Bound states and inverse scattering for the Schrödinger equation in one dimension

Tuncay Aktosun
Department of Mathematics, North Dakota State University, Fargo, North Dakota 58105

(Received 18 April 1994; accepted for publication 10 July 1994)

The one-dimensional Schrödinger equation is considered when the potential and its first moment are absolutely integrable. When the potential has support contained on the left (right) half-line, it is uniquely constructed by using only the reflection coefficient from the right (left). The bound state norming constants determine whether the potential has support contained on a half-line or on the full-line. The bound state energies and the unique set of norming constants yielding the potential with support contained on the left (right) half-line are completely determined by the reflection coefficient from the right (left). An explicit example is provided. © *1994 American Institute of Physics.*

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. When the potential vanishes as $x\to\pm\infty$ in some sense (the absolute integrability of the potential is sufficient for this purpose), there are two linearly independent solutions $\psi_l(k,x)$ and $\psi_r(k,x)$ of Eq. (1) known as the physical solutions satisfying the boundary conditions

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

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

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 Eq. (1) is defined as

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

and it satisfies $\mathbf{S}(-k)=\mathbf{S}(k)^*$, where the superscript $*$ denotes the complex conjugation. Due to the unitarity of $\mathbf{S}(k)$, we also have $R(k)T(-k)+L(-k)T(k)=0$.

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 $j=0,\dots,N$. We can then write $V(x)$ in terms of its fragments $V_{j,j+1}(x)$, using

$$V(x)=\sum_{j=0}^{N} V_{j,j+1}(x), \tag{3}$$

where we have defined

0022-2488/94/35(12)/6231/6/$6.00
J. Math. Phys. **35** (12), December 1994

$$V_{j,j+1}(x)=\begin{cases} V(x), & x\in(x_j,x_{j+1}),\\ 0, & x\notin(x_j,x_{j+1}). \end{cases} \tag{4}$$

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

$$\mathbf{S}_{j,j+1}(k)=\begin{bmatrix} T_{j,j+1}(k) & R_{j,j+1}(k)\\ L_{j,j+1}(k) & T_{j,j+1}(k)\end{bmatrix}, \tag{5}$$

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 already known[1] that $\mathbf{S}(k)$ can be written explicitly in terms of $\mathbf{S}_{j,j+1}(k)$ in the form of matrix product

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

where

$$\Lambda(k)=\begin{bmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)}\\[2mm] \dfrac{L(k)}{T(k)} & \dfrac{1}{T(-k)}\end{bmatrix},\quad \Lambda_{j,j+1}(k)=\begin{bmatrix} \dfrac{1}{T_{j,j+1}(k)} & -\dfrac{R_{j,j+1}(k)}{T_{j,j+1}(k)}\\[2mm] \dfrac{L_{j,j+1}(k)}{T_{j,j+1}(k)} & \dfrac{1}{T_{j,j+1}(-k)}\end{bmatrix}.$$

The bound states associated with $V(x)$ correspond to the square-integrable solutions of Eq. (1), and such solutions can occur only at certain discrete negative energies $k^2 = -\beta_1^2,\ldots,-\beta_{\mathcal{N}}^2$, where β_j are distinct and $\beta_j>0$ for $j=1,\ldots,\mathcal{N}$ and $\mathcal{N}$ is the number of bound states. For each fixed x, the physical solutions have meromorphic extensions in k to the upper half complex plane $\mathbf{C}^+$. At the bound states, the physical solutions of Eq. (1) become linearly dependent, and the ratio $c_j=\psi_r(i\beta_j,x)/\psi_l(i\beta_j,x)$ is a positive constant known as the norming constant associated with the bound state of energy $-\beta_j^2$. It was discovered by Levinson[2] that a potential with bound states cannot be determined uniquely from its scattering matrix and the bound state energies; the bound state norming constants must be specified separately in order to uniquely determine the potential from its reflection coefficient and bound state energies. It is already known[3–6] that a reflection coefficient, the bound state energies, and the bound state norming constants uniquely determine a potential in $L_1^1(\mathbf{R})$; here $L_1^1(\mathbf{R})$ denotes the class of potentials satisfying $\int_{-\infty}^{\infty}(1+|x|)|V(x)|dx<+\infty$, i.e., the class of potentials such that the potential and its first moment are absolutely integrable.

The question whether a unique potential can be obtained in a restrictive class when less information is known *a priori* was first discussed by R. G. Newton. For the radial Schrödinger equation, Newton[7] observed that if there is one potential with given phase shift and bound state energies and exponentially decaying at infinity with decay rate faster than twice the square root of the absolute value of the ground state energy, then this potential is the only one with that property.

It was recently discovered[8–10] that the bound state norming constants can be obtained from the scattering matrix $\mathbf{S}(k)$ if the corresponding potential vanishes for $x<a$ or for $x>b$ for some real numbers a and b, i.e., if the potential has support contained on a half-line. When the inverse scattering problem of recovery of $V(x)$ in Eq. (1) is transformed from the frequency domain into the time domain, it is now possible to understand why the bound state norming constants are not needed in the time domain in the recovery if the support of the potential is contained on a half-line. A surprising consequence of this discovery is the following: although each scattering matrix $\mathbf{S}_{j,j+1}(k)$ in Eq. (5) uniquely determines all the bound state norming constants related to the potential $V_{j,j+1}(x)$ in Eq. (4), none of the bound state norming constants associated with $V(x)$

in Eq. (3) are determined by $\mathbf{S}(k)$ in Eq. (2) unless the support of $V(x)$ is contained on a half-line. We now see that it is better to state Levinson's result as follows: a potential whose support is on the whole line cannot be determined from its reflection coefficient and the bound state energies alone; the bound state norming constants for a potential with support contained on a half-line are fixed by the reflection coefficient and the bound state energies. In fact, we will show that for a potential with support contained on the left (right) line, the reflection coefficient from the right (left) alone determines the bound state energies and hence determines also the bound state norming constants. The reflection coefficient from the right (left) alone cannot determine the bound state energies for a potential with support contained on the right (left) line; however, in practice, in the recovery of a potential with support contained on the left (right) line, it is more appropriate to use the reflection coefficient from the right (left) because the measuring instruments are expected to be placed outside the potential being probed.

We will now show that the reflection coefficient from the right (left) alone is sufficient to construct a potential with support contained on the left (right) half line. Without loss of generality, we can assume that $V(x)=0$ for $x>b$. Let $\overline{\mathbf{C}^+} = \mathbf{C}^+ \cup \mathbf{R}$. Then[8] $R(k)/T(k)$ can be extended from the real axis $\mathbf{R}$ to $\mathbf{C}^+$ in an analytic manner and $R(k)e^{2ikx}/T(k) \to 0$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$ for $x \geqslant b$. The poles of $T(k)$ in $\mathbf{C}^+$ correspond to the bound states;[3-6] since $R(k)/T(k)$ is analytic in $\mathbf{C}^+$ and cannot vanish at the bound states, the poles of $R(k)$ and those of $T(k)$ must coincide. Thus, the bound state energies are obtained from $R(k)$; from the reflection coefficient and the bound state energies one can construct the transmission coefficient by using[4]

$$T(k)=\left(\prod_{j=1}^{\cdot l \cdot} \frac{k+i\beta_j}{k-i\beta_j} \right) \exp \left(\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\log(1-|R(\omega)|^2)}{\omega-k-i0}\, d\omega \right). \tag{7}$$

The bound state norming constant corresponding to $k=i\beta_j$ is given by[8] $c_j=(R/T)(i\beta_j)$. Alternatively, c_j can be expressed using only the values of scattering coefficients for real values of k via

$$c_j=\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{k}{k+i0} \frac{R(k)}{T(k)} e^{2ikx+2\beta_j x} \frac{dk}{k-i\beta_j}, \quad x \geqslant b. \tag{8}$$

One can then use the Marchenko method[3-6,11] or one of the other methods[4,5,8,11] of inverse scattering to obtain the potential uniquely. Define

$$m_l(k,x)=e^{-ikx}\psi_l(k,x)/T(k), \quad m_r(k,x)=e^{ikx}\psi_r(k,x)/T(k),$$

$$B_l(x,y)=\frac{1}{2\pi} \int_{-\infty}^{\infty} [m_l(k,x)-1]e^{-iky}\, dk.$$

The potential is then given by[3-8,11] $V(x)=-2(d/dx)B_l(x,0+)$.

From (3.13) of Ref. 12, we have

$$B_l(x,y)=\frac{1}{2\pi} \int_{-\infty}^{\infty} ([T(k)-1]e^{iky}m_r(k,x)-R(k)e^{2ikx+iky}m_l(k,x))dk. \tag{9}$$

If $V(x)=0$ for $x>b$, we have $m_l(k,x)=1$ for $x \geqslant b$. Using[3-8,11] the analyticity of $m_l(k,x)$ in $k \in \mathbf{C}^+$, $m_r(i\beta_j,x) = c_j e^{-2\beta_j x} m_l(i\beta_j,x)$, and $m_l(k,x) \to 1$ for each $x \in \mathbf{R}$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$, from Eq. (9) we obtain

$$B_l(x,0+)=i\sum_{j=1}^{\cdot l \cdot} e^{-2\beta_j x}[\mathrm{Res}_{k=i\beta_j} T(k)][c_j-(R/T)(i\beta_j)], \quad x>b,$$

where Res denotes the residue. Since $\beta_1,...,\beta_{\mathcal{N}}$ are distinct, $e^{-2\beta_j x}$ for $j=1,...,\mathcal{N}$ are linearly independent; hence we must have $c_j=(R/T)(i\beta_j)$. Conversely, assume that $c_j=(R/T)(i\beta_j)$, $R(k)/T(k)$ has analytic extension to $\mathbf{C}^+$, and $R(k)e^{2ikx}/T(k)\to 0$ as $k\to\infty$ in $\overline{\mathbf{C}^+}$ for $x\geqslant b$. From Eq. (9) we then obtain $B_l(x,y)=0$ for $x\geqslant b$, and hence $V(x)=0$ for $x>b$. We have thus shown that the potential has support contained on the left half-line if and only if the bound state norming constants are chosen as in Eq. (8). Note that it is already known that nontrivial potentials corresponding to zero reflection coefficient cannot have support contained on a half-line, and hence such potentials need not be considered here.

The function $f_l(k,x)=\psi_l(k,x)/T(k)$ is known as the Jost solution of Eq. (1). Instead of the norming constants c_j, one can use $\kappa_j=[\int_{-\infty}^{\infty}f_l(i\beta_j,x)^2dx]^{-1}$ as norming constants; these are related to each other as[6,8]

$$c_j=i\kappa_j\left[\frac{d}{dk}\left(\frac{1}{T(k)}\right)\right]_{k=i\beta_j}.$$

In the Marchenko theory, $B_l(x,y)$ is obtained from the integral equation[3–8,11]

$$B_l(x,y)=\Omega_l(x,y)+\int_0^\infty \Omega_l(x,y+z)B_l(x,z)dz, \tag{10}$$

where

$$\Omega_l(x,y)=-\frac{1}{2\pi}\int_{-\infty}^{\infty}R(k)e^{2ikx+iky}\,dk-\sum_{j=1}^{\mathcal{N}}\kappa_j^2e^{-2\beta_j x-\beta_j y}, \tag{11}$$

and it is known[3–8,11] that Eq. (10) is uniquely solvable for $B_l(x,y)$. Hence, we have shown that knowing only $R(k)$, one can construct $\Omega_l(x,y)$ defined in Eq. (11) using the bound state norming constants as in Eq. (8) and construct the potential with support on the left half-line from the unique solution of Eq. (10). Note that the value of b is not used in the construction of the bound state norming constants and that for the construction of the potential it is sufficient to know the reflection coefficient only at real values of k. In fact, the value of b itself is constructed during the construction of the potential. One can also obtain b directly as

$$b=\inf\left\{x\in\mathbf{R}: \frac{R(k)}{T(k)}\,e^{2ikx}\to 0 \quad \text{as} \quad k\to\infty \quad \text{in} \quad \overline{\mathbf{C}^+}\right\}.$$

If one chooses c_j not as in Eq. (8), then the potential constructed will not have support contained on a half-line.

We can restate our result as in the following theorem.

Theorem: For a given reflection coefficient $R(k)$ there exists at most one potential in $L_1^1(\mathbf{R})$ with support on the left half-line. If such a potential exists, its bound states are the poles of the analytic continuation of $R(k)$ in the upper half plane, and the norming constants are given by Eq. (8).

The procedure outlined above can be illustrated with a simple example. Let us use $R(k)=-1/(2k^2+1)$ for $k\in\mathbf{R}$ with one bound state at energy $k^2=-1/2$. From Eq. (7) we obtain $T(k)=2k(k+i)/(2k^2+1)$. The potential constructed via the Marchenko method will have support contained on the half-line if and only if the norming constant c is chosen as $c=\sqrt{2}-1$, which is the value obtained from Eq. (8). Any other value of c leads to a potential with support on the whole line. In fact we have

$$V(x)=\begin{cases}\dfrac{[1-(\sqrt{2}+1)c]e^{-\sqrt{2}x}}{(1-\frac{1}{4}[1-(\sqrt{2}+1)c]e^{-\sqrt{2}x})^2}, & x>0,\\ \dfrac{d}{dx}\left[\dfrac{W_1(x)}{W_2(x)}\right], & x<0,\end{cases}\tag{12}$$

where

$$W_1(x)=e^{2x}\left[\frac{1}{c}[c-(\sqrt{2}-1)]e^{\sqrt{2}x}-4\right]+\frac{(\sqrt{2}+1)^2}{\sqrt{2}c}[1-(\sqrt{2}-1)^2e^{2x}][c-(\sqrt{2}-1)]e^{\sqrt{2}x},$$

$$W_2(x)=(1+e^{2x})\left[1-\frac{1}{4c}(\sqrt{2}+1)^2[c-(\sqrt{2}-1)]e^{\sqrt{2}x}\right]+\frac{\sqrt{2}}{c}[c-(\sqrt{2}-1)]e^{\sqrt{2}x+2x}.$$

For $c=\sqrt{2}-1$, from Eq. (12) we obtain

$$V(x)=\begin{cases}0, & x>0,\\ \dfrac{-8e^{2x}}{(1+e^{2x})^2}, & x<0,\end{cases}\tag{13}$$

and hence we see that $b=0$ in this case.

It is interesting to consider the fragments of the potential in Eq. (12). Let $V_1(x)=\theta(-x)V(x)$ and $V_2(x)=\theta(x)V(x)$, where $\theta(x)$ is the Heaviside function. Let $T_1(k)$ and $T_2(k)$ be the corresponding transmission coefficients for $V_1(x)$ and $V_2(x)$, respectively, $R_1(k)$ be the reflection coefficient from the right for $V_1(x)$ and $L_2(k)$ be the reflection coefficient from the left for $V_2(x)$. With the help of Eq. (6) we have

$$R_1(k)=\frac{1}{D_1(k)}\left[i\,\frac{(\sqrt{2}+1)^2c^2-18(\sqrt{2}+1)c+1}{2\sqrt{2}[3+(\sqrt{2}+1)c]^2}-k\,\frac{(\sqrt{2}+1)^2c^2+14(\sqrt{2}+1)c+1}{2[3+(\sqrt{2}+1)c]^2}\right],$$

$$T_1(k)=\frac{1}{D_1(k)}[k(k+i)(k+i/\sqrt{2})],\quad L_2(k)=\frac{1}{D_2(k)}\left[4\,\frac{1-(\sqrt{2}+1)c}{[3+(\sqrt{2}+1)c]^2}\right],$$

$$T_2(k)=\frac{1}{D_2(k)}[k(k+i/\sqrt{2})],$$

where

$$D_1(k)=k^3+\frac{ik^2}{\sqrt{2}}\,\frac{1+3(\sqrt{2}+1)c}{3+(\sqrt{2}+1)c}+\frac{k}{2}\,\frac{-3(\sqrt{2}+1)^2c^2+6(\sqrt{2}+1)c+13}{[3+(\sqrt{2}+1)c]^2}$$
$$-\frac{i}{2\sqrt{2}}\,\frac{(\sqrt{2}+1)^2c^2-18(\sqrt{2}+1)c+1}{[3+(\sqrt{2}+1)c]^2},$$

$$D_2(k)=k^2+\frac{ik}{\sqrt{2}}\,\frac{5-(\sqrt{2}+1)c}{3+(\sqrt{2}+1)c}-4\,\frac{1-(\sqrt{2}+1)c}{[3+(\sqrt{2}+1)c]^2}.$$

The poles of the transmission coefficients on the imaginary axis in $\mathbf{C}^+$ correspond to the bound states. When $0<c\leqslant\sqrt{2}-1$, $T_2(k)$ does not have poles in $\mathbf{C}^+$, and when $c>\sqrt{2}-1$, $T_2(k)$ has exactly one pole in $\mathbf{C}^+$; hence $V_2(x)$ has no bound states for $0<c\leqslant\sqrt{2}-1$ and exactly one bound

state for $c>\sqrt{2}-1$. When $c=\sqrt{2}-1$, we have $T_2(k)=1$; hence $T_2(k)$ does not vanish at $k=0$ if $c=\sqrt{2}-1$, otherwise $T_2(k)$ vanishes linearly at $k=0$. In other words, for $c=\sqrt{2}-1$ we have the exceptional case, otherwise we have the generic case.[3-8,11] Let $\xi_\pm = (9 \pm 4\sqrt{5})(\sqrt{2}-1)$. When $0<c<\xi_-$, $T_1(k)$ has exactly two poles in $\mathbf{C}^+$ and hence $V_1(x)$ supports exactly two bound states. When $\xi_- \leqslant c < \xi_+$, $T_1(k)$ has exactly one pole in $\mathbf{C}^+$ and hence $V_1(x)$ supports exactly one bound state. When $c \geqslant \xi_+$, $T_1(k)$ does not have any poles in $\mathbf{C}^+$ and hence $V_1(x)$ does not have any bound states. When $c=\xi_\pm$, $T_1(k)$ does not vanish at $k=0$; otherwise it vanishes linearly at $k=0$. Hence, for $V_1(x)$ we have the exceptional case for $c=\xi_\pm$ and the generic case for $c\neq\xi_\pm$. On the other hand, $V_1(x)+V_2(x)$ given in Eq. (12) always supports exactly one bound state independently of the value of c, and its transmission coefficient always vanishes linearly at $k=0$ and thus always corresponds to the generic case.

ACKNOWLEDGMENTS

The research leading to this article was supported in part by the National Science Foundation under Grant No. DMS-9217627. The author is indebted to Roger Newton, Paul Sacks, and Ricardo Weder for their comments.

[1] T. Aktosun, J. Math. Phys. **33**, 3865 (1992).
[2] N. Levinson, Kgl. Danske Viden. Sels. Mat. Fys. Medd. **25**, 1 (1949).
[3] L. D. Faddeev, Am. Math. Soc. Transl. **2**, 139 (1964).
[4] P. Deift and E. Trubowitz, Commun. Pure Appl. Math. **32**, 121 (1979).
[5] R. G. Newton, J. Math. Phys. **21**, 493 (1980).
[6] V. A. Marchenko, *Sturm-Liouville Operators and Applications* (Birkhäuser, Basel, 1986).
[7] R. G. Newton, Phys. Rev. **101**, 1588 (1956).
[8] T. Aktosun, M. Klaus, and C. van der Mee, J. Math. Phys. **34**, 2651 (1993).
[9] W. Rundell and P. E. Sacks, "On the determination of potentials without bound state data," J. Comput. Appl. Math. (to appear, 1994).
[10] B. Grebert and R. Weder, "Reconstruction of a potential on the line that is a priori known on the half line," SIAM J. Appl. Math. (to appear, 1994).
[11] K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory*, 2nd ed. (Springer-Verlag, New York, 1989).
[12] T. Aktosun, M. Klaus, and C. van der Mee, Integr. Eqs. Oper. Theor. **15**, 879 (1992).