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Limitations on the use of δ-function potentials as replacements for actual atomic potentials in one-dimensional studies [1])

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Abstract. In calculations involving one-dimensional disordered systems of atomic potentials, it is desirable to simplify the problem by representing the atomic potentials by δ-functions. We have investigated the claim that it is always possible to represent a single atomic potential by a δ-function, and have pointed out the limitations of extending this claim to include an array of atomic potentials.

1. Introduction

There has been considerable literature published concerning electron states in one-dimensional disordered systems of atomic potentials [see for example, Mott (1961), Mott (1967), Elliott (1974)]. For ease of calculation, δ-function potentials were often used to represent the actual atomic potentials. Consequently the question arose as to what extent the results obtained had features peculiar to the fact that δ-functions were used to represent the actual potentials.

Borland (1961) published an article in which he investigated the existence of energy gaps in a one-dimensional liquid. In this article Borland presented what he considered a proof of this statement that: '. . . it is always possible for a fixed positive electron energy E to replace the atomic potential by a δ-function surrounded by two regions of zero potential which together have the same transformation properties as the atomic potential upon the wave functions to the right and left of it.'

Borland (1961, 1963) as well as other authors [see for example, Dworin (1965), McCubbin (1972) and Eggarter (1972)] have accepted this statement as justification for the use of a δ-function representation for atomic potentials. We will show that the content of Borland's statement must be carefully interpreted in order to avoid misunderstanding. A δ-function potential is characterized by two energy independent parameters (strength and location). However, in general, three energy

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dependent parameters are necessary to specify the transfer matrix of a (not necessarily symmetric) potential. One of these parameters may always be interpreted as the 'location' of the potential. In general, the 'location' parameter is energy dependent, but we will show that for potentials with a line of symmetry, the location is energy independent and coincides with the line of symmetry of the potential.

Borland (1961), in arriving at his result, essentially wrote the transfer matrix for a general potential in a form that resembled the corresponding transfer matrix for a δ-function potential. It will be shown, that there are essential differences between what Borland considers as the transfer matrix for the 'equivalent δ-function potential' and the properties of the transfer matrix of an actual δ-function potential. Finally, a graphical representation of the transfer matrix is made to help clarify the distinction between the transfer matrices of a potential located at an arbitrary point and one located at the origin, and between those of symmetric and non-symmetric potentials.

In order to make our presentation clear, we will first develop the properties of the transfer matrix for the case of a general potential. Although this involves much rather trivial algebra, it is precisely this algebra, whose careless handling in the past has led to misunderstandings. With this done, we can then understand the content of Borland's statement and what limitations are contained therein, in particular with regard to representing an array of general atomic potentials by a series of δ-function potentials.

2. Properties of the transfer matrix R

The potential is assumed to be a single-valued, real (but not necessarily symmetric) function $V(x)$ such that

$$V(x) = 0 \quad \text{for} \quad \begin{cases} x \leq x_1 \\ x \geq x_2 \end{cases} \tag{2.1}$$

where $-\infty < x_1 \leq x_2 < \infty$. We will call such a potential *localized*. The region $-\infty < x \leq x_1$ will be denoted by I, and the region $x_2 \leq x < \infty$ by III. (Fig. 1.)

The time independent Schrödinger equation[2]) for a particle of energy κ^2 is, in units where $\hbar^2/2m = 1$,

$$[-d^2/dx^2 + V(x) - \kappa^2]\psi(x) = 0. \tag{2.2}$$

The solution of this equation is:

$$\psi_{\mathrm{I}}(x) = \mathrm{A}_{\mathrm{I}} \exp(i\kappa x) + B_{\mathrm{I}} \exp(-i\kappa x), \quad x \leq x_1$$

and (2.3)

$$\psi_{\mathrm{III}}(x) = A_{\mathrm{III}} \exp(i\kappa x) + B_{\mathrm{III}} \exp(-i\kappa x), \quad x \geq x_2.$$

If boundary conditions on ψ and $d\psi/dx$ at some point $x \leq x_1$ specify the complex constants A_{I} and B_{I}, then A_{III} and B_{III} are not free since the solution of a second-order differential equation is completely determined by only two arbitrary constants. We relate A_{III} and B_{III} to A_{I} and B_{I} by means of a 2×2 matrix **R** with complex elements.

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[2]) The periodic time dependence of the wave function may be omitted since it would cancel out in the calculated intensities.

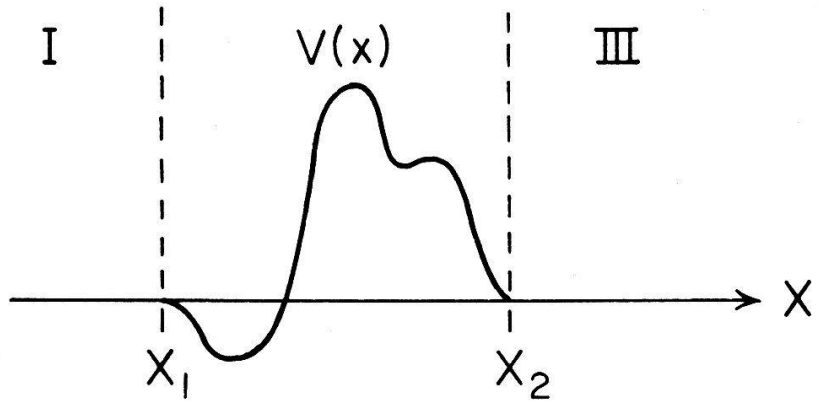

Figure 1
Localized potential: $V(x) = 0, \begin{cases} x \leqslant x_1 \\ x \geqslant x_2 \end{cases} \quad -\infty < x_1 \leqslant x_2 < \infty$

We define **R** by

$$\begin{pmatrix} A_{\mathrm{III}} \\ B_{\mathrm{III}} \end{pmatrix} = \mathbf{R} \cdot \begin{pmatrix} A_{\mathrm{I}} \\ B_{\mathrm{I}} \end{pmatrix}. \tag{2.4}$$

The column vectors in equation (2.4) will be denoted by $\mathbf{b}_{\mathrm{III}}$ and $\mathbf{b}_{\mathrm{I}}$, respectively; hence

$$\mathbf{b}_{\mathrm{III}} = \mathbf{R}\mathbf{b}_{\mathrm{I}}. \tag{2.5}$$

By making use of the linear superposition principle valid for solutions of (2.2), we can show that the matrix **R** is independent of A_{I} and B_{I} (or A_{III} and B_{III}). Further the property of time reversal invariance of (2.2) and the conservation of probability current density lead to the following relationships between the elements of **R**:

$$R_{22} = R_{11}^*; \qquad R_{12} = R_{21}^*,$$

and

$$\det \mathbf{R} = |R_{11}|^2 - |R_{12}|^2 = 1. \tag{2.6}$$

These are equivalent to five real equations connecting the eight real numbers which characterize the four complex matrix elements R_{mn}. These equations are such that **R** is completely determined by three real parameters. Since the solutions of the Schrödinger equation are functionals of $V(x)$ and κ only, the three parameters can only depend on $V(x)$ and κ. We should note that the transfer matrix **R** is unimodular (det **R** = 1) and it is not unitary. There are three additional properties of the transfer matrix we will use. We will call these three properties (P1), (P2) and (P3) in what follows.

(P1) A shift by x_0 of the origin of the x-coordinate (leaving the potential in place) induces the transformation $\mathbf{R} \to \mathbf{R}'$, defined by

$$R_{11} \to R'_{11} = R_{11} \tag{2.7}$$

and

$$R_{12} \to R'_{12} = R_{12} \exp(2i\kappa x_0). \tag{2.8}$$

Here $\mathbf{R}'$ is the transfer matrix relating the coefficients of $\psi_{\mathrm{III}}(x')$ and $\psi_{\mathrm{I}}(x')$, where $x' = x - x_0$.

To prove (P1) we note that a shift in the origin of the coordinate means that we replace x by $x' + x_0$ in the exponent of equation (2.3). This leads to coefficients $\mathbf{a}_A$

of the wave function with respect to the basis $\exp(i\kappa x')$, $\exp(-i\kappa x')$

$$\mathbf{a}_A = \mathbf{U}(x_0)\mathbf{b}_A, \quad A = \mathrm{I}, \mathrm{III} \tag{2.9}$$

where

$$\mathbf{U}(x_0) = \begin{pmatrix} \exp(i\kappa x_0) & 0 \\ 0 & \exp(-i\kappa x_0) \end{pmatrix}. \tag{2.10}$$

Therefore, if we set

$$\mathbf{a}_{\mathrm{III}} = \mathbf{R}'\mathbf{a}_{\mathrm{I}}, \tag{2.11}$$

we obtain from equations (2.5) and (2.9)

$$\mathbf{R}' = \mathbf{U}(x_0)\mathbf{R}\mathbf{U}(-x_0) = \mathbf{U}(x_0)\mathbf{R}\mathbf{U}^{-1}(x_0), \tag{2.12}$$

from which equations (2.7) and (2.8) follow immediately.

(P2) For a fixed coordinate origin $x = 0$ and for each value of κ, there exists a point $-\infty < x_0(\kappa) < \infty$ such that if $x_0(\kappa)$ is chosen as the origin of the coordinate y, and $\mathbf{M}$ is the matrix relating A_{I}, B_{I} and A_{III}, B_{III} as coefficients of $\psi_{\mathrm{I}}(x')$ and $\psi_{\mathrm{III}}(x')$, respectively, then in addition to the properties that

$$M_{22} = M_{11}^*; \qquad M_{21} = M_{12}^* \tag{2.13}$$

and

$$\det \mathbf{M} = |M_{11}|^2 - |M_{12}|^2 = 1,$$

the following relation exists:

$$\mathrm{Re}\, M_{12} = 0. \tag{2.14}$$

Equation (2.13) follows from equation (2.6).

To prove equation (2.14) and thereby (P2), we write the matrix element R_{12} as

$$R_{12} = |R_{12}| \exp[-i\phi], \quad \phi \text{ real}, \ -\pi \leq \phi \leq \pi. \tag{2.15}$$

Then choosing the new coordinate origin $x' = 0$ at

$$x_0(m, \kappa) \equiv [\phi - (m + \tfrac{1}{2})\pi]/2\kappa, \quad m = 0, \pm 1, \pm 2, \ldots \tag{2.16}$$

we find that equation (2.8) yields

$$M_{12} = (-1)^{m+1} i |R_{12}|. \tag{2.17}$$

Let us denote the value of m, for which

$$|x_0(m, \kappa) - \tfrac{1}{2}(x_1 + x_2)| \tag{2.18}$$

as a function of m is a minimum, by m_0. Here, x_1 and x_2 are defined by equation (2.1). The point $x_0(\kappa) \equiv x_0(m_0, \kappa)$ will be denoted as the *location* of the potential. We then obtain

$$M_{12} = (-1)^{m_0+1} i |R_{12}|. \tag{2.19}$$

Equation (2.14) reduces the number of independent parameters which define the transfer matrix $\mathbf{M}$ to two. Hence, $x_0(\kappa)$ may be considered as the third parameter characterizing $\mathbf{R}$ with respect to the original coordinate x.[3])

[3]) From now on when the transfer matrix $\mathbf{R}$ is expressed with respect to a coordinate whose origin coincides with the location of the potential, it will be denoted by $\mathbf{M}$.

(P3) If the potential is *symmetric*, its location x_0 is independent of κ, and is identical to the position, x_S, of its line of symmetry.

To prove (P3) we note that if the line of symmetry of the potential is at $x_S = 0$, then the transformation $x' = -x$ leaves the Schrödinger equation invariant. Therefore, along with $\psi(x)$ there exists another solution $\psi''(x')$ such that

$$\psi''_{\mathrm{I}}(x') = \psi_{\mathrm{III}}(-x), \tag{2.20}$$

and

$$\psi''_{\mathrm{III}}(x') = \psi_{\mathrm{I}}(-x).$$

Consequently, if $\mathbf{b}''_A (A = \mathrm{I}, \mathrm{III})$ denotes the coefficient of the wave function referred to $\exp(i\kappa x')$, $\exp(-i\kappa x')$, we have

$$\mathbf{b}''_{\mathrm{I}} = \boldsymbol{\sigma}_x \mathbf{b}_{\mathrm{I}}, \tag{2.21}$$

and

$$\mathbf{b}''_{\mathrm{III}} = \boldsymbol{\sigma}_x \mathbf{b}_{\mathrm{I}},$$

where $\boldsymbol{\sigma}_x$ is the Pauli spin matrix.

Since $\mathbf{R}$ is invariant under the space inversion $x \to x' = -x$, we have from equation (2.5),

$$\mathbf{b}''_{\mathrm{III}} = \mathbf{R}\mathbf{b}''_{\mathrm{I}}. \tag{2.22}$$

Combining equations (2.5), (2.21) and (2.22), we obtain

$$(\mathbf{R}\boldsymbol{\sigma}_x)^2 = (\boldsymbol{\sigma}_x \mathbf{R})^2 = 1. \tag{2.23}$$

Equation (2.23) used in conjunction with equation (2.6) leads to the additional relation that

$$\mathrm{Re}\, R_{12} = 0, \tag{2.24}$$

where equation (2.24) is valid regardless of the value of κ as long as the potential is symmetric with respect to $x_S = 0$. Hence, the line of symmetry of the potential is its 'location' in the sense defined in (P2), because it is the point which, when chosen as the coordinate origin, leads to equations (2.14) and (2.19).

We are now in the position to determine from the transfer matrix whether there exists a line of symmetry for a given potential. From equations (2.8) and (2.24) it follows that for a symmetric potential, located at x_s, the matrix element R_{12} of a symmetric potential fulfills the equation

$$\mathrm{Im}\,[\ln R_{12}] = -(2x_s\kappa + \pi/2 + n\pi), \quad n = 0, \pm 1, \pm 2, \ldots \tag{2.25}$$

where x_s is independent of κ. In contrast to this, for a nonsymmetric potential, it follows from equation (2.15) that

$$\mathrm{Im}\,[\ln R_{12}] = -\phi(\kappa) + n\pi, \quad n - 0, \pm 1, \pm 2, \ldots \tag{2.26}$$

where $\phi(\kappa)$ is not necessarily a linear function of κ.

Without loss of generality, we may express the elements of the transfer matrix $\mathbf{M}$ for a potential located at the origin $x' = 0$ in terms of two real κ-dependent parameters λ and γ such that

$$M_{11} = (ch\lambda) \exp(-i\gamma),$$

and (2.27)

$$M_{12} = -ish\lambda,$$

where we have made use of equations (2.13) and (2.14).

It should be borne in mind that the representation given by equation (2.27) is valid for a symmetric potential for all values of κ, since the location of the symmetric potential, once chosen, remains at $x' = 0$, independent of κ. In contrast to this, the location x_0 of a non-symmetric potential depends on κ, and, therefore, the two-parameter description, equation (2.27), is valid only for a particular value $\kappa = \kappa_0$, for which $x_0(\kappa_0) = 0$. For general values of κ, the third parameter $x_0(\kappa)$ is needed in addition to $\lambda(\kappa)$ and $\gamma(\kappa)$ to specify the transfer matrix.

The elements of the transfer matrix **R** for a potential *not located at the origin* are commonly written such that the unimodular property is explicitly taken into account similar to equation (2.27). In this case, however, $R_{12} \neq 0$, in general, and there are three real parameters α, λ, and γ as discussed previously:

$$R_{11} = (ch\lambda) \exp(-i\alpha); \qquad R_{12} = (sh\lambda) \exp(-i\gamma). \tag{2.28}$$

For our purposes, it is more convenient to use the parameters t, β and ϕ defined by

$$R_{11} = (1 - it) \exp(-i\beta); \qquad R_{12} = \mathrm{t} \exp(-i\phi), \tag{2.29}$$

where it is clear that the unimodular condition is still automatically satisfied.

From equation (2.12) and (2.29), we can find the matrix elements of **R**′ (or **M**):

$$M_{11} = (1 - it) \exp(-i\beta),$$

and (2.30)

$$M_{12} = t \exp[-i(\phi - 2\kappa x_0)].$$

In accord with the discussions under (P2), we interpret the parameter x_0 as the 'location' of the potential so that we may write

$$M_{12} = -it, \tag{2.31}$$

where we have made use of equations (2.15) through (2.19).

From equations (2.12) and (2.30) we find **R** to be

$$\mathbf{R} = \begin{pmatrix} (1 - it) \exp(-i\beta) & -it \exp(-2i\kappa x_0) \\ it \exp(2i\kappa x_0) & (1 + it) \exp(i\beta) \end{pmatrix} \tag{2.32}$$

It is important to note that β, t and x_0 are, in general, all κ dependent.

3. The transfer matrix as defined by Borland

Before proceeding further, it is necessary to comment upon the transfer matrix as used by Borland (1961). Whereas we have defined a transfer matrix **R** through equations (2.3) and (2.4), Borland chose to use a different basis for ψ_{I} and ψ_{II} [see equation (2.3)]. This means Borland makes use of plane wave solutions where the

coordinate x is measured from two different origins on the two sides of the potential such that

$$\psi_{\mathrm{I}} = A'_{\mathrm{I}} \exp\left[i\kappa(x - x_1)\right] + B'_{\mathrm{I}} \exp\left[-i\kappa(x - x_1)\right], \quad x \leq x_1$$

and (3.1)

$$\psi_{\mathrm{III}} = A'_{\mathrm{III}} \exp\left[i\kappa(x - x_2)\right] + B'_{\mathrm{III}} \exp\left[-i\kappa(x - x_2)\right], \quad x \geq x_2$$

so that Borland's transfer matrix, $\mathbf{R}_B$, is defined by

$$\begin{pmatrix} A'_{\mathrm{III}} \\ B'_{\mathrm{III}} \end{pmatrix} = \mathbf{R}_B \cdot \begin{pmatrix} A'_{\mathrm{I}} \\ B'_{\mathrm{I}} \end{pmatrix}. \tag{3.2}$$

Using equations (2.3) and (3.1), we can write the primed coefficients of the wave function in terms of the unprimed coefficients, thus relating the transfer matrices defined by equations (2.4) and (3.2): equation (3.2) may then be written as

$$\begin{pmatrix} A_{\mathrm{III}} \exp(i\kappa x_2) \\ B_{\mathrm{III}} \exp(-i\kappa x_2) \end{pmatrix} = \mathbf{R}_B \cdot \begin{pmatrix} A_{\mathrm{I}} \exp(i\kappa x_1) \\ B_{\mathrm{I}} \exp(-i\kappa x_1) \end{pmatrix} \tag{3.3}$$

or equivalently

$$\mathbf{b}_{\mathrm{III}} = \mathbf{U}^*(x_2)\mathbf{R}_B\mathbf{U}(x_1)\mathbf{b}_{\mathrm{I}} = \mathbf{R}\mathbf{b}_{\mathrm{I}}, \tag{3.4}$$

where we have made use of equation (2.5), and we have defined

$$\mathbf{U}(x_n) = \begin{pmatrix} \exp(i\kappa x_n) & 0 \\ 0 & \exp(-i\kappa x_n) \end{pmatrix}; \quad n = 1, 2. \tag{3.5}$$

From equation (3.4) we see that $\mathbf{R}$ and $\mathbf{R}_B$ are related through the relationship

$$\mathbf{R} = \mathbf{U}^*(x_2)\mathbf{R}_B\mathbf{U}(x_1), \tag{3.6}$$

or solving for $\mathbf{R}_B$ we have

$$\mathbf{R}_B = \mathbf{U}(x_2)\mathbf{R}\mathbf{U}^*(x_1). \tag{3.7}$$

For later reference we note that if a single coordinate origin is used ($x = 0$), the transfer matrix $\mathbf{R}$ which represents a line segment of zero potential between x_1 and x_2 (see Fig. 1), is given by

$$\mathbf{R} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.8}$$

However, from equation (3.7), we see that the transfer matrix $\mathbf{R}_B$ for a line segment of zero potential is

$$\mathbf{R}_B = \mathbf{U}(x_2)\mathbf{U}^*(x_1) = \mathbf{U}(x_2 - x_1) = \begin{pmatrix} \exp\left[i\kappa(x_2 - x_1)\right] & 0 \\ 0 & \exp\left[-i\kappa(x_2 - x_1)\right] \end{pmatrix}. \tag{3.9}$$

4. Transfer matrix for a δ-function potential

To understand what is meant by an 'equivalent' δ-function potential, we will need the transfer matrix for an actual δ-function potential for comparison. We will first find the transfer matrix for a δ-function potential located at the origin. We can

then use equation (2.12) to transform it to a δ-function potential located at an arbitrary point, $x = x_0$.

A δ-function potential of strength ξ located at $x = 0$ gives rise to the Schrödinger equation

$$[-d^2/dx^2 + \xi\delta(x) - \kappa^2]\psi(x) = 0, \tag{4.1}$$

where κ^2 is the energy of the particle in units $\hbar^2/2m = 1$. Integrating this equation from $x = -\varepsilon$ to $x = y > 0$, we obtain

$$-\psi'(y) + \psi'(-\varepsilon) + \xi \int_{-\varepsilon}^{y} \delta(x)\psi(x)\,dx - \kappa^2 \int_{-\varepsilon}^{y} \psi(x)\,dx = 0. \tag{4.2}$$

Integrating once more from $y = -\varepsilon$ to $+\varepsilon$ we obtain

$$-\psi(\varepsilon) + \psi(-\varepsilon) + 2\varepsilon\psi'(-\varepsilon) + \xi \int_{-\varepsilon}^{\varepsilon} dy \int_{-\varepsilon}^{y} \delta(x)\psi(x)\,dx - K^2 \int_{-\varepsilon}^{\varepsilon}\int_{-\varepsilon}^{y} \psi(x)\,dx = 0. \tag{4.3}$$

Subject to the condition that $|\psi(x)|$ remains finite, it is easy to see that in the limit of $\varepsilon \to 0$ the last three terms in equation (4.3) tend to zero. It follows:

$$-\psi(0^+) + \psi(0^-) = 0, \tag{4.4}$$

where $\psi(0^+)$ is the value of the wave function slightly to the right of $x = 0$ and similarly for $\psi(0^-)$. Using the fact that $\psi(x)$ is continuous across the δ-function, we obtain from equation (4.2) in the limit of $\varepsilon \to 0$:

$$-\psi'(0^+) + \psi'(0^-) + \xi\psi(0) = 0. \tag{4.5}$$

We now use the plane wave solutions given by equation (2.3) on each side of the δ-function potential (in this case $x_1 = x_2 = 0$). Inserting these solutions and their derivatives into equation (4.4) and (4.5), we obtain

$$A_{\mathrm{III}} = (1 - i\xi/2\kappa)A_{\mathrm{I}} - (i\xi/2\kappa)B_{\mathrm{I}},$$

and

$$B_{\mathrm{III}} = (i\xi/2\kappa)A_{\mathrm{I}} + (1 + i\xi/2\kappa)B_{\mathrm{I}}. \tag{4.6}$$

Therefore, from equation (2.4) we have for the elements of the transfer matrix of a δ-function potential situated at the origin

$$M_{11} = 1 - i\xi/2\kappa, \tag{4.7}$$

$$M_{12} = -i\xi/2\kappa. \tag{4.8}$$

The conditions given by equation (2.6) are fulfilled, as is easily seen by inspection. Further, in keeping with our convention, we denote this transfer matrix by the letter **M**, since it is expressed with respect to a coordinate origin at the location (line of symmetry) of the potential [see (P2) and (P3)] in Section 2].

Using equations (2.12), (4.7) and (4.8), we can write the transfer matrix $\mathbf{R}_\delta$, for a δ-function potential located at a point $x = x_0$ as

$$\mathbf{R}_\delta = \mathbf{U}^*(x_0)\mathbf{M}_\delta(\xi)\mathbf{U}(x_0), \tag{4.9}$$

where

$$\mathbf{U}(x_0) = \begin{pmatrix} \exp(i\kappa x_0) & 0 \\ 0 & \exp(-i\kappa x_0) \end{pmatrix}, \tag{4.10}$$

and

$$\mathbf{M}_\delta(\xi) = \begin{pmatrix} 1 - i\xi/2\kappa & -i\xi/2\kappa \\ i\xi/2\kappa & 1 + i\xi/2\kappa \end{pmatrix}. \tag{4.11}$$

The parameters ξ and x_0 are not κ dependent. [See (P3) in Section 2.]

5. Graphical representation of the transfer matrix

Let us represent the elements R_{11} and R_{12} of the transfer matrix in the complex plane $z = \sigma_1 + i\sigma_2$. The elements R_{21} and R_{22} are completely determined by R_{11} and R_{12} through equation (2.6) and, therefore, need not be considered.

The use of equation (2.6) allows the following graphical construction of a compatible set of matrix elements for a given value of the wave number κ (see Fig. 2).

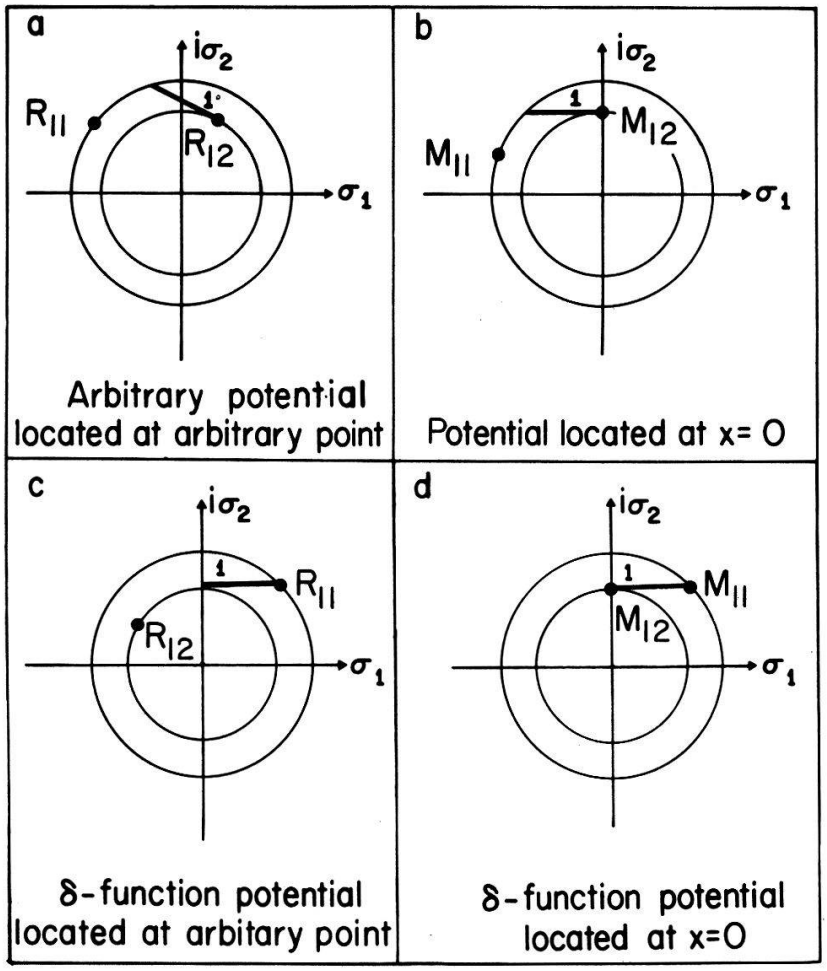

Figure 2
Argand diagrams of the transfer matrix elements.

(i) Choose R_{12} as an arbitrary point in the complex plane.

(ii) Draw a circle through R_{12} with the origin as center. At an arbitrary point on the circle draw a tangent of unit length measured from the point of contact. Draw a second circle through the end point of the tangent with the origin as center.

(iii) Choose R_{11} anywhere on the larger circle (see Fig. 2a). This will fulfill equation (2.6).

The construction could, of course, be reversed, choosing first R_{11} arbitrarily with obvious modifications. In either case there are three real parameters at our disposal: the modulus and angle of the complex number R_{12} and the phase angle of R_{11} (or vice versa).

It follows from equation (2.8) that a shift in the origin of the coordinate x is equivalent to moving R_{12} on the smaller circle. If the potential is located at $x = 0$ (see Fig. 2b), then R_{12} (or M_{12}) lies on the imaginary axis [refer to (P2) and (P3) in Section 2]. For an arbitrary potential $V(x)$, when κ is varied, both R_{11} and R_{12} move in the complex plane, always retaining the geometrical relationships given by (i), (ii) and (iii). A symmetric potential is characterized by the fact that M_{12} always moves along the imaginary axis if the potential is centered at the origin (see Fig. 2b).

Next let us construct the complex diagram of the matrix elements of a δ-function potential located at $x = 0$ and of strength ξ. From equations (4.7) and (4.8), the relationships

$$R_{11} = M_{11} = 1 + \varepsilon i|\xi| \tag{5.1}$$

and

$$R_{12} = M_{12} = \varepsilon i|\xi| \tag{5.2}$$

follow, where for attractive potentials ε is a positive sign and for repulsive potentials ε is a negative sign. In applying rules (i), (ii) and (iii) we have to choose M_{12} on the imaginary axis [equation (5.2)]: Furthermore, M_{11} has to be chosen at a distance 1 to the right of the imaginary axis on the larger circle in the same half plane as M_{12} (see Fig. 2d). Consequently, no freedom is left in the choice of M_{11} once M_{12} is chosen.

If the δ-function is moved to the point x_0, R_{12} moves on the inner circle of Fig. 2c. In this case, equation (5.1) still remains valid and R_{11} does not move; however, equation (5.2) no longer holds [see (P3), Section 2]. Note that for a δ-function potential

$$\operatorname{Re} R_{11} = 1, \tag{5.3}$$

and it is this relation which distinguishes a δ-function potential from a more general one.

6. Discussion

Let us now compare the transfer matrix given by equation (2.32) for a general potential with that given by equation (4.9) for a δ-function potential. Using equations (4.10) and (4.11) we can write equation (4.9) as

$$\mathbf{R}_\delta = \begin{pmatrix} 1 - i\xi/2\kappa & -\xi/2\kappa \exp(-2i\kappa x_0) \\ i\xi/2\kappa \exp(2i\kappa x_0) & 1 + i\xi/2\kappa \end{pmatrix}, \tag{6.1}$$

where it is important to keep in mind that the strength, ξ, and the location, x_0, are not dependent on κ for a δ-function potential. We can rewrite equation (2.32) as

$$\mathbf{R} = \begin{pmatrix} [1 - it'(\kappa)/2\kappa] \exp [-i\beta(\kappa)] & [-it'(\kappa)/2\kappa] \exp [-2i\kappa x_0(\kappa)] \\ [it'(\kappa)/2\kappa] \exp [2i\kappa x_0(\kappa)] & [1 + it'(\kappa)/2\kappa] \exp [i\beta(\kappa)] \end{pmatrix}, \tag{6.2}$$

where we have defined

$$t(\kappa) = t'(\kappa)/2\kappa, \tag{6.3}$$

and we have explicitly indicated that for a general potential the parameters t', β and x_0 are κ dependent.

It is clear from equations (6.1) and (6.2) that $\mathbf{R}$ and $\mathbf{R}_\delta$ have the same form only if $\beta(\kappa) = 0$. However, as we have seen in Sections 2 and 5, a general potential requires *three* independent parameters to specify the transfer matrix whereas the transfer matrix given by equation (6.1) for a δ-function potential has only two, the strength and the location. Therefore, it is inappropriate to say that the transfer matrix for a general atomic potential can always be expressed in terms of the transfer matrix for a δ-function potential. Borland stated that there exists an 'equivalent' δ-function potential surrounded by two regions of zero potential. To understand what this means let us use equation (3.7) to transform $\mathbf{R}$ into $\mathbf{R}_B$, the transfer matrix of a general potential, referred to the basis Borland used (see Section 3). Using equation (3.7) we can write equation (6.2) as

$$\mathbf{R}_B = \mathbf{U}(x_2)\mathbf{R}\mathbf{U}^*(x_1) = \mathbf{U}(x_2)\mathbf{U}^*(v_1)\mathbf{M}\mathbf{U}(v_2)\mathbf{U}^*(x_1), \tag{6.4}$$

where $\mathbf{R}$ has been written as

$$\mathbf{R} = \mathbf{U}^*(v_1)\mathbf{M}\mathbf{U}(v_2) \tag{6.5}$$

with

$$\mathbf{U}(v_1) = \begin{pmatrix} \exp(i\kappa v_j) & 0 \\ 0 & \exp(-i\kappa v_j) \end{pmatrix}, \quad j = 1,2 \tag{6.6}$$

$$\kappa v_1 = -(\beta/2 + \kappa x_0); \qquad \kappa v_2 = -(\beta/2 - \kappa x_0),$$

and

$$\mathbf{M} = \begin{pmatrix} 1 - it'/2\kappa & -it'/2\kappa \\ it'/2\kappa & 1 + it'/2\kappa \end{pmatrix}. \tag{6.7}$$

The form of equation (6.7) for the matrix $\mathbf{M}$ is the same as equation (4.11) for the matrix $\mathbf{M}_\delta$, for a fixed energy (t' in $\mathbf{M}$ is a function of κ, while ξ in $\mathbf{M}_\delta$ is not). According to Borland's point of view we would interpret equation (6.4) as representing an 'equivalent' δ-function potential, $\mathbf{M}$, given by equation (6.7), multiplied on the left and right, respectively, by the matrices $\mathbf{U}(x_2 - v_1)$ and $\mathbf{U}(v_2 - x_1)$, which represent line segments of zero potential in the same sense as equation (3.9).

It is however, deceptive to call the matrix $\mathbf{M}$ of equation (6.4) a transfer matrix for an 'equivalent' δ-function potential, since one would tend to attribute to it the properties of an actual δ-function potential transfer matrix. This idea of an 'equivalent' δ-function potential to represent a general potential is misleading, then, on the following counts:

(1) An actual δ-function potential has only two independent parameters, the strength and location, whereas for a general potential three parameters are necessary, all of which may be energy dependent.
(2) The matrices which multiply $\mathbf{M}_\delta$ in equation (4.9) contain only the location parameter which is energy independent, whereas the matrices which multiply $\mathbf{M}$ in equation (6.4) contain two parameters, both of which may be energy dependent.
(3) A total transfer matrix for an array of potentials may be written as the ordered product of the individual transfer matrices $\mathbf{R}$ [see, e.g. Erdös and Herndon (1972)]. This multiplicative property of the transfer matrices, $\mathbf{R}$, is highly desirable in investigations dealing with disordered arrays of potentials. On the other hand, it is clear from equation (3.7) that this *multiplicative property does not hold for* $\mathbf{R}_B$.

This is easily seen to be true by considering the following situation. Let $\mathbf{R}_1$ and $\mathbf{R}_2$ be the transfer matrices for the potentials V_1 and V_2, respectively, situated as shown in Fig. 3. Then from equation (3.6) we have

$$\mathbf{R}_1 = \mathbf{U}^*(x_2)\mathbf{R}_{B1}\mathbf{U}(x_1), \tag{6.8}$$

and

$$\mathbf{R}_2 = \mathbf{U}^*(x_4)\mathbf{R}_{B2}\mathbf{U}(x_3), \tag{6.9}$$

where $\mathbf{R}_{B1}$ and $\mathbf{R}_{B2}$ are the transfer matrices corresponding to V_1 and V_2, respectively, as expressed in the basis Borland used (see Section 3). Therefore

$$\mathbf{R}_2\mathbf{R}_1 = \mathbf{U}^*(x_4)\mathbf{R}_{B2}\mathbf{U}(x_3)\mathbf{U}^*(x_2)\mathbf{R}_{B1}\mathbf{U}(x_1), \tag{6.10}$$

and we see that the multiplicative nature of $\mathbf{R}_1$ and $\mathbf{R}_2$ does not carry over to $\mathbf{R}_{B1}$ and $\mathbf{R}_{B2}$ since the matrix $\mathbf{U}(x_3 - x_2)$ appears between them.

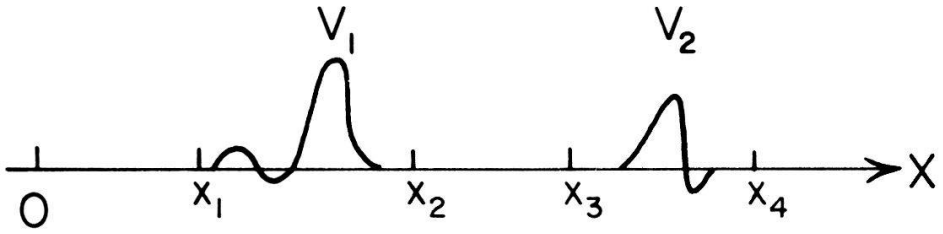

Figure 3
Two localized potentials $V_1(x)$ and $V_2(x)$ located on the x-axis between x_1 and x_2, and x_3 and x_4, respectively.

In summary, then, we may state that it is always possible to write the transfer matrix $\mathbf{R}$, which characterizes a general potential, $V(x)$ as the product of three matrices [see equation (6.5)], each of which contains one energy dependent parameter. In addition one of these matrices may be written in a form given by equation (6.7). However, as we have previously explained, it is misleading to identify equation (6.7) as an 'equivalent' δ-function potential transfer matrix.

A consequence of these conclusions is, that certain results, which were thought to be valid for chains of arbitrary atomic potentials, are only valid for chains of δ-function potentials. An example of this is found in the work of Dworin (1964). His criteria for the existence of electron energy gaps in the spectrum of a disordered chain

of potentials or chain of random potentials cannot be used, unless one would assume that the location of each potential is different for each value of the electron energy.

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