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Study of the S-matrix near bound states in the continuum

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Abstract. The behaviour of S-matrix for potentials generating bound states in continuum in the neighbourhood of the positive bound state energies is studied. It is shown that unlike the case of usual negative energy bound states, the S-matrix does not have a pole at the positive bound state energy but becomes unity at the energy corresponding to bound states in continuum. Calculations of S-wave S-matrix for a local potential constructed by Stillinger and Herrick and a separable nonlocal potential constructed by the present authors verify these results. Our results indicate that the bound states embedded in continuum constructed *via* the von Neumann and Wigner procedure cannot be interpreted as resonances with zero width.

Keywords. S-matrix; bound states in continuum.

1. Introduction

As early as 1929, von Neumann and Wigner (1929) demonstrated the possibility of constructing a potential for which the single particle Schrödinger equation could possess isolated eigenvalues embedded in the continuum of positive energy states. Their method was based on amplitude modulation of a free particle wavefunction, leading to a normalizable eigenfunction and a local potential which produces it. The potential was bounded and could be made to vanish at infinity.

The von Neumann and Wigner states gained importance recently following the work of Stillinger and others on some atomic and molecular systems (Stillinger 1966; Stillinger and Stillinger 1974; Stillinger and Weber 1974). They have shown that some atomic and molecular systems might exhibit bound states in the relevant continua. In view of this, the construction of potential by von Neumann and Wigner method was revived by Stillinger and Herrick (1975). The implications of the existence of such bound states in physical systems such as decaying radio active nuclei and 'tunnel junctions' where tunnelling plays an important role have also been discussed by them. Further, the present authors recently constructed a set of separable nonlocal potentials which can generate bound states in continuum (Jain and Shastry 1975).

The special nature of these bound states makes the study of the behaviour of S-matrix for such potentials near positive bound state energies quite interesting. At the usual negative bound state energies, the S-matrix is known to have a simple pole (Newton 1966). To find the behaviour of S-matrix in the neighbourhood of positive bound state energies is the main objective of this paper. We shall carry out this analysis both for local and nonlocal potentials. In section 2 we briefly review the construction of these potentials. In section 3 we discuss the problem of the poles of the S-matrix and show that the S-matrix does not have a pole at positive bound state energies. In section 4 we present the results of numerical calculations and discussions.

2. Potentials generating bound states in continuum

The method of construction of the potentials generating bound states in continuum has been described by Stillinger and Herrick (1975) for local potentials and by Jain and Shastry (1975) for separable nonlocal potentials. For simplicity we restrict ourselves only to the case of S-wave. The case of higher angular momenta can also be similarly studied. The essential idea in the construction of the potentials is to start with an amplitude modulated plane wave $\Psi(r)$ as a normalizable bound state wavefunction. Thus

$$\Psi(r) = f(r) \sin(kr)/(kr) \tag{1}$$

where k is the momentum ($\hbar=1=m$ units) and $f(r)$ is the modulating function. The behaviour of $f(r)$ should be such that it makes $\Psi(r)$ normalizable. This wavefunction is then plugged into the wave equation to yield the potential. The final expression for the potential for specific choices of $f(r)$ are as follows.

For a local potential $V(r)$, we get

for
$$f(r) = [A^2+s(r)]^{-1} \tag{2}$$

$$s(r) = \tfrac{1}{2}(2k_br)^2 - 2k_br \sin(2k_br) - \cos(2k_br) + 1,$$

$$V(r) = \frac{64k_b^4 r^2 \sin^4(k_br)}{[A^2+s(r)]^2} - \frac{4k_b^2 [\sin(k_br) + 2k_br \sin(2k_br)]}{A^2+s(r)}. \tag{3}$$

In the above expression, A is an arbitrary dimensionless parameter and $E_b=\frac{1}{2}k_b^2$ is bound state energy. Following Stillinger and Herrick (1975), we choose $A=ak_b^2$ with $a=1$ for local potential $V(r)$. The behaviour of this potential for small and large values of r is given by

$$V(r) \xrightarrow[r\to 0]{} -(20k_b^2/A^2)(k_br)^2 + O(k_br)^4 \tag{4a}$$

$$V(r) \xrightarrow[r\to\infty]{} -8k_b^2 \sin(2k_br)/(2k_br). \tag{4b}$$

In the case of separable nonlocal potentials (Jain and Shastry 1975) of the form

$$\langle \mathbf{r} | V | \mathbf{r}' \rangle = \sum_{l,m} \epsilon\, g_l(r)\, g_l(r')\, Y_{lm}(\hat{r})\, Y^*_{lm}(\hat{r}') \tag{5}$$

we have for $f(r) = [A^2 + (k_b r)^2]^{-1}$

$$g_0(r) = \chi_0(r)/\phi_0(k_b), \text{ where} \tag{6}$$

$$\chi_0(r) = \frac{8k_b^3 r \sin(k_b r)}{(A^2 + k_b^2 r^2)^3} - \frac{1}{(A^2 + k_b^2 r^2)^2}\left[\frac{2k_b \sin(k_b r)}{r} + 4k_b^2 \cos(k_b r)\right]$$

$$(\hbar = 1 = 2m), \tag{7}$$

and

$$\phi_0(k_b) = \left[\frac{\epsilon\pi}{48k_b A^5}\{e^{-2A}(3+6A-8A^3)-3\}\right]^{\frac{1}{2}}. \tag{8}$$

The behaviour of $g_0(r)$ for small and large values of r is given by

$$g_0(r) \xrightarrow[r \to 0]{} (6k_b^2/A^4)/\phi_0(k_b) \tag{9a}$$

and

$$g_0(r) \xrightarrow[r \to \infty]{} 4 \cos(k_b r)/k_b^2 r^4 \, \phi_0(k_b). \tag{9b}$$

In the next section we shall discuss the properties of S-matrix for the potentials given by eqs (3), (5) and (6).

3. Analysis of the S-matrix

As explained earlier, the special property of the potentials given in section 2 is that they generate bound state (localized, square integrable) wavefunction at a certain positive energy. Positive energy eigenvalues for bound states are however not uncommon; the harmonic oscillator problem is a good example of this. But in the case of harmonic oscillator, we have no continuum solutions and the bound state solutions themselves form the complete set. Our problem of positive energy bound states is of interest since it is embedded in continuum and hence they have considerable significance in scattering problems. Thus it is important to study how these bound states affect the S-matrix behaviour in their neighbourhood. The analytic S-matrix theory provides a set of interesting relations between the physical states and the poles of the S-matrix (Newton 1966). For example, in complex k-plane, some poles of S-matrix along the positive imaginary axis correspond to the bound states, the poles in the lower half of k-plane and lying close to the real axis correspond to resonances and other poles are classified as antibound state poles, unphysical poles or redundant poles (Newton 1966).

In order to study the behaviour of S-matrix in the neighbourhood of the positive energy eigenvalues, we use the well established results of non-relativistic potential scattering theory. Thus, for potentials obeying the conditions

$$\int_a^\infty |V(r)| \, dr < \infty, \tag{10a}$$

and

$$\int_0^b r\,|V(r)|\,dr<\infty;\ a,\ b>0 \tag{10b}$$

it is possible to obtain the following asymptotic expression for the regular solution of the modified S-wave radial Schrödinger equation:

$$\Phi(k,\ r)\xrightarrow[r\to\infty]{}\left[f(-k)e^{-ikr}-f(k)e^{ikr}\right]/(2ik) \tag{11}$$

Here $\Phi(k,\ r)=r\Psi(k,\ r)$ and $f(\pm k)$ are given by the Wronskian

$$f(\pm k)=\underset{r\to\infty}{\mathrm{Lt}}\ W[\Phi,\ e^{\mp ikr}] \tag{12}$$

$f(\pm k)$ are known as Jost functions and the S-wave S-matrix is related to these through the relation

$$S_0(k)=f(k)/f(-k). \tag{13}$$

However, the local potential described in section 2 does not satisfy the condition (10a) because it is essentially a long range potential as is clear from eq. (4b). As a result, the Jost functions are not defined as in eqs (11) and (12). The long range nature of the potential may lead to asymptotic distorted waves and the S-matrix has to be defined with respect to these distorted waves as is done in the case of ' Coulomb-nuclear ' problem. At this point it should be stressed that no potential seems to exist which generates a bound state in continuum and at the same time is a short range potential i.e., satisfying eqs (10a) and (10b). In the absence of a sound knowledge of the distorted asymptotic states, it is worthwhile to discuss the plane wave representation of the S-matrix. A similar study of another long range potential, namely the Coulomb potential is well known (Schwinger 1964; Shastry and Rajagopal 1970). Furthermore, it should be stressed that the conditions given by eqs (10) are only sufficient conditions because they are obtained by estimating the bounds on integrals for iterated solutions of integral form of the Schrödinger equation (Newton 1966). Therefore, it is quite possible that the results of the usual scattering theory are valid even for a potential which fails to satisfy these conditions. Specially in the case of the local potential of section 2, the plane wave representation may turn out to be a very good approximation to the actual S-matrix because of the extra factor of $\sin(2k_b r)$ over the Coulomb potential.

By definition, S-matrix is nothing but the ratio of the coefficient of spherically outgoing wave to the coefficient of the spherically incoming wave. These coefficients are the Jost functions. However, if Φ corresponds to a positive energy bound state, then as $r\to\infty$, there should not be any coefficient of $e^{\pm ikr}$, because then it will correspond to a scattering solution. This can be seen more clearly by substituting for $\Psi(r)$ from eq. (1) in eq. (12) for Jost functions. We have,

$$\begin{aligned} f(\pm k_b) &= \underset{r\to\infty}{\mathrm{Lt}}\ W[f(r)\sin(kr),\ e^{\mp ikr}]/k \\ &= \underset{r\to\infty}{\mathrm{Lt}}\ e^{\mp ikr}f(r)\,[f'(r)\sin(kr)/f(r) \\ &\qquad\qquad +k\{\cos(kr)\pm i\sin(kr)\}]/k\ (k=k_b). \end{aligned}$$

Now for $f(r)$ of the type given in eq. (2), $f'(r)/f(r) \to 0$ as $r \to \infty$.
We therefore get,

$$f(\pm k_b) = \underset{r \to \infty}{\mathrm{Lt}} f(r) \to 0. \tag{14}$$

From the symmetry relation $f(k) = f^*(-k^*)$, we see that for real k, $f(k) = f^*(-k)$. The S-matrix is then given by $f(k)/f^*(k)$ and thus cannot have a pole. As a result, at $k = k_b$ corresponding to positive energy bound state also, the S-matrix does not have a pole. Moreover, as is clear from eq. (14), both $f(k_b)$ and $f(-k_b)$ are real and tend to zero. Consequently, the value of the S-matrix at $k = k_b$ can be expected to become unity, and the wavefunction will go to the localized, square integrable wavefunction without the usual scattering wave boundary conditions. The generation of bound state and scattering states in its neighbourhood is demonstarated in figure 1 for $k_b = 0{\cdot}5$ and $V(r)$ given by eq. (3). In this connection it should be stressed that at $k = k_b$, there is no scattering solution and as such no phase shift or S-matrix can be defined in the usual sense. However, we have the S-matrix well defined for all $k \neq k_b$ and it is of interest to know how it behaves for $k = k_b$. Another similar example exists in the study of S-matrix for negative energies ($k^2 < 0$). In this case also,

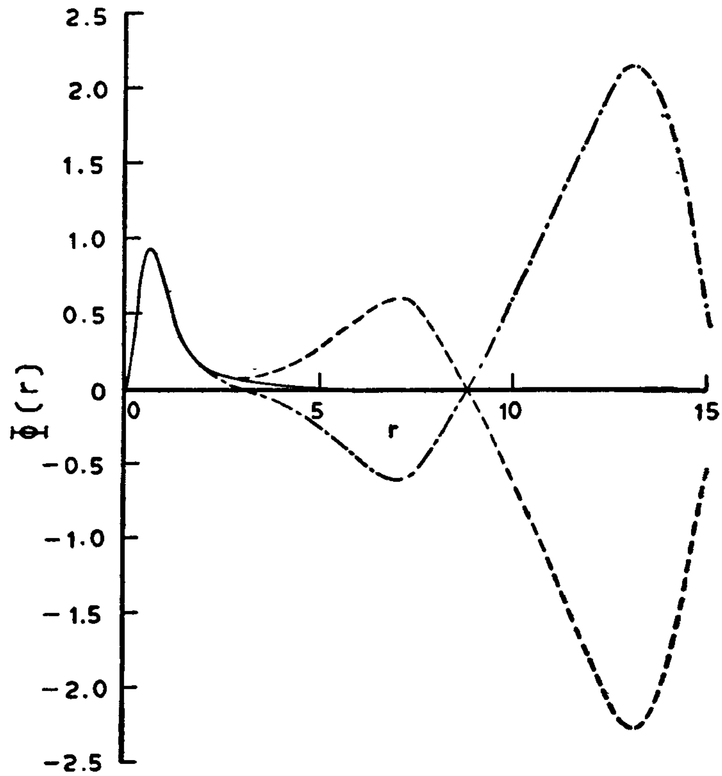

Figure 1. Scattering states in the neighbourhood of bound state energy for the local potential given by eq. (3): (a) at $k = k_b = 0{\cdot}5$ (Solid curve), (b) at $k = 0{\cdot}495$ (dotted curve) and (c) at $k = 0{\cdot}505$ (dash-dotted curve).

S-matrix is to be defined with respect to diverging and damping waves (not the scattering boundary condition) and when one tries to define it for $k^2=-k_n^2$ corresponding to a negative bound state energy, one finds that the S-matrix has a pole. Similarly, it is interesting to know how the ' analytically continued ' S-matrix behaves at $k=k_b$ corresponding to a bound state in continuum.

For separable nonlocal potentials, a general study of the Jost function has been carried out by Warke and Bhaduri (1971). However, the form factors given in section 2 are of short range type (Shastry and Singh 1974) and plane wave representation of the S-matrix is valid in this case. Thus all the arguments given earlier in this section regarding S-matrix for a local potential also hold good for the separable nonlocal potential defined by eqs (5) and (6). The S-matrix is therefore expected to become unity at $k=k_b$ in the case of this nonlocal potential also. In the next section we verify these arguments with the help of suitable calculations.

4. Calculations and discussion

In the previous section we had shown that the S-matrix cannot have a pole at a positive energy bound state, but is expected to have a value one. In other words, the on-shell T-matrix element for the potentials discussed in section 2 is zero at $k=k_b$, because it is given by (Newton 1966)

$$t_0(k) = [1-S_0(k)]/(2\pi ikm). \tag{15}$$

The subscript in eq. (15) refers to S-wave ($l=0$). In this section we shall present some calculations carried out for the potentials discussed in section 2. Let us first take the case of T-matrix element for separable nonlocal potential because closed form expression makes the calculation of T-matrix much simpler. For separable nonlocal potential of the type given by eq. (4), the on-shell S-wave T-matrix element is given by (see for example, Gupta *et al* 1975).

$$t_0(k) = \xi_0^2(k) \Big/ \left[1 - \int_0^\infty \frac{\xi_0^2(k')k'^2\, dk'}{k^2-k'^2+i\delta}\right] (\hbar=2m=1;\ \epsilon=1) \tag{20}$$

where
$$\xi_0(k) = (2/\pi)^{\frac{1}{2}}\left[\int_0^\infty \frac{\sin(kr)}{kr}\chi_0(r)r^2\, dr\right] \Big/ \phi_0(k_b) \tag{21}$$

and $\delta\to 0$. For $\chi_0(r)$ given by eq. (7), the integral in eq. (21) can be evaluated to get

$$\xi_0(k) = (2/\pi)^{\frac{1}{2}}(X+Y)/\phi_0(k_b) \tag{22}$$

where

$$X=(k_+^2 e^{-k_+}-k_-^2\, e^{-k_-})/(4kA^3)$$

$Y= -\pi(k_+\, e^{-k_+} \pm k_-\, e^{-k_-})/(2kA^2)$, (plus sign if $k \geqslant k_b$ and minus sign if $k \lessgtr k_b$),

$$k_+ = (k+k_b)\, B,\ k_- = B\,|k-k_b|\,,\ B = A/k_b.$$

From eq. (22) it is easy to see that at $k = k_b$, $\xi_0(k)$ becomes zero. Equation (20) immediately gives the result that the T-matrix element is zero at $k=k_b$:

$$t_0(k_b) = 0. \tag{23}$$

For $k \neq k_b$, the value of $t_0(k)$ can be evaluated numerically. We calculated the T-matrix for several values of k_b and k in the neighbourhood of k_b. The results of calculation for a typical case of $k=2{\cdot}0$ are shown in figure 2. The value of A was arbitrarily chosen to be 2. It can be seen that at $k=k_b$, both the real and imaginary parts of T-matrix vanish. This is exactly what we expected from our analysis in the previous section.

In the case of local potentials, the calculation of S-matrix is usually done by numerically solving the Schrödinger equation and then matching the solution at large r to a combination of spherically outgoing and incoming waves. However, the method of wavefunction matching is not suitable for potentials of the type in eq. (3) because the

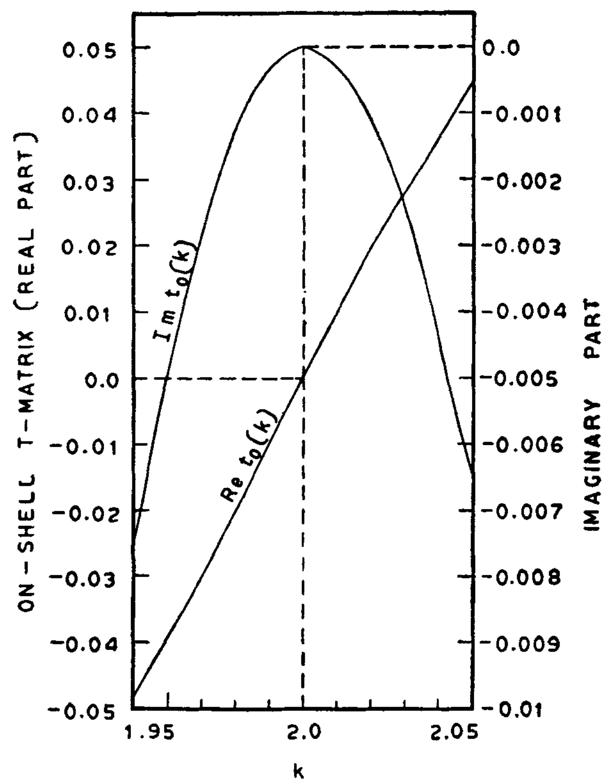

Figure 2. S-wave on-shell T-matrix for separable nonlocal potential given by eqs (5) and (6) for $k_b = 2{\cdot}0$, $A = 2{\cdot}0$ ($\hbar = 2m = 1$ unit).

error introduced in the wavefunction is large at large r due to the highly oscillating nature of the potential. We therefore used the following expression for the S-wave Jost function (Newton 1964)

$$f(k) = 1 + \int_0^\infty V(r) e^{-ikr} \Phi(k,r)\, dr \tag{24}$$

and calculated the S-matrix from the relation $S_0(k) = f(k)/f^*(k)$ for real k. This method makes use of the values of the wavefunction $\Phi(k, r)$ at all points and does not depend on the value at large r only. The T-matrix elements can then be found using eq. (15). The wavefunction $\Phi(k, r)$ was evaluated numerically using modified Noumerov method (Melkanoff *et al* 1966) and was normalized to satisfy the condition (Newton 1964)

$$\Phi(k, r) \xrightarrow[r \to 0]{} r \text{ (for } S\text{-wave).} \tag{25}$$

The results of our calculation show that the imaginary part of the Jost function vanishes for $k=k_b$ whereas the real part has a minimum at this value. The real part does not vanish because the integration in eq. (24) is performed only up to a finite value of r. The value of $f(k_b)$ decreases as the upper limit of the integration is increased. A very large upper limit cannot be taken because the wavefunction is in error at large r. In any case, since $f(k_b)$ is real, the S-matrix given by $f(k)/f^*(k)$ still goes to unity as $k \to k_b$. The results of the calculation for a typical case of $k=0{\cdot}5$ are shown in figures 3a and 3b. The potential (3) for this energy has been plotted in figure 3 of Stillinger and Herrick (1975). It is seen that the T-matrix element vanishes at $k=k_b$. Thus our analysis in the previous section regarding the behaviour of the

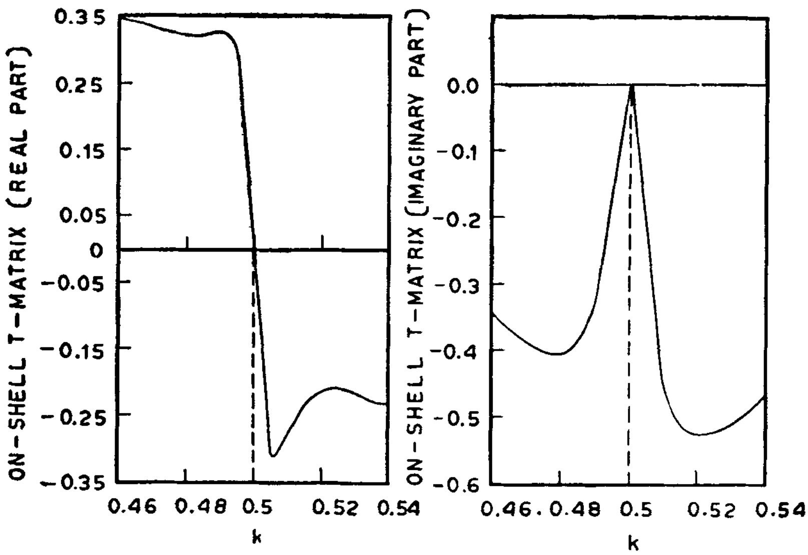

Figure 3. S-wave on-shell T-matrix for local potential given by eq. (3) for $k = 0{\cdot}5$ ($\hbar = m = 1$ unit).

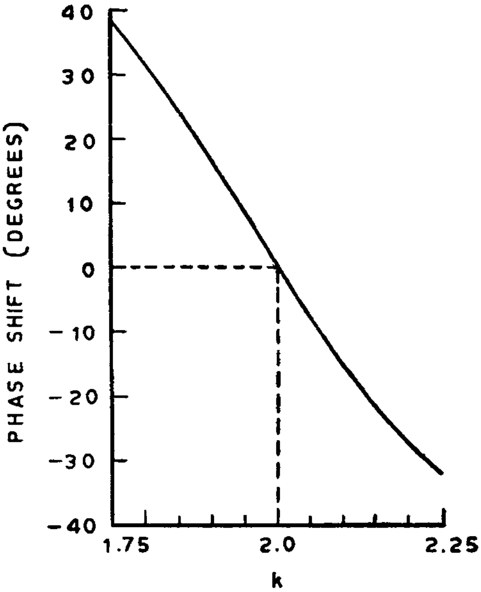

Figure 4. S-wave phase shifts for separable nonlocal potential given by eqs (5) and (6) for $k_b = 2{\cdot}0$, $A = 2{\cdot}0$.

S-matrix near a positive energy bound state is supported by actual calculations carried out for separable nonlocal as well as local potentials. An analysis of Jost function for separable nonlocal potentials which also gives conditions for occurrence of bound states in continuum was recently made by Mulligan *et al* (1976).

In this connection, it may be further pointed out that the bound states in continuum constructed via the von Neumann and Wigner procedure do not correspond to an infinitely narrow resonance. This is because at a resonance, the scattering cross-section should have a maxima whereas our calculations show that the cross-section is zero at $k=k_b$ (in fact there is no scattering). Figure 4 gives a plot of phase shift δ_0 versus k for the separable nonlocal potential with $k_b = 2{\cdot}0$. It can be seen that $\delta = 0$ at $k = k_b$ and the variation of δ_0 with k is smooth without any discontinuous increase by π. This clearly shows that these bound states in continuum of the above type cannot be interpreted as resonances. However, in the many body case a bound state in continuum may be thought of as a resonance of zero width (Stillinger and Herrick 1975; Beregi 1973).

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