PARTITION OF THE POTENTIAL OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

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Abstract: The one-dimensional Schrödinger equation is considered when the potential and its first moment are absolutely integrable. The transmission coefficient vanishes at zero energy in the generic case, and it never vanishes in the exceptional case. It is shown that any nontrivial exceptional potential can always be fragmented into two generic potentials. Furthermore, any nontrivial potential, generic or exceptional, can be fragmented into all generic pieces in infinitely many ways. The results remain valid when Dirac delta functions are included in the potential, in which case even the trivial potential can be fragmented into generic pieces.

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Consider the one-dimensional Schrödinger equation

$$\frac{d^2\psi(k,x)}{dx^2} + k^2\psi(k,x) = V(x)\,\psi(k,x), \tag{1}$$

where k^2 is energy, x is the space coordinate, and $V(x)$ is the potential; appropriate units are used in which $\hbar = 1$ and $m = 1/2$. When the potential is absolutely integrable, there are two linearly independent solutions $f_l(k,x)$ and $f_r(k,x)$ of (1) known as the Jost solutions from the left and from the right, respectively, satisfying the boundary conditions

$$f_l(k,x) = \begin{cases} e^{ikx} + o(1), & x \to +\infty, \\ \dfrac{1}{T(k)} e^{ikx} + \dfrac{L(k)}{T(k)} e^{-ikx} + o(1), & x \to -\infty, \end{cases}$$

$$f_r(k,x) = \begin{cases} \dfrac{1}{T(k)} e^{-ikx} + \dfrac{R(k)}{T(k)} e^{ikx} + o(1), & x \to +\infty, \\ e^{-ikx} + o(1), & x \to -\infty, \end{cases}$$

where $T(k)$ is the transmission coefficient and $R(k)$ and $L(k)$ are the reflection coefficients from the right and from the left, respectively. The scattering matrix associated with (1) is defined as

$$\mathbf{S}(k) = \begin{bmatrix} T(k) & R(k) \\ L(k) & T(k) \end{bmatrix}. \tag{2}$$

We have

$$R(k)\,T(-k) + L(-k)\,T(k) = 0. \tag{3}$$

We will assume that $\int_{-\infty}^{\infty} dx\,(1+|x|)\,|V(x)|$ is finite. For such potentials, the corresponding scattering matrix is well understood. Generically, the transmission coefficient vanishes linearly as $k \to 0$ and $R(0) = L(0) = -1$. In the exceptional case, we have $T(0) \neq 0$ and hence $|R(0)| = |L(0)| < 1$. In fact, the potential $V(x)$ is exceptional if and only if

$$\int_{-\infty}^{\infty} dx\, V(x)\, f_l(0,x) = 0, \tag{4}$$

where $f_l(k,x)$ is the corresponding Jost solution from the left. Note that (4) is equivalent to $\int_{-\infty}^{\infty} dx\, V(x)\, f_r(0,x) = 0$ because $f_l(0,x)$ and $f_r(0,x)$ are linearly dependent in the exceptional case.

The exceptional case is unstable in the sense that a small change in the potential usually makes the case generic. As an example, consider the square-well potential: the exceptional case occurs at the exact depths when a bound state is added to the potential; at any other depth the square-well potential is generic. A zero-energy particle tunnels through an exceptional potential whereas such tunneling is impossible through a generic potential.

The distinction between the generic and exceptional cases becomes obvious when the small energy behavior of the scattering coefficients or the wavefunctions is considered [1-5]. In many instances one has to deal with quantities involving the factor $\frac{T(k)}{2ik}$; in the generic case this factor remains bounded and continuous as $k \to 0$. However, in the exceptional case, this factor behaves as $O(1/k)$ and one often has to obtain detailed estimates and prove that the remaining multiplicative terms have $o(k^\gamma)$ behavior for some $\gamma \in (0,1)$ or $O(k)$ behavior in order to insure integrability or continuity at $k = 0$, respectively. In general, the proofs corresponding to exceptional potentials are much more difficult and elaborate than those corresponding to generic potentials. In this Letter we show that an exceptional potential can always be fragmented into two generic pieces; since the quantities related to a potential can be written in terms of those related to the fragments of this potential, the result presented here offers drastic simplifications in dealing with exceptional potentials. The reader is referred to the existing literature for additional information on the difference between the generic and exceptional cases [1-5].

Let us partition the real axis $\mathbf{R}$ as $\mathbf{R} = \cup_{j=0}^{N}(x_j, x_{j+1})$, where $x_0 = -\infty$, $x_{N+1} = +\infty$, and $x_j < x_{j+1}$ for $j = 0, \ldots, N$. We can then write $V(x)$ in terms of its fragments $V_{j,j+1}(x)$ as

$$V(x) = \sum_{j=0}^{N} V_{j,j+1}(x), \tag{5}$$

where we have defined

$$V_{j,j+1}(x) = \begin{cases} V(x), & x \in (x_j, x_{j+1}), \\ 0, & x \notin (x_j, x_{j+1}). \end{cases}$$

Let $\mathbf{S}_{j,j+1}(k)$ denote the scattering matrix associated with the potential $V_{j,j+1}(x)$; in analogy with (2) we have

$$\mathbf{S}_{j,j+1}(k) = \begin{bmatrix} T_{j,j+1}(k) & R_{j,j+1}(k) \\ L_{j,j+1}(k) & T_{j,j+1}(k) \end{bmatrix},$$

where $T_{j,j+1}(k)$ is the transmission coefficient and $R_{j,j+1}(k)$ and $L_{j,j+1}(k)$ are the reflection coefficients from the right and from the left, respectively, corresponding to the potential $V_{j,j+1}(x)$. It is known [6] that $\mathbf{S}(k)$ can be written explicitly in terms of $\mathbf{S}_{j,j+1}(k)$ in the form of the matrix product

$$\Lambda(k) = \Lambda_{0,1}(k)\,\Lambda_{1,2}(k)\,\cdots\,\Lambda_{N,N+1}(k), \tag{6}$$

where

$$\Lambda(k) = \begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(-k)} \end{bmatrix}, \qquad \Lambda_{j,j+1}(k) = \begin{bmatrix} \dfrac{1}{T_{j,j+1}(k)} & -\dfrac{R_{j,j+1}(k)}{T_{j,j+1}(k)} \\ \dfrac{L_{j,j+1}(k)}{T_{j,j+1}(k)} & \dfrac{1}{T_{j,j+1}(-k)} \end{bmatrix}.$$

In the special case $N = 2$, from the factorization formula (6), with the help of (3), we obtain

$$\frac{1}{T(k)} = \frac{1 - R_{0,1}(k)\,L_{1,2}(k)}{T_{0,1}(k)\,T_{1,2}(k)}, \qquad \frac{1}{T_{1,2}(k)} = \frac{1 - L_{0,1}(-k)\,L(k)}{T_{0,1}(-k)\,T(k)}. \tag{7}$$

The following proposition shows that a potential is necessarily exceptional if both of its two fragments are exceptional, and that it is necessarily generic if one fragment is exceptional and the other is generic.

Proposition Consider the potential $V(x)$ given in (5). If all the fragments are exceptional, then $V(x)$ is exceptional. In the special case $N = 2$, if one fragment is generic and the other is exceptional, then $V(x)$ is generic; if both fragments are generic then $V(x)$ can be either generic or exceptional. For $N \geq 3$, if at least one of the fragments is generic, then $V(x)$ can be either generic or exceptional.

PROOF: We can omit trivial fragments in the summation (5) and assume that none of $V_{j,j+1}(x)$ are identically zero. For $N = 2$ from (7) we see that if neither of $T_{0,1}(k)$ and $T_{1,2}(k)$ vanish at $k = 0$, then the transmission coefficient $T(k)$ corresponding to $V(x)$

cannot vanish at $k = 0$. Using induction, it then follows that if none of the transmission coefficients corresponding to $V_{j,j+1}(x)$ vanish at $k = 0$, then the transmission coefficient corresponding to $V(x)$ cannot vanish at $k = 0$, i.e. if all $V_{j,j+1}(x)$ are exceptional, then $V(x)$ is also exceptional. When $N = 2$, from (7) it follows that, if $T(0) \neq 0$ and $T_{0,1}(0) \neq 0$, we must have $T_{1,2}(0) \neq 0$. Consequently, if both $V_{0,1}(x)$ and $V(x)$ are exceptional, $V_{1,2}(x)$ has to be exceptional. A similar argument shows that if $T(0) \neq 0$ and $T_{1,2}(0) \neq 0$, we must have $T_{0,1}(0) \neq 0$. Hence, if one fragment is generic and the other is exceptional, the total potential must be generic. The example given below shows that if both fragments are generic then the total potential can be generic or exceptional. Through induction, we then obtain the result that, for $N \geq 3$, if at least one of $V_{j,j+1}(x)$ is generic, then $V(x)$ can be generic or exceptional. ∎

The next example shows that in the factorization formula, if both of the fragments of $V(x)$ are generic, then $V(x)$ can be generic or exceptional.

Example Let $\theta(x)$ denote the Heaviside function, i.e. $\theta(x) = 1$ if $x > 0$ and $\theta(x) = 0$ if $x < 0$. Assume

$$V_{0,1}(x) = \frac{-4e^{\sqrt{2}x}}{(1+e^{\sqrt{2}x})^2}\theta(-x), \qquad V_{1,2}(x) = \frac{-4e^{-\sqrt{2}x}}{(1+e^{-\sqrt{2}x})^2}\theta(x).$$

Both $V_{0,1}(x)$ and $V_{1,2}(x)$ are generic, and in fact we have

$$T_{0,1}(k) = T_{1,2}(k) = \frac{k(k+i/\sqrt{2})}{k^2+1/4}, \qquad R_{0,1}(k) = L_{1,2}(k) = \frac{-1}{4k^2+1}.$$

Note that corresponding to $V(x) = V_{0,1}(x) + V_{1,2}(x)$ we have

$$T(k) = \frac{k+i/\sqrt{2}}{k-i/\sqrt{2}}, \qquad R(k) = 0,$$

which is an exceptional potential. On the other hand, let

$$V_{0,1}(x) = \frac{u(x)}{v(x)^2}\theta(-x), \qquad V_{1,2}(x) = \frac{-e^{-\sqrt{2}x}}{(1+e^{-\sqrt{2}x}/4)^2}\theta(x), \tag{8}$$

both of which are generic with the transmission coefficients

$$T_{0,1}(k) = \frac{50k(k+i)(\sqrt{2}k+i)}{50\sqrt{2}k^3+70ik^2+13\sqrt{2}k+31i}, \qquad T_{1,2}(k) = \frac{25k(\sqrt{2}k+i)}{25\sqrt{2}k^2+15ik+4\sqrt{2}}.$$

In (8) the quantities $u(x)$ and $v(x)$ are given by

$$u(x) = 8\left[4(3+2\sqrt{2})e^{\sqrt{2}x} - 64e^{2x} + 8e^{(2+\sqrt{2})x} - e^{(2+2\sqrt{2})x} + 4(3-2\sqrt{2})e^{(4+\sqrt{2})x}\right],$$

$$v(x) = 8 + 8e^{2x} - (3+2\sqrt{2})e^{\sqrt{2}x} - (3-2\sqrt{2})e^{(2+2\sqrt{2})x}.$$

The sum $V(x) = V_{0,1}(x) + V_{1,2}(x)$ is a generic potential with scattering coefficients

$$T(k) = \frac{2k(k+i)}{2k^2+1}, \qquad R(k) = \frac{-1}{2k^2+1}.$$

By a trivial potential we mean a potential that vanishes almost everywhere. The next theorem shows that any nontrivial potential, generic or exceptional, can be decomposed, in an infinite number of ways, as in (5), where all the fragments are generic.

Theorem Any nontrivial potential, generic or exceptional, can be fragmented such that all the pieces are generic. There are infinitely many ways of fragmenting a given potential into generic pieces.

PROOF: Consider any fragmentation (5). Since trivial fragments can be omitted from (5), we can assume that none of the fragments of $V(x)$ vanish identically. If any one of the fragments is exceptional, we can fragment that piece further into two generic subpieces as follows. Assume the piece $V_{j,j+1}(x)$ is exceptional. Let $f_{l;j,j+1}(k,x)$ be the corresponding Jost solution from the left. From (4) we have

$$\int_{x_j}^{x_{j+1}} dx\, V_{j,j+1}(x)\, f_{l;j,j+1}(0,x) = 0. \tag{9}$$

Then for any $z \in (x_j, x_{j+1})$, consider the fragmentation of $V_{j,j+1}(x)$ as

$$V_{j,j+1}(x) = \theta(z - x_j)\, V_{j,j+1}(x) + \theta(x_{j+1} - z)\, V_{j,j+1}(x). \tag{10}$$

There are infinitely many such z. The fragments given in (10) have to be generic for almost every $z \in (x_j, x_{j+1})$; otherwise, as seen by replacing the upper integration limit in (9) by z, we could conclude that $V_{j,j+1}(z)\, f_{l;j,j+1}(0,z) = 0$, which cannot happen unless $V_{j,j+1}(x)$ is almost everywhere zero. ∎

The fragmentation of an exceptional potential into two generic pieces has important consequences in scattering, inverse scattering, and wave propagation, where the governing equations are related to the Schrödinger equation or its variants. One such differential equation is given by

$$\frac{d^2\psi(k,x)}{dx^2}+\frac{k^2}{c(x)^2}\,\psi(k,x)=Q(x)\,\psi(k,x), \tag{11}$$

or its time domain equivalent

$$\frac{\partial^2\phi(t,x)}{\partial^2 x}-\frac{1}{c(x)^2}\frac{\partial^2\phi(t,x)}{\partial^2 t}=Q(x)\,\phi(t,x). \tag{12}$$

These equations describe the quantum mechanical behavior of a particle when the potential also depends on the particle's energy. They also describe the propagation of waves in a one-dimensional nonhomogeneous, nonabsorptive medium where the wavespeed is $c(x)$ and the restoring force density is $Q(x)$. These equations can be analyzed by transforming them into (1) through local Liouville transformations [7]. In the special (but still significant) case $Q(x)=0$, the potential in the transformed Schrödinger equation is always exceptional. One important outcome of the theorem given here is that it is possible to choose all the local Liouville transformations in such a way that all the resulting fragments of the transformed Schrödinger equation are generic. This should offer drastic simplifications in the analysis of (11) and (12).

As an illustrative example, consider (3.25) of Ref. [7] where the Jost solutions and their space derivatives are expressed as a product of matrices, each of which is expressed in terms of the quantities related to one fragment only; in that reference the problem of the recovery of the wavespeed from the scattering data is considered when the properties of the medium change abruptly at a finite number of interfaces. Some of the multiplicative matrices in (3.25) of Ref. [7] contain the factor $\dfrac{T(k)}{2ik}$. By fragmenting the exceptional pieces into generic ones, it becomes obvious that the Jost solutions and their space derivatives are continuous at $k=0$; this result is difficult to obtain without fragmenting an exceptional potential into two generic pieces. With the use of the results presented here, we expect a simplification of many proofs involving exceptional potentials for the Schrödinger equation and the wave equation with variable speed.

The results presented here are also valid if we allow the potential $V(x)$ to contain a finite number of Dirac delta functions. In fact, when delta functions are included, our theorem can be extended even to include trivial potentials. We will now elaborate on the inclusion of delta function potentials.

The factorization formula (6) remains unchanged if some or all the fragments of potential are delta functions. The potential $V(x) = \alpha\delta(x-a)$ corresponds to

$$T(k) = \frac{k}{k+i\alpha/2}, \qquad R(k) = \frac{-i\alpha/2}{k+i\alpha/2}e^{2ika}, \qquad L(k) = \frac{-i\alpha/2}{k+i\alpha/2}e^{-2ika}. \tag{13}$$

Note that a delta function potential is always generic. Since the support of a delta function potential is a point, it is possible to decompose $\alpha\delta(x-a)$ in an arbitrary manner in the form $V(x) = \sum_{j=1}^N V_j(x)$, where $V_j(x) = \alpha_j\delta(x-a)$ in such a way that $\sum_{j=1}^N \alpha_j = \alpha$. Using (6) and (13) we obtain

$$\frac{1}{k}\begin{bmatrix} k+\frac{i}{2}\alpha & \frac{i}{2}\alpha e^{2ika} \\ -\frac{i}{2}\alpha e^{-2ika} & k-\frac{i}{2}\alpha \end{bmatrix} = \frac{1}{k^N}\prod_{j=1}^N \begin{bmatrix} k+\frac{i}{2}\alpha_j & \frac{i}{2}\alpha_j e^{2ika} \\ -\frac{i}{2}\alpha_j e^{-2ika} & k-\frac{i}{2}\alpha_j \end{bmatrix}, \tag{14}$$

where the matrix product is commutative. We can write (14) in the equivalent form

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{i\alpha}{2k}\begin{bmatrix} 1 & e^{2ika} \\ -e^{-2ika} & 1 \end{bmatrix} = \frac{1}{k^N}\prod_{j=1}^N \begin{bmatrix} k+\frac{i}{2}\alpha_j & \frac{i}{2}\alpha_j e^{2ika} \\ -\frac{i}{2}\alpha_j e^{-2ika} & k-\frac{i}{2}\alpha_j \end{bmatrix},$$

which holds for any positive integer N, $a \in \mathbf{R}$, and real numbers $\alpha_1, \cdots, \alpha_N$ with sum α.

We can write the zero potential, which is an exceptional potential with $T(k) = 1$, as the sum of two delta function potentials, which are always generic. Letting $V_1(x) = \alpha\,\delta(x-a)$ and $V_2(x) = -\alpha\,\delta(x-a)$, from (14) we obtain

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1+\frac{i\alpha}{2k} & \frac{i\alpha}{2k}e^{2ika} \\ -\frac{i\alpha}{2k}e^{-2ika} & 1-\frac{i\alpha}{2k} \end{bmatrix} \begin{bmatrix} 1-\frac{i\alpha}{2k} & \frac{-i\alpha}{2k}e^{2ika} \\ \frac{i\alpha}{2k}e^{-2ika} & 1+\frac{i\alpha}{2k} \end{bmatrix}. \tag{15}$$

We can generalize (15) to

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \prod_{j=1}^N \begin{bmatrix} 1+\frac{i\alpha_j}{2k} & \frac{i\alpha_j}{2k}e^{2ika} \\ -\frac{i\alpha_j}{2k}e^{-2ika} & 1-\frac{i\alpha_j}{2k} \end{bmatrix} \qquad \text{if} \quad \sum_{j=1}^N \alpha_j = 0,$$

where N is an arbitrary natural number, a is an arbitrary real number, and α_j are arbitrary real numbers satisfying $\sum_{j=1}^{N} \alpha_j = 0$. Thus, when delta function potentials are included, the theorem presented becomes true even for the trivial potential: the zero potential can be fragmented into delta function potentials in an infinite number of ways.

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