Levinson's Theorem and Bound States in the Continuum

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Abstract

As is well known, the use of nonlocal potentials in the description of many particle systems is an attempt to account for the suppression of degrees of freedom by an effective equation for the relative motion of two particles. Furthermore, such potentials are useful in creating phase-equivalent potentials for the study of nucleon- nucleus and nucleus- nucleus scattering and cluster models of light nuclei. These potentials can support positive energy bound states, that is, states embedded in the continuous energy spectrum. There is some controversy in the literature on how such bound states are to be included in Levinson's theorem, that is, should the phase shift be taken continuous at the energy of the bound state or should one introduce a discontinuity of π. This paper examines this issue and gives a general expression for the phase shift.

1 Introduction

Levinson's theorem states that

$$\delta(0) = \pi(n + q/2) \tag{1}$$

where the phase shift $\delta(k)$ is evaluated at zero momentum, n is the number of bound states, and q is either 1 nor 0 depending on whether or not a "half bound" state exists. There has been some disagreement in the literature on the application of this theorem to the case of nonlocal potentials which support bound states with energy embedded in the continuous spectrum. Bolsterli [1] suggests that a jump of π should be added to the phase shift at the energy of the bound state whereas Newton [2] states that the phase shift should be taken continuous. The following analysis confirms Newton's analysis and gives a specific expression for the phase shift in the general case that includes a local potential.

The analysis is restricted to the radial s wave Schrödinger equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\Psi(r) + V(r)\Psi(r) + \int_0^\infty U(r,r')\Psi(r')\,\mathrm{d}r' = k^2\Psi(r), \tag{2}$$

where $\hbar = 2m = 1$ and $E = k^2$.

The nonlocal potential is taken to be separable,

$$U(r,r') = \sum g_i\, v_i(r)\, v_i(r'), \tag{3}$$

where $v_i(r)$ are real and well behaved, and the g_i are real constants, positive or negative. These conditions ensure that the hamiltonian is hermitian. Only one term in the sum will be used in the following analysis; the results are easily generalized.

The physical solution of Eq. (1) is defined by the mixed boundary conditions

$$\Psi(0,k) = 0 \tag{4a}$$

and

$$\Psi(r,k) \underset{r\to\infty}{\longrightarrow} \frac{1}{2}\,\mathrm{i}\left[e^{-\mathrm{i}kr} - S(k)e^{\mathrm{i}kr}\right], \tag{4b}$$

where $S(k)$ is the scattering matrix element which can be written in terms of the phase shift,

$$S(k) = e^{2\mathrm{i}\delta(k)}. \tag{5}$$

In these equations, k is taken to be real positive. The usual notation of a superscript "+" indicating the physical solution and the corresponding Green's function is not used here since there is little likelihood of confusion. In the following, the Fredholm determinant of the physical solution written as an integral equation is constructed. The zeros of this determinant give the energies of solutions to the homogeneous equation and these solutions, if normalizable, are bound states. In this introduction the local potential is taken to be zero.

The physical solution to the Schrödinger equation (2) is,

$$\Psi(k,r) = \sin kr + \int_0^\infty \mathrm{d}s\; K(r,s)\,\Psi(s,k), \tag{6}$$

where the kernel is

$$K(r,s) = g\,v(s)\int_0^\infty \mathrm{d}r'\; G(k,r,r')\,v(r'), \tag{7}$$

and the Green's function for the physical solution is

$$G(k,r,r') = -\frac{1}{k}\,e^{\mathrm{i}kr_>}\sin kr_< \;, \tag{8}$$

where $r_>$ indicates the larger of r and r' while $r_<$ denotes the smaller. For simplicity, the separable potential is taken to have only one term

$$U(r,r') = g\,v(r)\,v(r'). \tag{9}$$

Note that the integral for the kernel is convergent for $\mathrm{Im}\,k > 0$, that is, the solutions will be analytic in the upper half of the complex k-plane. If $v(r)$ is of finite range, the solutions will also be analytic functions of k in the lower half plane while if $v(r)$ is exponentially damping, the solutions will be analytic in a strip along the real k axis in the lower half plane.

The Fredholm determinant is easily found to be

$$\begin{aligned} D &= 1 - \int_0^\infty K(r,r)\,\mathrm{d}r \\ &= 1 - g\int_0^\infty v(r)\,\mathrm{d}r \int_0^\infty \mathrm{d}r'\; G(k,r,r')\,v(r'). \end{aligned} \tag{10}$$

Sine transforms are used to write this determinant in the momentum representation on the half line,

$$v(r) = \frac{2}{\pi}\int_0^\infty \tilde{v}(p)\,\sin pr\; p\,\mathrm{d}p, \tag{11}$$

and

$$\tilde{v}(p) = \int_0^\infty v(r)\,\frac{\sin pr}{p}\,\mathrm{d}r. \tag{12}$$

In doing the resulting integrals, it is assumed that k has a positive complex part so that the need for using distributions is avoided. The result is

$$D(k) = 1 + \frac{2g}{\pi}\int_0^\infty p^2\,\mathrm{d}p\;\frac{\tilde{v}^2(p)}{p^2 - k^2}\;, \tag{13}$$

which can be easily generalized to the sum of separable terms by replacing in the integrand,

$$g\,\tilde{v}^2(p) \Longrightarrow g_1\tilde{v}_1^2(p) + g_2\tilde{v}_2^2(p) + \ldots \tag{14}$$

The expression for the Fredholm determinant given in Eq. (13) is analytic in the upper half complex k-plane. To evaluate D for real momentum values, k is taken to approach the real positive axis from above. The result is,

$$D(k_0) = 1 + \frac{2g}{\pi}\,\wp\int_0^\infty p^2\,\mathrm{d}p\;\frac{\tilde{v}^2(p)}{p^2 - k_0^2}\;-\;g\,\mathrm{i}\,k_0\,\tilde{v}^2(k_0)\,, \tag{15}$$

where k_0 is real positive. The symbol $\wp$ indicates the Cauchy principal part. For the conjugate physical solution, k is taken to approach the negative real axis. To analytically continue $D(k)$ into the lower half plane, the path of integration is distorted around the simple pole at k as k is moved from the upper half plane to the lower. Finally the contour of integration is pinched off as k passes to the lower half plane. The result for D is exactly the same as given in Eq. (13) but with the addition of the residue at the pole:

$$D(k) = 1 + \frac{2g}{\pi} \int_0^\infty p^2\,\mathrm{d}p\, \frac{\tilde{v}^2(p)}{p^2 - k^2} \;+\; 2g\,\mathrm{i}\,k\,\tilde{v}^2(k)\,. \tag{16}$$

This last result is valid provided $v(r)$ has finite range or is exponentially damping for large r. It is not difficult to show that $D(k)$ given by Eq. (13) or the continuation given in Eq. (16) satisfies the condition,

$$D(k) = D^*(-k^*). \tag{17}$$

The condition for a solution to the homogeneous equation for real k is that the Fredholm determinant given in Eq. (15) is zero, that is,

$$1 + \frac{2g}{\pi}\, \wp \int_0^\infty p^2\,\mathrm{d}p\, \frac{\tilde{v}^2(p)}{p^2 - k_0^2} \;=\; 0 \tag{18a}$$

and

$$\tilde{v}^2(k_0) = 0. \tag{18b}$$

The solution for the homogeneous equation can be written,

$$\Psi(r, k_0) = C \int_0^\infty \sin k_0\xi\;\, v(\xi + r)\;\mathrm{d}\xi, \tag{19}$$

where C is a constant. It is apparent that if $v(r)$ is of finite range or decreases exponentially the solution will be normalizable. It can be shown that if $v(r)$ goes as $r^{-\alpha}$ then the wave function also goes as $r^{-\alpha}$. Thus if α is greater than $1/2$ the solution will be normalizable and thus represent a bound state with energy embedded in the continuous spectrum.

2 The Fredholm determinant and the phase shift

It is not difficult to show that the t matrix is proportional to the reciprocal of the Fredholm determinant and that the Jost function is proportional to the determinant [5] with a real proportionality factor [3]. Therefore, the phase shift can be taken to be negative the phase of $D(k)$, that is,

$$D(k) = \mid D(k) \mid e^{-\mathrm{i}\delta_D(k)}, \tag{20}$$

where the subscript denotes that the phase shift so defined has a discontinuity of π at k_0, the k_0 value associated with the bound state. This jump of π comes about because $D(k)$ goes through zero at k_0 where the real part changes sign but not the imaginary. But the S matrix element,

$$S(k) = \frac{D^*(k)}{D(k)} = e^{2\mathrm{i}\delta_D(k)}, \tag{21}$$

is continuous at k_0. There are no zeros for $D(k)$ in the upper half plane except possibly on the positive imaginary k axis. Such zeros correspond to conventional bound states with negative real energies. If the continuation to the lower half plane is possible then D given by Eq. (16) may have zeros there. In the rest of the analysis, it will be assumed that D has a zero at k_1. Then it follows from Eq. (17) that $D(k)$ has a zero at $-k_1^*$, symmetrically placed with respect to the imaginary axis, and furthermore for real k,

$$\delta(k) = -\delta(-k). \tag{22}$$

Suppose that the two zeros at k_1 and $-k_1^*$ can be moved around in the complex k-plane by varying the parameters of the potential. With the only zeros in the lower half plane, that is, no conventional bound states nor bound states in the continuum,

$$I = \int_{-\infty}^{\infty} \mathrm{d}\ln D(k) = \int_{-\infty}^{\infty} \frac{D'(k)}{D(k)}\;\mathrm{d}k = 0. \tag{23}$$

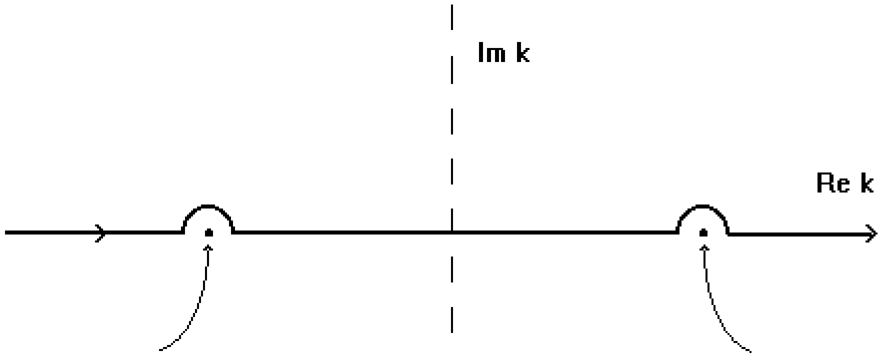

Figure 1: Path of integration for Levinson's theorem.

This is readily seen by closing the contour of integration by a large semi-circle in the upper half plane and letting the radius go to infinity. Doing the integral along the real axis and noting the definition of the phase shift in terms of $D(k)$, one obtains

$$\delta_{\mathrm{C}}(0) = 0 \tag{24}$$

where the phase shift for infinite wave number is taken to be zero. Since there are no zeros on the real axis, this phase shift is continuous. Imagine how the phase shift changes when k is real but is passing near a simple pole at k_1 due to the zero of D. The phase shift will increase sharply but continuously through π. This behavior of the phase shift is usually taken to indicate a resonance at $k \simeq \mathrm{Re}\ k_1$.

Now imagine that the parameters are varied such that the zeros approach the real axis from below as shown in figure 1. It should be noted that it is not possible to have the zero pop up into the upper half k-plane for Re $k > 0$ and still have an hermitian hamiltonian. The integral is again zero as can be seen by closing the contour by a large semi circle. Assuming that the zeros are simple. one obtains

$$I = \wp \int_{-\infty}^{\infty} \mathrm{d} \ln D(k) - 2\pi\mathrm{i} = 2\mathrm{i}\delta_{\mathrm{C}}(0) - 2\pi\mathrm{i} = 0. \tag{25}$$

The -2πi comes from the integration around the two semi-circles. The principal part defines a continuous phase shift so that in this case of a bound state with energy embedded in the continuum Levinson's theorem reads,

$$\delta_{\mathrm{C}}(0) = \pi, \tag{26}$$

where the phase shift is defined continuously. If the zero is of order m then

$$\delta_{\mathrm{C}}(0) = m\pi, \tag{27}$$

It may surprise one that the principal part defines a continuous phase shift since, for a simple pole at k_0 real, the integration from 0 to k_0 will give a logarithmic singularity. But one must remember to include the integration from $-k_0$ to zero which results in a cancellation of the logarithmic singularity and gives a continuous phase shift as k passes through k_0. These results are in agreement with those obtained by Newton [2].

3 General case

For the case in which a local potential exists, the Fredholm determinant is

$$D(k) = 1 - g \int \mathrm{d}r\, \mathrm{d}r'\, G(k, r, r')\, v(r)\, v(r'), \tag{28}$$

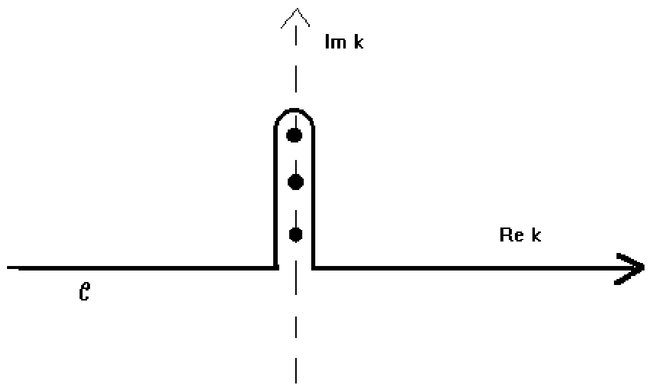

Figure 2: Integration contour for the completeness relation.

where the Green's function for the physical solution is

$$G(k,r,r') = -\frac{f(k,r_>)\varphi(k,r_<)}{\Im(k)} \ . \tag{29}$$

The Jost solution for the local potential is defined by its asymptotic form

$$f(k,r)) \underset{r\to\infty}{\longrightarrow} e^{\mathrm{i}kr}, \tag{30}$$

while the regular solution, $\varphi(k,r)$, is defined such that, at the origin, the function and its first derivative at the origin are zero and one respectively. The Jost function is defined in terms of the wronskian of these two solutions,

$$\Im(k) = W\left[f(k,r),\ \varphi(k,r)\right]. \tag{31}$$

This Jost function will have zeros on the imaginary axis in the upper half complex k-plane at the location of bound states of the local potential. The nonlocal potential can be expanded in terms of the Jost solution and the regular solution of the local potential by use of the completeness relation [4],

$$\int_{\mathcal{C}} \frac{k\mathrm{d}k\ \varphi(k,r)\,f(k,r')}{\Im(k)} = \mathrm{i}\pi\delta(r-r'), \tag{32}$$

where the contour $\mathcal{C}$ goes along the real k axis from minus infinity to plus infinity and over any zeros of $\Im(k)$ in the upper half plane (see figure 2). In this way the bound states are included in the expansion.

Using the completeness relation gives,

$$v(r) = \int_{\mathcal{C}} \frac{p\mathrm{d}p\ \varphi(p,r)\,\bar{v}(p)}{\Im(p)} \ , \tag{33}$$

where,

$$\bar{v}(r) = \frac{1}{\mathrm{i}\pi}\int_0^\infty v(r)\,f(p,r)\ \mathrm{d}r. \tag{34}$$

Substituting for $v(r)$ from Eq. (33) into $D(k)$ gives,

$$D(k) = 1 + g\int_{\mathcal{C}} \frac{p\mathrm{d}p}{\Im(p)}\ \frac{\bar{v}(p)\tilde{v}(p)}{p^2-k^2} \ , \tag{35}$$

where,

$$\tilde{v}(p) = \int_0^\infty v(r')\,\varphi(p,r')\ \mathrm{d}r. \tag{36}$$

To arrive at this result it is useful to use the relation,

$$\frac{\mathrm{d}}{\mathrm{d}r}\, W\left[\varphi(k_1,r),\ \psi(k_2,r)\right] = \frac{\varphi(k_1,r)\,\psi(k_2,r)}{k_1^2-k_2^2}\ , \tag{37}$$

valid for any solution of the Schrödinger equation for the local potential, regardless of boundary conditions.

For the particular case of no bound states this leads to

$$D(k) = 1 + \frac{2g}{\pi}\int_0^\infty \frac{p^2\mathrm{d}p\ \tilde{v}^2(p)}{(p^2-k^2)\ |\Im(p)|^2}\ , \tag{38}$$

as given in [6].

But $D(k)$ given in Eq. (35) cannot tell the whole story since for $v(r)=0$, $D(k)=1$. This appears to say there are no bound states even if the local potential supports a bound state. Examination of the t matrix [5] suggests that for the general case, one should take

$$\mathcal{D}(k) = \Im(k)\left\{1 + g\int_{\mathcal{C}} \frac{p\mathrm{d}p}{\Im(p)}\ \frac{\bar{v}(p)\tilde{v}(p)}{p^2-k^2}\right\} \tag{39}$$

as the general expression for determining the phase shift.

4 Example

For a simple example we suppose that $v(r)$ for the nonlocal potential is chosen to be the same as one of the bound states eigenfunctions of the local potential, say at $E=k_0^2<0$. Then the contour of integration for completeness reduces to a contour around the simple pole due to the zero of F at k_0. One obtains

$$\mathcal{D}(k) = \Im(k)\left\{1 + \frac{4\mathrm{i}gk_0^2\tilde{v}^2(k_0)}{\Im^*(k_0)\Im'(k_0)(k^2-k_0^2)}\right\}, \tag{40}$$

where the prime on $\Im$ denotes differentiation. This can be rewritten as

$$\mathcal{D}(k) = \Im(k)\left\{\frac{k^2+K^2-gN^2\tilde{v}^2(k_0)}{k^2+K^2}\right\}, \tag{41}$$

where

$$k_0 = \mathrm{i}K \tag{42}$$

with K real and positive, and N is the normalization of the regular solution of the local potential,

$$N^2\int \mathrm{d}r\,\varphi^2(k_0,r) = 1. \tag{43}$$

It is apparent that $\mathcal{D}(k)$ is not equal to zero at $k=\mathrm{i}K$. The zero now appears at

$$k^2 = -K^2 + gN^2\tilde{v}^2(k_0), \tag{44}$$

which, for a positive g large enough, gives an energy embedded in the continuous spectrum [7].

5 Discussion

In an actual experiment, the measurement of the phase shift for various wave numbers will be continuous since any jumps of π will not affect the cross section. It appears that there will be nothing in the phase shift that would signify the existence of a bound state with energy embedded in the continuous spectrum. The existence of the bound state, however, shows up in the modification of the phase shift at zero energy as described by Levinson's theorem. But if the system is perturbed such that the bound state can interact with other states, that is, the state becomes a resonance with a finite width, then the phase shift will change rapidly but continuously by π as the energy is varied through the original energy of the bound state.

The simple example given above was studied in an earlier paper [7]. In that paper a bound state of the local potential was moved to positive energy by use of a nonlocal potential. The phase shift was found to be equal to the negative phase of the Jost function of the local potential, that is, the term in the brackets of Eq. (41) was missing. The resulting cross section is the same in either case since the missing term is real. But in the earlier work, Levinson's theorem held because of the zero in the Jost function at the original energy of the bound state, as if its ghost remained. The situation as described in this paper is much more satisfactory.

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