} \phi_{j'} \phi_{j''} \cdots \phi_{j_{m-1}} \phi_{j_m} \right)$$

$$+ \prod_{j'=1}^{j-1} (1 + \alpha_{j'}) \left( e^{-2ikx_1} \sum_{m(\text{odd}) = 1}^{m_{\text{max}}} \sum_{j'=1}^{j-1} \sum_{l_{m-1} = 0}^{l_{m-1}} \phi_{j'} \phi_{j''} \cdots \phi_{j_{m-1}} \phi_{j_m} \right)$$

(2.14)
and
\[ \bar{y}_j(b_i; \{a_i\}, \{x_i\}) = y_j(-b_i; \{-a_i\}, \{x_i\}) \]  
(2.15)

In (2.14), \( \phi^*_j = \phi_j([+a_i], +k) \) [see (2.10)] and
\[ \sum_{\text{even}} + \sum_{\text{odd}} \]  
mean, respectively, a sum over even values of \( m \) and a sum over odd values of \( m \). The proof of this assertion is by induction.

Expressions (2.13), of course, conform to the prescriptions of (2.14) and (2.15), so let us assume that (2.14) and (2.15) are correct for all values of \( j < J \). Using Eqs. (2.11) and (2.12) for \( j < J \) and looking at the coefficients of \( A_i \), we have
\[ \gamma_{j-1}(b_i; a_1 \cdots a_{J-2} x_1 \cdots x_{J-1}) = 1 + \sum_{j=1}^{J-2} \alpha_j \gamma_j(b_i; \{a_i\}, \{x_i\})(e^{2ik(x_j-x_{j+1})} - 1) \]  
(2.16)

Similarly, we have
\[ \gamma_j(b_i, a_1 \cdots a_{J-1} x_1 \cdots x_J) \]

Collecting together the terms in each of the curly brackets in (2.19), we observe that this equation can be rewritten in the form (2.14). This completes the induction. It is now a simple matter to establish that \( \bar{y}_j(k, \{a_i\}, \{x_i\}) = y_j(-k, \{-a_i\}, \{-x_i\}) \); we shall not give the details here. We remark, however, that when \( k \) is real,
\[ \bar{y}_j = y^*_j \]  
(2.20)

To complete the determination of \( u_j \), we must now remove \( S(+) \) from (2.12). Multiplying (2.12) by \( e^{ikx_j a_j} \) and summing, we have
\[ S(+) = \left( A \sum_{j_1=1}^{K} y_j e^{ikx_j a_j} + B \sum_{j_1=1}^{K} \alpha_j \bar{y}_j \right) / \left( 1 + \sum_{j_1=1}^{K} \alpha_j \bar{y}_j \right) \]  
(2.21)

We then get
\[ u_j = A \left[ e^{ikx_j \gamma_j} - e^{-ikx_j \bar{y}_j} \left( \sum_{j_1=1}^{K} \gamma_j e^{ikx_j a_j} \right) \right] \]
\[ + \left( 1 + \sum_{j_1=1}^{K} \alpha_j \bar{y}_j \right) \left[ B e^{-ikx_j \bar{y}_j} \left( 1 + \sum_{j_1=1}^{K} \alpha_j \bar{y}_j \right)^{-1} \right] \]  
(2.22)

We can finally obtain a solution of (2.3) by inserting into it the result (2.22). Thus for \( x_j < x < x_{j+1} \), we get
\[ u(x) = A e^{ikx} + \left[ B - S(+) \right] e^{-ikx} \]
\[ + \sum_{j=1}^{J-2} \alpha_j u_j \left( e^{ik(x_j-x)} - e^{-ik(x_{j+1}-x)} \right) \]  
(2.23)

Noting that the only difference between (2.11) for \( u_{j-1} \) and (2.23) is the replacement of \( x_{j+1} \) by \( x \) [except where it occurs in \( S(+) \)], we can immediately write
In obtaining this result, we have used expression (2.21). The formula (2.24) also suffices for \( x < x_1 \) and \( x > x_h \) if we think of \( x_0 = -\infty \), \( x_h = +\infty \), and \( \alpha_0 = \alpha_{-1} = 0 \). Equation (2.24) is the exact solution to the Schrödinger equation (2.3).

We remark here that Eq. (2.3) is an integral equation of rank \( N \) which can be attacked by the Fredholm method.\(^5\) The solution provided by that method involves complicated power series in \( \{ \alpha \} \) and thus does not lead unambiguously to estimates of the sizes of the various quantities of interest. Our approach overcomes some of these difficulties: In effect, we have successfully summed together all terms with equivalent dependence on the positions of the scattering sites. For example, in expression (2.14) for \( \gamma_j \) the term involving no \( \phi \)'s is independent of the positions of the scattering centers and its size is thus unaffected by the incoherence introduced when the sites are randomly located. The terms with the simplest dependence on position are those for which \( m = 1 \) or \( m = 2 \) in the sums in (2.14); these involve one or two factors \( e^{ikx_j} \) and thus, in the random case, we expect them to be small because of incoherence. Of course, all terms with more factors \( \phi \) (higher \( m \) values) are presumably affected to a greater extent by incoherence. If, in fact, the terms involving one or more factors \( \phi \) are forced to be small by the randomness of the system, then we can estimate for large \( j \)

\[
\gamma_j \sim \prod_{j=1}^{j-1} (1 + \alpha_j),
\]

and in the special case that all the \( \alpha \)'s are the same, we have (for positive energies)

\[
|\gamma_j| \sim e^{j |\alpha|^{1/2}} (|\alpha| < 1).
\]

These results imply a tendency of the \( \gamma \)'s to increase in magnitude exponentially with \( j \). Along with this goes the expectation that the solution \( u(x) \) is increasing in magnitude as \( x \) goes deeper into the chain. The behavior we describe here was previously noted by Borland\(^6\) (but only for the averaged wave function).

We discuss in Appendix A the application of the methods described above to the form of the solution of (2.3) found by starting from the other end of the chain (i.e., from \( x_h \)). The same conclusions regarding growth can be arrived at, so that, once again, if incoherence is effective, then the wave function grows from that end as well. In Sec. IV we discuss the implications of this apparent growth from both ends.

We add here that a connection between the work we have done here and the transfer matrix method is made in Appendix B.

III. T MATRIX AND INVERSE OF M

In this section we show how the use of the results and techniques described in Sec. II enables us to obtain an exact expression for the \( T \) matrix associated with the potential \( V(x) \),\(^8\) both on and off the energy shell. To obtain this result we shall have to determine completely the matrix \( M^{-1} \) and we shall find an useful relation for \( \det M \). The value of having an expression for the \( T \) matrix lies in its relationship to the density of states and to the formalism of linear transport theory; we shall, in this section, discuss these connections.

The \( T \)-matrix operator satisfies the equations

\[
T(E) = V + V \frac{1}{E-H_0} T(E),
\]

\[
T(E) = V + T(E) \frac{1}{E-H_0} V.
\]

(3.1)

Here \( H_0 = -\frac{d^2}{dx^2} \) is the kinetic-energy operator; we no longer restrict \( E \) to be real (\( k \) is still taken to be the root in the upper half-plane). Because \( V(x) \) is a sum of \( \delta \) functions, it turns out that

\[
\langle \delta | T(E) | \delta \rangle = \sum_{j,j'} e^{i\gamma_j \beta_{j',j}} \delta_{j,j'}. \]

(3.2)

Inserting (3.2) into (3.1), we have

\[
\sum_{j,j'} \delta_{j,j'} \langle \delta | T(E) | \delta \rangle \frac{1}{E - \beta^\delta_{j,j'}} = \beta_{j,j'}.
\]

(3.3)

The integral is easily done and we get

\[
\sum_{j,j'} T_{j,j'} \langle \delta | T(E) M_{j,j'} | \delta \rangle = \beta_{j,j'}.
\]

(3.4)

where \( M \) is the matrix defined by (2.5). It follows that a complete knowledge of the \( T \) matrix on and off the energy shell requires a determination of \( M^{-1} \). It is this task to which we now turn our attention.

In order to find \( M^{-1} \), we must solve the equation [which is more general than (2.4)]

\[
u(x) = \frac{1}{T - E} \left[ \sum_{j=1}^{N} (1 + \alpha_j) \left( A e^{ikx_j} + B \bar{\gamma}_j \right) \right], \quad x_j < x < x_{j+1}.
\]

(2.24)
\[ \sum_{j'} M_{jj'} u_{j'} = A_j ; \quad (3.5) \]

when \( A_j = \delta_{jj'} \) then \( u_j = (M^{-1})_{jj'} \). We begin by finding a solution when \( A_j = a_j e^{ikx_j} \delta_{jj'} \). In this case we can rewrite (3.5) as

\[
\sum_{j'} M_{jj'} u_{j'} = a_j e^{ikx_j}, \quad \sum_{j'} M_{jj'} u_{j'} = a_j e^{ikx_j} - \bar{a}_j e^{ikx_j} \quad (j > 1),
\]

where in the end we must set \( \bar{a}_1 = a_1 \). Reintroducing \( S(+) \), we can write after some manipulation

\[
\begin{align*}
u_1 &= a_1 e^{ikx_1} - S(+) e^{ikx_1}, \\
u_2 &= a_1 e^{ikx_2} \gamma_2(k_j, \{x_j\}, \{x_l\}) - S(+) e^{ikx_2} \\
u_3 &= a_1 e^{ikx_3} \gamma_3(k_j, \{x_j\}, \{x_l\}) - S(+) e^{ikx_3} \\
&= a_1 e^{ikx_2} \gamma_2(k_j, \{x_j\}, \{x_l\}) - a_1 e^{ikx_2} \\
&- a_1 e^{ikx_3} \gamma_3(k_j, \{x_j\}, \{x_l\}).
\end{align*}
\]

By setting \( \bar{a}_2 = a_2 \), we get a coefficient of \( a_2 \), for example, in \( u_2 \) of the form \( \gamma_3 - \gamma_2 \). In general, we have (with \( \bar{a}_1 = a_1 \))

\[
u_j = (a_1 e^{ikx_1}) \Omega_j^2(k_j, \{x_j\}, \{x_l\}) - S(+) e^{ikx_j} \gamma_j(k_j, \{x_j\}, \{x_l\}), \quad (3.8)
\]

where

\[
\begin{align*}
\Omega_j^2 &= 0, \quad (j > j'), \\
\Omega_j^2 &= 1, \\
\Omega_j^2 &= \gamma_{j'-1} \gamma_{j} (k_j, a_j \cdots a_{j'-1}, x_j \cdots x_{j'}) e^{ik(x_j-x_{j'})} \\
&- \gamma_{j'-1} (k_j, a_j \cdots a_{j'-1}, x_j \cdots x_{j'}) e^{ik(x_j-x_{j'})}.
\end{align*}
\]

By an analysis like that given above we now can readily find for the case \( A_j = A_0 \delta_{jj} \) that

\[
\begin{align*}
u_j &= - S(+) e^{ikx_j} \gamma_j(k_j, \{x_j\}, \{x_l\}) \gamma_j(k_j, \{x_j\}, \{x_l\}) \\
&= - S(+) e^{ikx_j} A_0 \gamma_j(k_j, \{x_j\}, \{x_l\}) \gamma_j(k_j, \{x_j\}, \{x_l\}) \quad (j < j), \\
u_0 &= - S(+) e^{ikx_0} \gamma_0 A_0 \\
&= - S(+) e^{ikx_0} A_0 + \Omega_j^2 A_0 \\
&\text{and, as well,} \\
u_j &= - S(+) e^{ikx_j} \gamma_j \gamma_j A_0 \quad (j > j). \\
\end{align*}
\]

Thus for all values of \( j \) we have the same form as, for example, shown in (3.12). The remarks following (3.5) lead, upon replacement of \( S(+) \) by its value, to the result

\[
(M^{-1})_{jj'} = \Omega_j^2 - \gamma_j e^{ikx_j} / (1 + \sum_{j'} \alpha_j \gamma_j^j). \quad (3.13)
\]

Note that we can obtain other expressions for \( M^{-1} \)
by use of the "solution from the other end" or a "solution from the middle" as described in Appendix A.

The denominator which occurs in (3.13) has been encountered before [see (2.21) et seq.], which leads us to the conclusion that it is an important invariant. We shall now show that

\[
1 + \sum_{j=1}^{N} \alpha_j \gamma_j = \det M ; \quad (3.14)
\]

we further remark that \( \det M \) is the Fredholm determinant. The proof is by induction on the rank of \( M \). For \( N = 1 \) we have

\[
\det M(N=1) = M_{11}(N=1) = 1 + \alpha_1 = 1 + \alpha_1 \gamma_1. \quad (3.15)
\]

We suppose that (3.14) holds for \( N - 1 \). Note, then, that

\[
[M^{-1}(N)]_{NN} = (\text{cofactor } M(N))_{NN}/\det M(N), \quad (3.16)
\]

but \( \text{cofactor } M(N)_{NN} = \det M(N-1) \). From (3.9) and (3.13) we have

\[
[M^{-1}(N)]_{NN} = 1 - \alpha_N \gamma_N / (1 + \sum_{i=1}^{N} \alpha_i \gamma_i) = (1 + \sum_{i=1}^{N} \alpha_i \gamma_i) / (1 + \sum_{i=1}^{N} \alpha_i \gamma_i). \quad (3.17)
\]

The induction hypothesis identifies the numerator in the second form of (3.17) with \( \det M(N-1) \); thus it follows from (3.16) that the denominator is \( \det M(N) \); this completes the proof. By using similar arguments it is easy to show that in terms of \( \{ p_j^N \} \) (see Appendix A)

\[
\det M = 1 + \sum_{j=1}^{N} \alpha_j p_j^N. \quad (3.18)
\]

For the special case in which \( E \) is real and positive (so that \( k \) is real) we shall now verify a useful inequality, namely,

\[
|\det M| \geq 1 \quad (E > 0). \quad (3.19)
\]

When \( k \) is real and positive, we can discuss a wave, of wave vector \( k \), traveling in the positive \( x \) direction, incident on the array of \( \delta \) functions, through which some of the wave is transmitted and from which some of it is reflected. This situation is described mathematically by (2.3) with \( A = 1, \ B = 0 \). We have

\[
\begin{align*}
u(x) &= e^{ikx} - S(+) e^{ikx} \quad (x < x_1), \\
u(x) &= e^{ikx} [1 - S(-)] \quad (x > x_N). \quad (3.20)
\end{align*}
\]

It follows that the reflection coefficient \( R = -S(+) \) and the transmission coefficient \( \tau = 1 - S(-) \). Using the results of Appendix A, we get
where $M^{-1}$ is determined from (3.13). This result is completely general; there is no requirement that $p^2 = E$. We remark here that the result (3.21) implies that for positive energy $E$ the $T$ matrix remains finite (i.e., has no poles).

The connection between linear response theory and the $T$ matrix lies in the fact that for an external disturbance of frequency $\omega$ and wave vector $q$ all linear response properties involve expressions of the form

$$
\langle \rho | T(E + \frac{i}{2} \omega - i0^+) | \rho' \rangle = \sum_{jj'} e^{i\rho_j \beta_j (M^{-1})_{jj'}} e^{i\rho_j' \beta_j' (M^{-1})_{jj'}}
$$

(3.22)

Thus to obtain a complete knowledge of the transport properties of the system we are required to have all the matrix elements of the $T$ matrix, both on and off the energy shell, as we do in (3.22).

We now discuss the connection of $T$ matrix to the average density of states per unit length in the sample. The sample, which encompasses a region of length $L$, contains all the scattering centers. The local density of states $s$ is given by

$$
D(E, x) = -(1/\pi) Im \langle x | G(E + i0^+) | x \rangle,
$$

(3.24)

where

$$
G(x) = \frac{1}{z - H_0} + \frac{1}{z - H_0} \frac{T(z)}{z - H_0}.
$$

(3.25)

The average density of states in the region between positions $y_1$ and $y_2$ is defined as

$$
D(E; y_1, y_2) = \frac{1}{y_2 - y_1} \int_{y_1}^{y_2} dx D(E, x).
$$

(3.26)

Using (3.2) and assuming that the sample lies between $-\frac{1}{2} L$ and $\frac{1}{2} L$, we have, upon carrying out the integral in (3.26),

$$
D(E, -\frac{1}{2} L, \frac{1}{2} L) = -\frac{1}{\pi} \text{Im} \left[ \frac{-1}{2k} \sum_{jj'} \frac{d}{dk} \left( e^{iak\xi_j - \xi_j'} \right) \right] T_{jj'} \left( \frac{-1}{2k}, \frac{-1}{2k} \right) + \frac{2}{\pi L} \sum_{jj'} \text{Im} \left[ \frac{-i}{2k} \right] e^{iak} \cos(k(x_j + x_{j'})) T_{jj'}.
$$

(3.27)

The last term in (3.27) is, of course, a boundary term. If $E < 0$ and $|k| L > 1$, then, since $k$ is pure positive imaginary, the boundary term is negligible. When $E > 0$, then $e^{iak}$ is of magnitude unity and the boundary term does not appear to be small. If, however, we do not have exact knowledge of the length of the sample but only know that $L_0 - \frac{1}{2} L < L < L_0 + \frac{1}{2} L$, where $k \ll k_0$, then averaging over the possible values $L$, we find that the boundary term is proportional to $(kl)^{-1}$; thus if $kl > 1$, the uncertainty in the size of the sample makes the boundary term in (3.27) negligible. Of course, since $k \ll k_0$, averaging over $L$ leaves the other two terms unchanged.

The second term in (3.27) may be simplified by observing that

$$
\sum_{jj'} \frac{1}{2k} \frac{d}{dk} \left( e^{iak\xi_j - \xi_j'} \right) T_{jj'} = \sum_{jj'} \frac{1}{2k} \frac{d}{dk} \left( e^{iak\xi_j - \xi_j'} \right) (M^{-1})_{jj'} = \frac{d}{dE} \text{ln det} M(E + i0^+) .
$$

(3.28)

For negative energies we have

$$
D(E < 0, -\frac{1}{2} L, \frac{1}{2} L)
$$

(3.28)
understand the phenomenon of localized states in the continuum (positive-energy) region for a system with randomly distributed scattering centers. We believe that the exact solution which we have exhibited will produce new understanding in this area. Here we present a few ideas on this important subject.

First we note that for a system involving a finite number of scattering sites, there can be no state of positive energy which is localized in the sense that its wave function vanishes at \( \pm \infty \). This, of course, does not preclude the possibility that states exist for which the wave-function amplitude is much greater in some region inside the sample than it is outside. If we assume that a state with vanishing amplitude at \( \pm \infty \) exists, then it follows from the work of Sec. II that

\[
\lim_{\xi \to \pm \infty} A e^{i k x} + [ B - S(\pm)] e^{-i k x} = 0,
\]

\[
\lim_{\xi \to \pm \infty} [A - S(-\pm)] e^{i k x} + B e^{-i k x} = 0.
\]

(4.1)

Clearly, from these equations we must have \( A, B, \) and \( S(\pm) \) all vanishing, but this implies [see (2.4)]

\[
\sum_{J} M_{J^*} v_{J} = \lambda v_{J},
\]

(4.2)

The only solution of this equation is \( u(x) = 0 \), as follows from the fact that \( |\det M| \approx 1 \) for positive energy [see (3.19)].

We are thus led to consider the case of the infinite sample to understand the meaning of localized states. If we again assume the existence of a state vanishing at \( \pm \infty \), we can define \( S(\pm) \) for it and we are again led to the conclusion that \( u(x) \) must satisfy (4.2). The difference is, of course, that, as the matrix \( M \) is now infinite in rank, the fact that \( \det M \) cannot vanish does not imply there is no solution of (4.2): if one of the eigenvalues of \( M \) is zero [i.e., (4.2)], then the product of all the others is infinite. Thus localized states are eigenvectors of zero eigenvalue of the matrix \( M \) and we may approach them from a study of the matrix \( M \) for the finite case. What we are interested in is the eigenvector (in the finite case) with the smallest eigenvalue. This presumably is what we call the localized state even in the finite case.

Let us, then, consider the eigenvalue equation

\[
\sum_{J^*} M_{J^*} v_{J} = \lambda v_{J},
\]

(4.3)

where \( \lambda \) is the smallest eigenvalue of \( M \) (\( |\lambda| \approx 1 \)).

From the equations

\[
\sum_{J^*} |\alpha_{J}|^{2} M_{J^*} v_{J} = \lambda \sum_{J} |\alpha_{J}| |v_{J}|^{2},
\]

\[
\sum_{J^*} |\alpha_{J}| v_{J} M_{J^*} v_{J}^{*} = \lambda^{*} \sum_{J} |\alpha_{J}| |v_{J}|^{2},
\]

(4.4)

we can show that for positive energy

\[
\Im \lambda = \frac{\sum_{J} \alpha_{J} v_{J} \cos k x_{J}}{\sum_{J} |\alpha_{J}| |v_{J}|^{2}},
\]

(4.5)

where to get this result we have assumed that all \( \beta_{J} \)'s have the same sign; also the \( \pm \) sign in front corresponds to the sign of \( \Im \alpha_{J} \). Defining

\[
S_{\pm}(\lambda) = \sum_{J} e^{i k x_{J}} \alpha_{J} v_{J},
\]

(4.6)

we get from (4.5) that for \( \lambda \to 0 \), \( S_{\pm}(\lambda) \to 0 \). Now the solution to (4.3) is easily written as

\[
v_{J} = S_{\pm}(\alpha) e^{i k x_{J}},
\]

(4.7)

which, when \( |\lambda| \approx 1 \), looks very much like a nearly perfect transmission solution to (2.3). To see this, note that for perfect transmission the reflection coefficient \( R = -S(\pm) = 0 \) and thus the solution to (2.3) in this case (with \( B = 0 \)) is

\[
v_{J} = A \gamma_{J}(\alpha), [\alpha_{J}], [x_{J}] e^{i k x_{J}},
\]

(4.8)

Thus, with \( |\lambda| \approx 1 \), if we are at an energy \( E \) such that perfect transmission exists, then we can identify \( v_{J} \) and \( u_{J} \) as zero from a normalization factor, i.e.,

\[
v_{J} = S_{\pm}(\alpha) e^{i k x_{J}}, [\alpha_{J}], [x_{J}] e^{i k x_{J}},
\]

\[
\cong S_{\pm}(\alpha) e^{i k x_{J}}.
\]

(4.9)

Here we have used the positive-energy result (2.20). It appears, therefore, that localized states are the infinite \( N \) limit of perfectly transmitting or resonant states.

As noted by Borland, wave functions generally grow in from the ends; this is indicated by the average growth of the \( \gamma_{J} \)'s as noted at the end of Sec. II. (Of course, precisely, the \( \gamma_{J} \)'s do a random walk about this average behavior.) If we start from the transmitted end (i.e., from \( \gamma_{J} \) [assuming \( B = 0 \) in (2.3)], then this growth of the \( \gamma_{J} \)'s (or \( \rho_{J} \)'s) makes it appear that the majority of states correspond to perfect reflection. Borland has understood this feature in terms of the likelihood of picking the phase at one end of the chain so that the phase at the other end is independent of it. We can see this feature by referring to the transfer matrix method (see Appendix B): The transfer matrix for the whole chain is a \( 2 \times 2 \) matrix with determinant equal to unity. Its eigenvalues are such that one is much greater and the other much less than 1. Any state \( (\alpha) \) (see Appendix B) at the end is a linear combination of the two nonorthogonal eigenvectors of the transfer matrix. When this matrix operates on \( (\alpha) \), the part of it corresponding to the eigenvector with the large eigenvalue gets tremendously enhanced while the other part is decreased in size. Thus, if the initial vector \( (\alpha) \) has any significant
part corresponding to the large eigenvalue eigenvector, that part will completely dominate at the other end of the chain and the final end wave function will be much larger than the initial. The likelihood that the initial vector has these features is very large. (Note: This explains why \( \gamma \) increases, since \( \gamma \) is a matrix element of the transfer matrix taken between particular vectors which are generally not equal to the smallest-eigenvalue eigenvector of the transfer matrix.)

In a finite chain there is a small set of vectors that are nearly in the direction of the eigenvector with smallest eigenvalue. A vector in this set corresponds to a wave function which decreases in magnitude as we follow it into the chain. We remark that the longer the chain (or, in other words, the larger and smaller the eigenvalues of the transfer matrix), the smaller the set of vectors which decrease in magnitude as we come in from the end. These states are again states of nearly perfect reflection, the difference being that we now are looking at them from the end of the chain from which they reflect instead of, as above, from the other end. What we observe, then, is that it is trivial to find nearly perfectly reflecting states if we look at the end to which the wave is trying to penetrate but nearly impossible to find these states viewed from the reflecting end. This feature is what Borland\(^5\) noted to be the fact that states which rise in magnitude from one end to the other satisfy extremely tight boundary conditions at the large end with little regard to the conditions at the small end.

How then can we understand localized states? Considering the infinite case, we can think of the semi-infinite chains to the right and left of the area of localization separately; then the wave function as it enters these semi-infinite chains must correspond to the smallest-eigenvalue eigenvector of the transfer matrix for each of them simultaneously. This only occurs at special values of the energy (i.e., the case of perfect transmission, as discussed above). In this case the \( \gamma 's \) do not increase indefinitely.

**APPENDIX A: OTHER FORMS OF SOLUTION OF RÖDINGER EQUATION**

We discuss here, very briefly, the modifications of the method described in Sec. II necessary to produce solutions starting from the other end (i.e., from \( x_0 \)) or from the middle (i.e., from \( x_0, \)).

In starting from \( x_0 \) we are led to use \( S(-) \), as given by (2.7), instead of \( S(+) \). Defining

\[
\eta_j(N, \{ \alpha \}, k) = \frac{-\alpha_j}{1 + \alpha_j} e^{\pm ikx_j} \prod_{j'=2}^{j} \left( 1 + \frac{\alpha_j}{1 - \alpha_j} \right),
\]

(A1)

and

\[
\bar{\eta}_j(k, \{ \alpha \}, \{ x \}) = \eta_j(-k, \{ -\alpha \}, \{ x \}),
\]

(A2)

we get

\[
u_j = \rho_j^N [A - S(-)] e^{ikx_j} + B \bar{\rho}_j^N e^{-ikx_j},
\]

(A3)

with

\[
S(-) = \left( \sum_{j = 1}^N \alpha_j \rho_j^N + B \bar{\rho}_j^N e^{-2ikx_j} \right) \left( 1 + \sum_j \alpha_j \rho_j^N \right).
\]

(A4)

An equation analogous to (2.24) can also be easily written down in terms of \( \bar{\rho}_j^N \) and \( \bar{\eta}_j^N \).

We can regard (2.24) and the above result as "solutions from the ends"; it is also possible to obtain a "solution from the middle." Introducing

\[
\eta_j(N, \{ \alpha \}, \{ x \}) = \frac{-\alpha_j}{1 + \alpha_j} e^{\pm ikx_j} \prod_{j'=2}^{j} \left( 1 + \frac{\alpha_j}{1 - \alpha_j} \right),
\]

(A5)

we get for \( j > j_0 \)

\[
u_j = A e^{ikx_j} \gamma_j \bar{\eta}_j \prod_{j=1}^{j_0} A \alpha_j + B \bar{\rho}_j^N e^{-2ikx_j},
\]

(A6)

while for \( j \leq j_0 \) we get

\[
u_j = [A - S_{10}^N(-)] e^{ikx_j} \rho_j^N \prod_{j=1}^{j_0} A \alpha_j + \prod_{j=1}^{j_0} \eta_j^N \left( 1 + \frac{\alpha_j}{1 - \alpha_j} \right),
\]

(A7)
These expressions can be used to obtain values for 
$S_0(x)$ and also for finding other forms for $u(x)$;
we shall not present these details here.

**APPENDIX B: CONNECTION WITH TRANSFER MATRIX METHOD**

In this appendix we discuss the connection between the technique we have developed and the transfer matrix method. This allows us, for example, to see how our approach is applied to the well-known Kronig-Penney problem.

We begin by introducing (ad hoc) a two-state fermion system; we call the states $|0\rangle$ and $|1\rangle$. We introduce the operators $a$ and $a'$ obeying $aa' + a'a = 1$; $a^2 = 0$ and $a|0\rangle = 0$; and $a'|0\rangle = |1\rangle$.

Next we define

$$\psi_j = 1 + \phi_j a^2 + \phi_j a' ,$$

where $\phi_j$ and $\phi'_j$ are as defined by (2.10) et seq.

Now note that $\langle 0 | \psi_1 | 0 \rangle = 1$ and $\langle 1 | \psi_1 | 0 \rangle = \phi_0^*$. It follows that

$$\gamma_1 = |0\rangle|0\rangle = 1 ,$$

$$\gamma_2 = (1 - \alpha_1) \langle 0 | \psi_1 | 0 \rangle + (1 + \alpha_1) e^{-2ikx_N} \langle 1 | \psi_1 | 0 \rangle .$$

A little more algebra shows that

$$\gamma_3 = (1 - \alpha_1)(1 - \alpha_2) \langle 0 | \psi_2 \psi_1 | 0 \rangle$$

and a relatively simple exercise proves that

$$\gamma_j = \left( \prod_{j'=1}^{j-1} (1 - \alpha_{j'}) \right) \langle 0 | \psi_1 | 0 \rangle + \prod_{j'=1}^{j-1} (1 + \alpha_{j'}) e^{-2ikx_{j'-1}} \langle 1 | \psi_1 | 0 \rangle \times \psi_{j-1} \psi_{j-2} \cdots \psi_1 |0\rangle .$$

In all these equations $\gamma_j$ is as defined by (2.14). It is also clear that

$$\bar{\gamma}_j = \left( \prod_{j'=1}^{j-1} (1 - \alpha_{j'}) \right) e^{2ikx_N} \langle 0 | \psi_1 | 0 \rangle + \prod_{j'=1}^{j-1} (1 + \alpha_{j'}) \langle 1 | \psi_1 | 0 \rangle \times \psi_{j-1} \psi_{j-2} \cdots \psi_1 |1\rangle .$$

To make the connection with the transfer matrix method we write this result in terms of a matrix notation; thus

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} ,$$

$$a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} , \quad a' = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} ;$$

then

$$\psi_j = \begin{pmatrix} 1 \\ \phi_j \end{pmatrix} = \mu_j .$$

We easily get

$$\gamma_j = (1, e^{-2ikx_j}) \begin{pmatrix} \prod_{j'=1}^{j-1} (1 - \alpha_{j'}) & 0 \\ 0 & \prod_{j'=1}^{j-1} (1 + \alpha_{j'}) \end{pmatrix} \begin{pmatrix} \mu_{j-1} \cdots \mu_1 \\ 0 \end{pmatrix} ,$$

while

$$\bar{\gamma}_j = (e^{2ikx_j}, 1) \begin{pmatrix} \prod_{j'=1}^{j-1} (1 - \alpha_{j'}) & 0 \\ 0 & \prod_{j'=1}^{j-1} (1 + \alpha_{j'}) \end{pmatrix} \begin{pmatrix} \mu_{j-1} \cdots \mu_1 \\ 0 \end{pmatrix} .$$

From (B7) and the definition of $\phi_j$, we find that

$$\begin{pmatrix} \prod_{j'=1}^{j-1} (1 - \alpha_{j'}) & 0 \\ 0 & \prod_{j'=1}^{j-1} (1 + \alpha_{j'}) \end{pmatrix} \begin{pmatrix} 1 - \alpha_{j-1} & 0 \\ 0 & 1 + \alpha_{j-1} \end{pmatrix} \begin{pmatrix} \prod_{j'=1}^{j-2} (1 - \alpha_{j'}) & 0 \\ 0 & \prod_{j'=1}^{j-2} (1 + \alpha_{j'}) \end{pmatrix} ;$$

Inserting this result into (B9) and repeating the procedure for each $\mu_j$, we obtain

$$\gamma_j = (1, e^{-2ikx_j}) \nu_{j-1} \cdots \nu_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} ,$$

where

$$\bar{\gamma}_j = (e^{2ikx_j}, 1) \nu_{j-1} \cdots \nu_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$
EXACT SOLUTION OF THE ONE-DIMENSIONAL...

\[
\nu_j = \left( \begin{array}{c} 1 - \alpha_j & -\alpha_j e^{-2i\xi_j} \\ \alpha_j e^{2i\xi_j} & 1 + \alpha_j \end{array} \right),
\]

(B12)

The matrix \( \nu_j \) is not quite the transfer matrix \( \theta_j^{-1} \); this matrix has the form

\[
\theta_j^{-1} = \left( \begin{array}{cc} (1 - \alpha_j) e^{i\hbar(x_{j+1} - x_j)} & -\alpha_j e^{i\hbar(x_{j+1} - x_j)} \\ \alpha_j e^{-i\hbar(x_{j+1} - x_j)} & (1 + \alpha_j) e^{-i\hbar(x_{j+1} - x_j)} \end{array} \right).
\]

(B13)

We recall the fact that if the wave function has the form \( A_j e^{i\hbar x} + B_j e^{-i\hbar x} \) for \( x_{j-1} \leq x \leq x_j \), then it follows that

\[
\begin{pmatrix} A_j e^{i\hbar x_j} \\ B_j e^{-i\hbar x_j} \end{pmatrix} = \theta_j^{-1} \begin{pmatrix} A_j e^{i\hbar x_j} \\ B_j e^{-i\hbar x_j} \end{pmatrix}
\]

(B14)

[this can be shown by a simple manipulation of the Schrödinger equation (2.1)]. It is easy to see that

\[
\theta_j^{-1} = \begin{pmatrix} e^{i\hbar x_{j+1}} & 0 \\ 0 & e^{-i\hbar x_{j+1}} \end{pmatrix} \nu_j \begin{pmatrix} e^{-i\hbar x_j} & 0 \\ 0 & e^{i\hbar x_j} \end{pmatrix},
\]

from which it follows that

\[
\gamma_j = (e^{-i\hbar x_j}, e^{i\hbar x_j}) \theta_j^{-1} \cdots \theta_1^{-1} \begin{pmatrix} e^{i\hbar x_1} \\ 0 \end{pmatrix}
\]

(B15)

and

\[
\tilde{\gamma}_j = (e^{i\hbar x_j}, e^{i\hbar x_j}) \theta_j^{-1} \cdots \theta_1^{-1} \begin{pmatrix} 0 \\ e^{-i\hbar x_1} \end{pmatrix}.
\]

(B16)

The connection is thus made between the transfer matrix method and the method described in Sec. II for finding the exact solution to (2.1).

We note that for a regular array of \( \delta \)-function potentials we have the well-known Kronig-Penney model. We have made some investigations in this area with our method; these were facilitated by the connection, just made, with the transfer matrix method. We shall not report the details here.

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For an up-to-date set of references on the one-dimensional problem see E. N. Economou and M. H. Cohen, Phys. Rev. B 4, 396 (1971).

5Any standard text discusses this method, for example, P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill, New York, 1953), Vols. I and II.


8See, for example, E. Merzbacher, Quantum Mechanics (Wiley, New York, 1961).