Continuity of Phase Shift at Continuum Bound State*

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(Received 17 October 1968)

When a separable potential has a bound state in the continuum, there are two possible definitions of the phase shift. It is shown that if the phase shift is chosen to be the boundary value of the phase of an analytic function, then it has a jump discontinuity of magnitude π at each continuum bound state. Some advantages of this definition, as opposed to one giving a continuous phase shift, are presented.

Since the introduction by Yamaguchi and Yamaguchi[1] of separable potentials as a tool for investigating scattering phenomena, there has been a substantial effort devoted to investigating their properties. In particular, several papers[2–4] have treated the special case in which there occur discrete states in the continuum. This paper is intended to clear up some apparent conflicts in the literature. The notation used is that of a previous paper[5] (I), in which the formulas were given for determining the separable potential from the phase shift (units $\hbar=2\mu=1$, where μ is the reduced mass).

If there is an s-wave separable potential of the form

$$V(k,k')=gv(k)v(k') \tag{1}$$

in momentum space, with $v(k)$ real and g either $+1$ or -1, then the t matrix is given by

$$t(k,k',z)=gv(k)v(k')/D(z), \tag{2}$$

where z is a complex variable and

$$D(z)=1+\frac{1}{\pi}\int_0^\infty \frac{\tau(\epsilon)d\epsilon}{z-\epsilon}, \tag{3}$$

$$\tau(k^2)=-(k/4\pi)gv^2(k); \tag{4}$$

the function $D(z)$ is analytic in the cut plane (cut from 0 to $+\infty$). The phase shift $\delta(E)$ is related to t by

$$\exp[i\delta(E)]\sin\delta(E)=-(E^{1/2}/4\pi)t(E^{1/2},E^{1/2},E+i0)$$
$$=\tau(E)/D^+(E), \tag{5}$$

where

$$D^\pm(E)=\lim_{\epsilon\to+0}D(E\pm i\epsilon). \tag{6}$$

Since it follows easily from (3) that

$$D^+(E)-D^-(E)=-2i\tau(E), \tag{7}$$

we also have

$$\exp(i\delta)\sin\delta=(D^- - D^+)/2iD^+, \tag{8}$$

and hence

$$\exp(2i\delta)=D^-/D^+. \tag{9}$$

Moreover,

$$D^-(E)=D^+(E)^*, \tag{10}$$

so that δ *can be* chosen to be the phase of $D^-(E)$. We lable this choice $\delta_A(E)$:

$$\delta_A(E)=\text{phase}[D^-(E)], \tag{11}$$

and since $D(z)$ is analytic in the cut plane and, by (3), goes to unity as z becomes infinite (all integrals are assumed to converge), we can choose $\delta_A(E)$ to be zero at $E=\infty$, and it is then uniquely defined for all E. The phase $\delta_A(E)$ is the boundary value of the phase of the function $D(z)$ analytic in the cut plane.

An alternative definition of $\delta(E)$ is obtained by solving for the scattering wave function in the potential (1) and determining $\delta(E)$ from the asymptotic behavior at energy E as $r\to\infty$:

$$\psi(r)\to A\sin[E^{1/2}r+\delta(E)]/r. \tag{12}$$

The result is[3,4]

$$\tan\delta(E)=\tau(E)\bigg/\left(1+\frac{P}{\pi}\int_0^\infty\frac{\tau(\epsilon)d\epsilon}{E-\epsilon}\right)=\frac{\text{Im}D^-(E)}{\text{Re}D^-(E)}, \tag{13}$$

and this is obviously consistent with (11). However, *if we impose the additional condition* that the phase shift determined in this way be continuous, and call the resulting phase shift $\delta_C(E)$, then it is not necessarily true that $\delta_C(E)$ and $\delta_A(E)$ are the same. It is only required that

$$\delta_C(E)=\delta_A(E)+n(E)\pi, \tag{14}$$

where $n(E)$ is a function that takes on only integral values.

To illustrate that these distinctions are not completely trivial, consider the example of Refs. 2–4. Here τ is chosen so that $\tau(E)$ and $\text{Re}D^-(E)$ both vanish at $E=E_0$. Since (4) shows that τ cannot change sign, τ is made quadratic in $E-E_0$ near E_0, while $\text{Re}D^-(E)$ is chosen to be linear in $E-E_0$ near E_0. Then, by (13), $\tan\delta$ clearly changes sign at E_0, and therefore $\sin\delta_C(E)$ changes sign.

* Work performed under the auspices of the U.S. Atomic Energy Commission.
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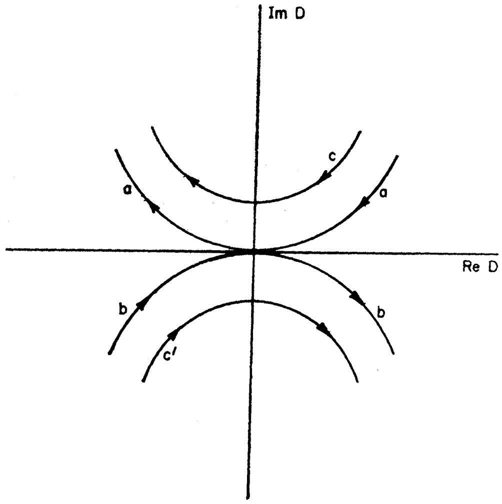

FIG. 1. Paths followed by the function $D(E)$. See text for explanation of various cases.

On the other hand, it is shown in I that (3) and (11) together allow the inverse problem of finding $v(k)$ in terms of $\delta_A(E)$ to be solved, with the result (assuming no bound state)

$$\tau(E)=\sin\delta_A(E)\exp\left(\frac{P}{\pi}\int_0^\infty\frac{\delta_A(\epsilon)d\epsilon}{E-\epsilon}\right). \quad (15)$$

Since the exponential is positive and $\tau(E)$ cannot change sign, it follows that $\sin\delta_A(E)$ cannot change sign.

The resolution of this apparent contradiction is most simply seen by considering the path on an Argand diagram of the function $D^-(E)$ near the point E_0. Since its real and imaginary parts are, respectively, linear and quadratic in $E-E_0$, $D^-(E)$ follows a parabola as in Fig. 1. Clearly, as E goes through E_0, $D^-(E)$ goes through zero, and its phase jumps by π. At the point $E=E_0$, the function $n(E)$ of Eq. (14) jumps by -1. If δ_C is chosen so that $\delta_C(\infty)=0$, then

$$\begin{aligned}\delta_C(E)&=\delta_A(E)+\pi, && E<E_0\\ &=\delta_A(E), && E>E_0.\end{aligned} \quad (16)$$

The sign of the jump in δ_A follows from

$$(d/dE)D(E)|_{E=E_0}=-\frac{1}{\pi}\int_0^\infty\frac{\tau(\epsilon)d\epsilon}{(E_0-\epsilon)^2}, \quad (17)$$

where the integral is nicely convergent. If $\tau>0$, then $\mathrm{Im}D^->0$, $dD/dE<0$ at E_0, and D^- follows curve a of Fig. 1. If $\tau<0$, then $\mathrm{Im}D^-<0$, $dD/dE>0$ at E_0, and D^- follows curve b of Fig. 1. In both cases, the phase of D^- jumps by $+\pi$ at $E=E_0$.

We can further verify this behavior of δ_A by looking at the behavior of $D(z)$ as z goes past (below) E_0 with a finite imaginary part ξ, that is, the behavior of $D(E-i\xi)$ for ξ small and fixed.

$$D(E-i\xi)=1+\frac{1}{\pi}\int_0^\infty\frac{\tau(\epsilon)(E-\epsilon)}{(E-\epsilon)^2+\xi^2}d\epsilon+i\frac{\xi}{\pi}\int_0^\infty\frac{\tau(\epsilon)}{(E-\epsilon)^2+\xi^2}. \quad (18)$$

It can easily be seen that $D(E-i\xi)$ follows the path c or c' of Fig. 1, so that the phase of D^- is, in fact, increased by π on the curves a and b.

The sign of the jump is also consistent with (15); it is easy to see that a jump of π at E_0 gives a contribution $\ln|E-E_0|$ to the exponent in (15), so that near E_0

$$\tau(E)=f(E)\sin\delta_A(E)\,|E-E_0|, \quad (19)$$

with $f(E)$ slowly varying. Since $\sin\delta_A(E)$ is proportional to $|E-E_0|$ near E_0, we again obtain $\tau(E)\propto(E-E_0)^2$ as required for consistency.

This jump in $\delta_A(E)$ is also connected with the fact that the solution of the Schrödinger equation at E_0 is not a scattering state at all, but has the Fourier transform

$$\phi_{E_0}(\mathbf{k})=N[v(k)/(E_0-k^2)], \quad (20)$$

with N a normalization factor. A scattering state would have an additional term $\delta(\mathbf{k}-\mathbf{p})$, with $p^2=E_0$. As shown in I, it is consistent and convenient to let $\delta_A(E)$ have a jump of π at the energy $-B$ of a bound state; similarly, δ_A jumps by π at the special state (20), which can be regarded as a "bound state in the continuum," since its configuration-space wave function goes to zero at infinity.

Of course, with δ_A it is easy to prove Levinson's theorem in the standard way by using the domain of analyticity of $D(z)$; it follows that

$$\delta_A(0)-\delta_A(\infty)=n_B\pi, \quad (21)$$

where n_B is the number of bound states in the potential (1) (at most one). If δ_C is used, Levinson's theorem requires the elaborate arguments of Ref. 3.

Finally, it is clear that a "bound state in the continuum" is the same as a resonance with zero width. Such a resonance would be a special type of accidental degeneracy, and hence unphysical. In an actual physical situation there are always interactions (electromagnetic, weak) that spread such a resonance. It follows that it is more reasonable not to require the exact coincidence of the zeros of $\tau(E)$ and $\mathrm{Re}D(E)$. Then there is a resonance in the scattering, and the phase shift goes from near zero to near π in a continuous way.

I would like to thank A. Kerman for stimulating this investigation and L. Heller, K. W. McVoy, and F. Tabakin for helpful discussions.