Determination of the S-wave scattering shape parameter P from the zero-energy wave-function

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We show that for S-wave scattering at an energy k^2 by a local potential which supports no more than one bound state, the shape parameter P and coefficients of higher powers of k^2 in the effective range expansion function $k\cot\delta = -1/a + \frac{1}{2}r_0k^2 - Pr_0^3k^4 + Qr_0^5k^6 + \cdots$, where δ is the phase shift, may be obtained from the zero-energy wave function, $u_0(r)$. Thus δ itself may be determined from u_0. We show that $Pr_0^3 = \int_0^R[\beta(r)u_0^2(r) - \bar{\beta}(r)\bar{u}_0^2(r)]dr$, where r_0 is the effective range, $\beta(r)$ is determined from an integral involving the wave function, and $\bar{\beta}(r)$ is a simple function of r which involves the scattering length and effective range.

I. INTRODUCTION

Recently, Klarsfeld *et al.*[1] have discussed in detail the importance of the shape dependence in low-energy NN scattering. The shape-dependent parameter P occurs in the (energy)^2 term in the effective range expansion of the S-state function $y = k\cot\delta$, where $k = (2mE/\hbar^2)^{1/2}$ and δ is the S-wave phase shift,

$$y(k^2) = k\cot\delta = -\frac{1}{a} + \tfrac{1}{2}r_0k^2 - Pr_0^3k^4 + k^6(\cdots). \quad (1)$$

In this expansion, a is the scattering length and r_0 is the effective range which may be obtained from the well-known expression,[2]

$$r_0 = 2\int_0^R [\bar{u}_0^2(r) - u_0^2(r)]dr, \quad (2)$$

where $\bar{u}_0$ is the zero-energy solution of the Schrödinger equation in the absence of a potential, normalized to $\bar{u}_0(0) = 1$ and equal to $u_0(r)$, the zero-energy wave function, for $r > R$, where R is a distance beyond which the potential may be neglected. In more recent work[3,4,5] involving the deuteron radius, the importance of the shape dependence has been further emphasized.

For a given potential $V(r)$ one can calculate the phase shift for a number of small energies using standard procedures, calculate values of the function $y(k^2)$ and use a least-squares-fit method to determine P. This is not always straightforward. For example, if we consider the triplet state $^3S_1$-$^3D_1$ of the neutron-proton system for the particular case of the Reid potential[6] and perform an expansion similar to Eq. (1) using the bar phase shift $\bar{\delta}(^3S_1)$, we find that the calculation of P is not simple.[7] This is because P is small for the Reid potential and more recent, unpublished, work suggests that it may actually be negative, in contradiction to the results obtained by Kermode and Allen.[7]

Thus, we were led to consider whether P for potential models could be determined more directly. In the next section we show that our attempt was successful by deriving an expression for P which involves integrals of the zero energy wave function.

II. THE SHAPE PARAMETER P

Consider a local potential $V(r)$ which supports no more than one bound state and the corresponding Schrödinger equations for the energies k^2 and 0 and for the S state ($\ell = 0$):

$$-u'' + V(r)u = k^2u, \quad (3)$$

$$-u_0'' + V(r)u_0 = 0. \quad (4)$$

The wave functions in Eqs. (3) and (4) satisfy the boundary conditions $u(0) = 0$ and $u_0(0) = 0$. Multiplying Eq. (3) by u_0, Eq. (4) by u, subtracting and integrating from the origin to some distance R beyond which the potentials are negligible, we have

$$(-u_0u' + uu_0')_0^R = k^2\int_0^R uu_0dr. \quad (5)$$

If we consider the solutions $\bar{u}(r)$ and $\bar{u}_0(r)$ of Eqs. (3) and (4) respectively in the absence of a potential [i.e., $V(r) \equiv 0$] with the boundary conditions $\bar{u}(R) = u(R)$ and $\bar{u}_0(R) = u_0(R)$, then

$$(-\bar{u}_0\bar{u}' + \bar{u}\bar{u}_0')_0^R = k^2\int_0^R \bar{u}\bar{u}_0dr \quad (6)$$

and

$$\bar{u}'(0)-\bar{u}_0'(0)=y(k^2)-y(0)=k^2\int_0^R(\bar{u}\bar{u}_0-uu_0)dr, \tag{7}$$

since $\bar{u}_0(0)=1=\bar{u}(0)$.

From Eqs. (1), (2), and (7), we have

$$Pr_0^3k^2-k^4(\cdots)=\int_0^R(\bar{u}_0^2-\bar{u}\bar{u}_0-u_0^2+uu_0)dr. \tag{8}$$

Hence,

$$Pr_0^3=\lim_{k^2\to 0}\frac{1}{k^2}\int_0^R(\bar{u}_0^2-\bar{u}\bar{u}_0-u_0^2+uu_0)dr. \tag{9}$$

For low energies, by considering a Taylor expansion in k^2 for the wave functions, neglecting terms of order k^4 and asssuming $u(r), u_0(r)$ have no zeros for $0<r<R$ (i.e., no more than one bound state), we may write

$$u(r)=[1+\beta(r)k^2]u_0(r), \tag{10}$$

$$\bar{u}(r)=[1+\bar{\beta}(r)k^2]\bar{u}_0(r), \tag{11}$$

from which it follows that Eq. (9) may be written

$$Pr_0^3=\int_0^R[\beta(r)u_0^2(r)-\bar{\beta}(r)\bar{u}_0^2(r)]dr, \tag{12}$$

the required result. We need now to determine the functions $\beta(r)$ and $\bar{\beta}(r)$. The determination of $\bar{\beta}(r)$ is simple, since

$$\begin{aligned}\bar{u}(r)&=\sin(kr)\cot\delta+\cos(kr)\\&=\left(1-\frac{r}{a}\right)+k^2\left(\frac{1}{2}rr_0+\frac{r^3}{6a}-\frac{r^2}{2}\right),\end{aligned} \tag{13}$$

to order k^2, from the expansions for $\sin(kr)$, $\cos(kr)$ and $k\cot\delta$ [Eq. (1)]. Hence,

$$\frac{\bar{u}(r)}{\bar{u}_0(r)}=1+k^2\frac{r(3ar_0+r^2-3ar)}{6(a-r)}, \tag{14}$$

giving, from Eq. (11),

$$\bar{\beta}(r)=\frac{r[3a(r_0-r)+r^2]}{6(a-r)}. \tag{15}$$

We note immediately that $\bar{\beta}(0)=0$, as required.

To determine $\beta(r)$, we substitute $u(r)$ from Eq. (10) into the Schrödinger Eq. (3),

$$\beta''u_0+2\beta'u_0'+(1+\beta k^2)u_0=0. \tag{16}$$

Letting $k^2\to 0$, we have a first-order differential equation for β', which may be written

$$(u_0^2\beta')'=-u_0^2. \tag{17}$$

Integrating from 0 to r,

$$u_0^2\beta'=-\int_0^r u_0^2(s)ds, \tag{18}$$

the constant of integration being zero. Dividing by $u_0^2(r)$ (which is nonzero for $0<r<R$ in the cases of no or one bound state) and integrating once again, we have

$$\beta(r)=-\int_0^r\frac{dt}{u_0^2(t)}\int_0^t u_0^2(s)ds+\text{const.} \tag{19}$$

Since $\beta(R)=\bar{\beta}(R)$, the constant of integration is determined and we have

$$\begin{aligned}\beta(r)&=\bar{\beta}(R)+\int_r^R\frac{dt}{u_0^2(t)}\int_0^t u_0^2(s)ds \text{ for } r\le R,\\&=\bar{\beta}(r) \text{ for } r\ge R.\end{aligned} \tag{20}$$

Eqs. (15), (20), and (12) enable P to be determined once the effective range r_0 and the scattering length a are known.

Before applying our formula to particular models, we note that Eqs. (10) and (16) may be extended to higher order terms in energy. Equation (10) may be generalized to

$$u(r)=\left(1+\sum_{n=1}^N\beta_{2n}(r)k^{2n}\right)u_0(r), \tag{21}$$

where $\beta_2(r)$ is our original $\beta(r)$. Equation (17) becomes

$$\sum_{n=1}[\beta_{2n+2}''+2\beta_{2n+2}'(u_0'/u_0)+\beta_{2n}]\,k^{2n+2}=0 \tag{22}$$

from which it follows that

$$\beta_{2n+2}''+2\beta_{2n+2}'(u_0'/u_0)+\beta_{2n}=0, \qquad n=1,2,\ldots. \tag{23}$$

Thus β_{2n+2}, and consequently higher-order terms in the expansion of $k\cot\delta$ may be determined. When the potential has a hard core within which the wave functions are zero, the β's need to be defined only for values of r greater than the core radius and the formulae still hold. By expanding Eq. (13) to higher order in k^2, the corresponding $\bar{\beta}_{2n}$ can be explicitly determined.

III. APPLICATION TO THE SQUARE WELL POTENTIAL

We apply our new formula to the simple case of the square well potential of depth K^2 and range R. The appropriate information is given in Table I. The evaluation of the integrals in Eq. (20) is straightforward and gives

$$\beta(r)=C+\frac{r}{2K}\cot(Kr), \tag{24}$$

where

TABLE I. Relevant quantities for the square well potential.

$u_0=A\sin(Kr),\ 0\le r\le R$
$\bar{u}_0=(a-r)/a$
$\tan(KR)=-K(a-R)$
$A^2=(K^2(a-R)^2+1)/(K^2a^2)$
$a=[KR-\tan(KR)]/K$
$r_0=R-R^3/(3a^2)-1/(K^2a)$

$$C = \bar{\beta}(R) - \frac{R}{2K}\cot(KR) = \frac{R^3}{6a}, \tag{25}$$

after substitution for r_0.

The second integral in Eq. (12) involves only a polynomial,

$$\int_0^R \bar{\beta}\bar{u}_0^2 dr = \frac{R^2}{60a^2}[\,15a^2r_0 + 10aR^2 - 10a^2R - 10ar_0R - 2R^3]. \tag{26}$$

The first integral is

$$\int_0^R \beta u_0^2 dr = A^2 \int_0^R \left[C + \frac{r}{2K}\cot(Kr)\right]\sin^2(Kr)dr \tag{27}$$

$$= A^2\left[\frac{CR}{2} - \frac{C}{4K}\sin(2KR) - \frac{R}{8K^2}\cos(2KR) + \frac{1}{16K^3}\sin(2KR)\right] \tag{28}$$

$$= \frac{R^3}{12a}\left[RA^2 + \frac{(a-R)}{K^2a^2}\right] + \frac{1}{8K^4a^2}\left[K^2a^2RA^2 - 2RKa^2 - (a-R)\right]. \tag{29}$$

From Eqs. (28) and (29), with a little help from the computer algebra software MAPLE we obtain

$$Pr_0^3 = (-45a^2 + 30K^4a^2R^4 - 30K^4a^3R^3 + 15K^2aR^3 - 18K^4aR^5 + 45K^2a^3R + 10K^4R^6)/(360K^4a^3), \tag{30}$$

in exact agreement with the expression obtained by the expansion of $k\cot\delta$ for a square well potential (see Preston and Bhaduri[8]), again using computer algebra.

IV. NUMERICAL APPLICATION

We have performed numerical integrations of Eqs. (12) and (20) for the cases of (i) the square well potential mentioned above and (ii) the Eckart potential which has a shape parameter with a value of zero.

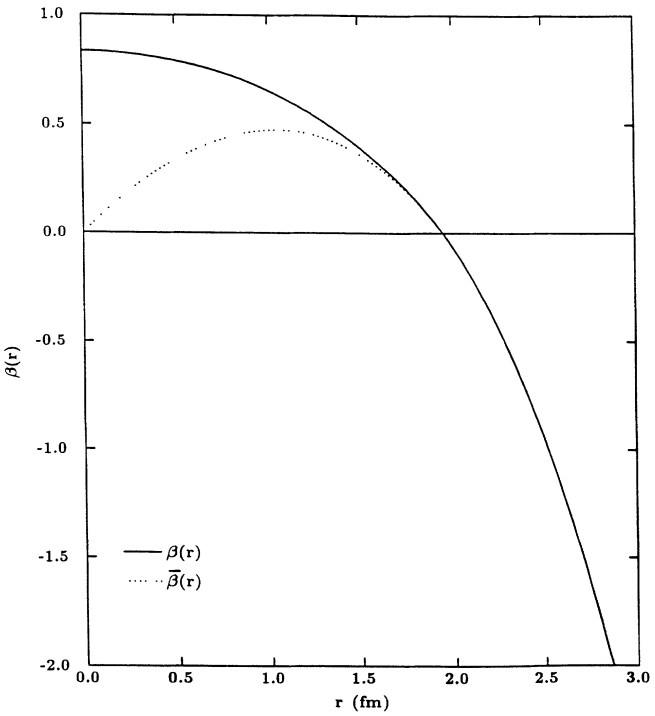

FIG. 1. The function $\beta(r)$ and $\bar{\beta}(r)$ for the square well potential.

First, with the square well potential (for which R is taken to be the range of the potential) an application of Simpson's rule for each of the three required integrations (over s, t, and r) gave a result in agreement with that from the formula (30). We used $R = 2.02$ fm and $K = 0.9343$ fm^{-1} for which $P = -0.040$. In Fig. 1, we show the behavior of the functions $\beta(r)$ and $\bar{\beta}(r)$. The numerical values agree with those obtained using Eqs. (24) and (15).

For the Eckart potential (see, for example, van Dijk and Kiang[9]),

$$V(r) = -\frac{2\lambda\gamma^2 e^{-\gamma r}}{(1+\lambda e^{-\gamma r})^2}, \tag{31}$$

the zero energy wave function is

$$u_0(r) = 1 - \frac{r}{a} - \frac{1}{2}[\gamma(1-\lambda)r + 2 + 2\lambda]\frac{e^{-\gamma r}}{1+\lambda e^{-\gamma r}} \tag{32}$$

and

$$y(k^2) = \frac{\gamma(1-\lambda)}{4\lambda} + \frac{1+\lambda}{\lambda\gamma}k^2. \tag{33}$$

For this potential the shape parameter is zero. Thus it provides a good test of our method. Considering, approximately, the singlet np state[2] with $a = -23.71$ fm and $r_0 = 2.4$ fm, we determined λ and γ from $\lambda = (1-2r_0/a)^{-1/2}$ and $\gamma = 2(1+\lambda)/(r_0\lambda)$, respectively. In Table II, we give the values of P for various choices of

TABLE II. Values for the shape parameter P for the Eckart potential.

R (fm)	P
5.0	−0.00097
6.0	−0.00026
7.0	−0.00006
8.0	−0.00002
9.0	−0.00000

R. In this table R has a slightly different meaning from that earlier in the text: for $r < R$, the wave function is that given by Eq. (32) and for $r > R$ the wave function has its asymptotic form. Thus there is a small discontinuity in the wave function if R is too small. In other words we have not amended the value of the scattering length in Eq. (33) to ensure continuity at R. This is not important here. We see that, for this case, our formula works very well.

In summary, we have shown that the coefficients of the effective range expansion can all be expressed in terms of the zero energy wave function. This feature is especially useful in the determination of the shape parameter, which is calculated in a straightforward manner by integrating simple functions made up of the square of the zero energy wave function. The presence of a hard core in the interaction is easily incorporated in the formalism. The numerical examples show that the method can be implemented for realistic local interactions whose wave functions tend to be known only numerically.

The extensions of our formula to the case of coupled channels and for the case when $u_0(r)$ has a zero for $r < R$ are under active consideration.

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