Phase shift behavior at degenerate continuum bound states

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A special case of a nonlocal potential which has a degenerate continuum bound state is studied using the Bolsterli criterion for defining the phase shift, and is found to be consistent with Levinson's theorem and the Wigner inequality.

NUCLEAR REACTIONS Phase shift behavior for nonlocal potentials, degenerate continuum bound states, Levinson's theorem.

It has long been known that nonlocal potentials can give rise to continuum bound states (CBS's) which require a change of viewpoint with respect to the generalization of Levinson's theorem,¹ originall proved for local potentials. The statement of the theorem is meaningful in this generalized context only if one makes an appropriate choice of the phase shift at each energy since direct scattering information only fixes the phase shift modulo π . In the case of local potentials, this prescription consists simply in requiring continuity of the phase shift for all energies $E > 0$ and

$$
\delta(0) = \lim_{E \to 0} \delta(E) ,
$$

provided there is no zero-energy bound state. In the presence of (nondegenerate) continuum bound states, one has two equivalent options: (a) to continue to insist on the continuity of $\delta(E)$ whence the theorem becomes

$$
\delta(0) - \delta(\infty) = \pi(N + M) , \qquad (1)
$$

where N is the number of negative energy bound states and M the number of positive energy bound states (this is the option exercised by Gourdin and Martin²); (b) alternatively³, insist that the phase shift is continuous everywhere except at the energy of each CBS where it jumps discontinuously by π ; hence, clearly

$$
\delta(0) - \delta(\infty) = N\pi \tag{2}
$$

The advantage of the latter choice is that the phase shift is then the phase of a meromorphic function in the complex plane (with a cut extending from $E=0$ to $E=\infty$ along the real axis) as the axis is approached from above.³ In such cases the CBS is a simple pole on the real E axis. If a small perturbation causes this pole to move down onto the second sheet of the Riemann surface, the CBS disappears

and a scattering resonance at a nearby energy replaces it.⁴ The phase shift then increases continuously but rapidly in this region by approximately π . Thus one gains not only the analytic properties, but a "stability" of the phase shift with respect to at least certain small perturbations. The relationship of the two choices has been carefully reviewed by Dreyfuss.⁵

Arguments in favor of (2) were raised again more recently by Foldy and Lock^{6} in response to a suggestion in the literature⁷ that the phase shift be defined such that it has a discontinuity of $-\pi$ at what has come to be called a spurious state. Foldy and Lock argued that (a) since such a spurious state gave no obvious "signature" of its presence, and (b) if the discontinuity could be smoothed out by some perturbation, one would encounter a violation of Wigner's phase shift theorem⁶; little advantage, if any, could be secured by this last convention. Hence they opted in favor of the stability considerations favoring the Bosterli choice (2). Unfortunately this is not sufficient for all purposes since we do not know that we get the same results independent of the nature of "allowed" perturbations.

However, the results of this earlier paper left the present author uncomfortable on one score. It was shown in the Appendix of Ref. 6 that one could construct a potential which had a doubly degenerate CBS and here there is the possibility that such a question of uniqueness could arise. Thus one could impose a perturbation such that the original degenerate CBS is split into two slightly separate nondegenerate CBS's whence the application of the results of that paper would predict a jump by π of the phase shift at each giving rise in the limit as the perturbation is removed to a jump of 2π at the degenerate CBS. On the other hand, if the scattering amplitude had a simple pole at the position of a degenerate CBS, the jump in the phase shift would be

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only π . To satisfy the requirements of the desired theorems the first of these results would have to hold. As might be expected the former was found to be the case, the latter failing because the singularity is not a simple pole but a *dipole* singularity⁸ on the real axis.

The question was resolved by examining the potential given by Eq. (A15) of Ref. 6, hereafter referred to as I, which we write with a slight notational change as

$$
\langle r | V | r' \rangle = \lambda_1 \Delta_0^{R_1}(r) \Delta_0^{R_1}(r')
$$

$$
+ \lambda_2 \Delta_{R_1}^{R_2}(r) \Delta_{R_1}^{R_2}(r')
$$
, (3)

where

$$
\Delta_a{}^b(r) = \begin{cases} 1 & a < r < b \\ 0 & \text{otherwise} \end{cases}
$$

We shall particularly be concerned with the special case where $\lambda_1 = \lambda_2 = \lambda$ and $R_2 = 2R$, $R_1 = R$ (though one other case is also examined). Under these circumstances the condition for a doubly degenerate eigenvalue in the continuum located at $E = \hbar^2 k^2 / 2m$ with $k = 2\pi n / R$, $n = 1, 2, \ldots$, is

 $R^3 = (2\pi n)^2$.

The linearly independent and orthogonal CBS

eigenfunctions are then

$$
u_1 = \begin{cases} A_1(1 - \cos kr) & 0 < r < R \\ 0 & \text{otherwise} \end{cases}
$$
\n
$$
u_2 = \begin{cases} A_2(1 - \cos kr) & R < r < 2R \\ 0 & \text{otherwise} \end{cases}
$$

The calculation of the phase shift as a function of k can be readily accomplished by the method employed in the Appendix of I but the resultant formula is too complicated to allow its behavior to be simply explored analytically. Numerical calculation has therefore been employed using the following relations which are valid for the more general case where the two λ 's are different and R_1 and R_2 are unrelated; we use the abbreviations $x_1 = kR_1$,
 $x_2 = kR_2$, $\sigma_1 = \lambda_1 R_1^3$, $\sigma_2 = \lambda_2 (R_2 - R_1)^3$.

$$
\delta(\text{mod}\pi) = -x_2 + \tan^{-1}(U_2/V_2) ,
$$

\n
$$
U_2 = U_1 + A(\sin x_2 - \sin x_1) + B(\cos x_2 - \cos x_1) ,
$$

\n
$$
V_2 = A\cos x_2 - B\sin x_2 .
$$

Here A and B are to be determined from U_1 and V_1 by solution of the equations

$$
\left[\sin x_1 - \frac{\sigma_2(\cos x_2 \cos x_1)}{(x_2 - x_1)^3 - \sigma_2(x_2 - x_1)}\right]A + \left[\cos x_1 + \frac{\sigma_2(\sin x_2 - \sin x_1)}{(x_2 - x_1)^3 - \sigma_2(x_2 - x_1)}\right]B = U_1,
$$

I

 $[\cos x_1]A - [\sin x_1]B = V_1$,

while U_1 and V_1 are given by

$$
U_1 = \frac{\sigma_1 (1 - \cos x_1)^2}{x_1^3 - \sigma_1 (x_1 - \sin x_1)} + \sin x_1,
$$

$$
V_1 = \frac{\sigma_1 (1 - \cos x_1) \sin x_1}{x_1^3 - \sigma_1 (1 - \sin x_1)} + \cos x_1.
$$

Even numerical computation using these formulas is difficult because of the rapid variation of the phase shift with energy in the regions where resonances produced by perturbations lie. The sharpmances produced by perturbations lie. The sharp-
ness of these resonances with $\lambda_1 = \lambda_2 = \lambda$ and $R_1=R_2=R$ when $\sigma-\lambda R^3$ differs from the critical value of $4\pi^2$ for a degenerate CBS by as much as 15 can be seen in Fig. 1, where the phase shift has been plotted as a function of $x \equiv kR$ varying from 0 to 10 for $\sigma = 55$. However, a clear answer to our question emerges immediately: The phase shift jumps by 2π . as the energy increases through the region of the degenerate CBS. The perturbation of σ from $4\pi^2$ causes the singularity in the scattering amplitude on the positive real axis associated with the CBS to move down from the axis onto the lower unphysical sheet, generally splitting into two simple poles, but possibly as a dipole. The motion of these poles is difficult to determine quantitatively. In Fig. ¹ we have also indicated the phase shift variation if the perturbation is introduced by choosing $\sigma_1 = 25$ and σ_2 =55 while the condition $R_1 = R_2 = R$ is retained. In this case the phase shift shows two successive rapid increases by π as x increases through 2π , but hovers around $-\pi$ in the intervening interval.

In summary, results for a particular nonlocal potential, but one representative of many (if not all) others, tempt one to conclude that:

(a) Levinson's theorem in either of its forms is satisfied for nonlocal potentials possessing degenerate

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FIG. 1. Phase shift $\delta(k)$ as a function of kR for the nonlocal potential given in Eq. (3). The dashed curve represents the case for a doubly degenerate continuum bound state occurring for the condition $\sigma = \sigma_1 = \sigma_2 = 4\pi^2$. The two solid curves labeled $\sigma = 25$ and $\sigma = 55$ represent the effect of perturbations which transform the continuum bound state into closely spaced pairs of resonances. The dashed-dotted curve corresponds to another perturbation corresponding to values of the parameters $\sigma_1 = 25$, σ_2 =55, in which case the resonances are more widely separated. All curves show the increase of the phase shift by 2π as kR increases through the region of the resonance. (The label on the abcissa should be kR rather than kr.) The remarkable sharpness of the resonances as measured by the steepness with which the phase shifts increase through $-\pi/2$ and $-3\pi/2$ should be noted.

continuum bound states (and degenerate negative energy bound states (see the Appendix) for any partial wave phase shift, with the understanding that M in (1) is the number of linearly independent continuum bound states, and in the case of (2), the jump in δ at the energy of a CBS is $m\pi$, where m is the number of linearly independent continuum

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(b) Presumably Bolsterli's analyticity properties continue to hold but with higher order poles in place of simple poles at degenerate CBS energies on the positive real axis.

(c) The limiting form of Wigner's inequality then also continues to hold.

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APPENDIX

The possibility of degenerate negative energy bound states with nonlocal potentials is demonstrated by an example for such a bound s state. The radial wave function multiplied by r satisfies the Schrödinger equation (units: $2m/\hbar^2 = 1$):

$$
d^{2}u/dr^{2}-\alpha^{2}u = \int_{0}^{\infty} V(r,r')u(r')dr',
$$

$$
\alpha = (-E)^{1/2}, \quad (A1)
$$

with

$$
V(r,r') = -g_1(r)g_1(r')/(g_1, L_1)
$$

\n
$$
-g_2(r)g_2(r')/(g_2, L_2),
$$

\n
$$
(g_i, L_j) = \int_0^\infty g_i(r)L_j(r)dr,
$$

\n
$$
L_j(r) = \int_0^\infty K(r,r')g_j(r')dr',
$$

and K is the Green's function:

$$
K(r,r') = -[e^{-\alpha r} \sinh \alpha r \cos \alpha r \cos \alpha]
$$

Then if $(g_1,L_2)=(g_2,L_1)=0$, which can easily be arranged, Eq. (Al) is clearly satisfied for any constants C_1 and C_2 by

$$
u = C_1 L_1(r) + C_2 L_2(r) .
$$

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