Counting the Bound States for Central Potentials

PETER SWAN
Département de Physique, Université Laval, Québec, Canada
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An interaction potential is fitted by a multiple-step function, step width $\Delta R \to 0$, to yield a first-order differential equation for phase function $\eta_l(k,r)$, and also an integral for the wave-function amplitude $A_l(k,r)$. Both neutral- and charged-particle scattering is treated. The number of bound states follows by integration of the $\eta_l(0,r)$ equation and Levinson's theorem $\eta_l(0,\infty)=n_l\pi$; also, for $U'(r\geq R)\geq 0$, one has $|\psi_0(r\geq R)|\leq 1$. An approximate method of evaluating all the eigenenergies via scattering phase shifts is discussed.

I. INTRODUCTION

THE number of bound states in a potential may be directly counted via numerical integration of the wave equation to find the corresponding eigenenergies. As one boundary condition is at $r=\infty$ and involves the unknown binding energy parameter, the latter must be guessed. The radial wave equation is integrated out from $r=0$ to a large r value, where the solution is checked for consistency with the asymptotic (parametrized) form. If inconsistent, the trial eigenvalue parameter must be changed, and the whole process repeated until consistent.

The process is very laborious, a large number of integrations being required. Moreover, it must be repeated for each bound state, with no assurance that some may have been missed, particularly loosely bound ones. However, extensive calculations of this type have been reported for the Debye–Hückel (Yukawa) potential.[1–3]

An alternative procedure[4] makes use of the properties of the zero-energy scattering length for neutral particles:

$$a_l=[(2l+1)!!]^2 \lim_{k\to 0} [-\tan\eta_l(k)/k^{2l+1}]. \tag{1}$$

If the strength parameter ω of the potential is steadily increased from zero, a_l changes sign each time a new bound state is formed, and the number of bound states for a given strength ω_s is given by the number of zeros of $a_l(\omega)$, $0<\omega\leq\omega_s$. The problem thus reduces to numerical integration of the radial wave equation at zero energy for a number of values of ω.

This is safer, more straightforward, and less work than the first method, although still somewhat laborious. The eigenenergy values, however, are not found at all.

A third method is to find conditions for the potential to have bound states. Writing

$$U(r)=(2\mu/\hbar^2)V(r), \tag{2}$$

Jost and Pais[5] showed that a necessary condition for bound states is

$$\int_0^\infty r|U(r)|dr \geqslant 1. \tag{3}$$

Bargmann[6] extended this result to a necessary condition for n_l bound states:

$$(2l+1)n_l \leqslant \int_0^\infty r|U(r)|dr, \tag{4}$$

which was later proved for tensor forces also by Schwinger.[7]

The condition (3) for a bound state of zero energy has been extended[8] to give a necessary condition for a bound S state of energy $-W$. Writing $\kappa^2=(2\mu|\hbar^2)|W|$, this is

$$\int_0^\infty r|U(r)|[1-e^{-2\kappa r}]/(2\kappa r)dr > 1. \tag{5}$$

Calogero[9–12] has derived both upper and lower limits to the number of bound states in a central potential. His upper limit for S states gives

$$n_l \leqslant n_0 \leqslant (2/\pi)\int_0^\infty |U(r)|^{1/2}dr, \quad U'(r)\geqslant 0. \tag{6}$$

Equation (6) is a better estimate for n_0 than (4), giving much smaller allowed values for $n_0\geq 2$. The example of a square well of depth U_0 and range b leads to $2n_0\leq U_0b^2$ from (4), $(\pi^2/4)n_0^2\leq U_0b^2$ from (6), and $(\pi^2/4)(2n_0-1)^2\leq U_0b^2$ in the exact calculation. Thus the true upper limit for S states is a good deal smaller than given even by the estimate (6), at least for $n_0\geqslant 2$.

In the fourth method following, we show how to count exactly the number of bound states in a very simple manner. The S-wave neutral scattering particle case is particularly straightforward and has special characteristics, so will be tackled first.

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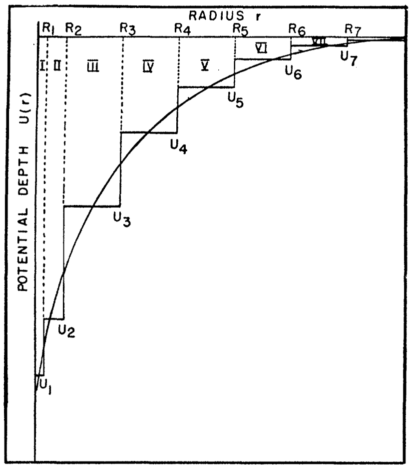

FIG. 1. Multiple-step approximation to a central potential.

II. AMPLITUDE AND PHASE-SHIFT EQUATIONS FOR NEUTRAL-PARTICLE SCATTERING, $l=0$

In Fig. 1, an attractive interaction potential between two particles is approximated by a multiple step function, defined in the region N by

$$U(r)=(2\mu/\hbar^2)V(r)=U_n \quad (R_{n-1}\leqslant r\leqslant R_n,\quad n\geqslant 1). \quad (7)$$

We restrict attention here to S-wave scattering of neutral particles, the wave function in region N being

$$\Psi_n(r)=A_n\sin(\kappa_n r+\eta_n)\,, \quad (8)$$

where

$$\kappa_n{}^2=-U_n+k^2,\quad U_n\leqslant 0. \quad (9)$$

Continuity of $\Psi'(r)/\Psi(r)$ at $r=R_n$ leads to

$$(\kappa_{n+1}/\kappa_n)\tan(\kappa_n R_n+\eta_n)=\tan(\kappa_{n+1}R_n+\eta_{n+1})\,. \quad (10)$$

Upon writing

$$\Delta U_n=U_{n+1}-U_n\,,\quad \Delta\eta_n=\eta_{n+1}-\eta_n\,,\quad \Delta A_n=A_{n+1}-A_n\,. \quad (11)$$

Equation (9) gives

$$\kappa_{n+1}{}^2=\kappa_n{}^2-\Delta U_n\,,\qquad \kappa_{n+1}=\kappa_n-\Delta U_n/(2\kappa_n)\,. \quad (12)$$

Equations (10), (11), and (12) may be combined, leading to the result

$$\Delta\eta_n=-(\Delta U_n/2\kappa_n)[(1/2\kappa_n)\sin 2(\kappa_n R_n+\eta_n)-R_n]\,. \quad (13)$$

In the limit as $\Delta R=R_{n+1}-R_n\to 0$, $\Delta U_n\to 0$, $\Delta\eta_n\to 0$, and we take $n\to\infty$. Equation (13) may then be put in the first-order differential equation form:

$$\eta'(r)=-\frac{1}{2\kappa(r)}\left\{\frac{1}{2\kappa(r)}\sin 2[\kappa(r)r+\eta(k,r)]-r\right\}U'(r)\,, \quad (14)$$

with boundary conditions $\eta(k,0)=0$, $\eta(k,\infty)=\eta_0(k)$.

Writing $\phi(k,r)=\kappa(r)r+\eta(k,r)$, an alternative statement of Eq. (14) is

$$\phi'(r)=[U'(r)/4\kappa^2(r)]\sin 2\phi(r)=\kappa(r)=[k^2-U(r)]^{1/2}. \quad (15)$$

Next, one considers the continuity relation

$$\kappa_{n+1}{}^2\Psi_n{}^2(R_n)+\{\Psi_n'(R_n)\}^2=\kappa_{n+1}{}^2\Psi_{n+1}{}^2(R_n)+\{\Psi_{n+1}'(R_n)\}^2, \quad (16)$$

which, with Eqs. (11) and (12), leads to

$$\Delta A_n/A_n=(\Delta U_n/2\kappa_n{}^2)\cos^2(\kappa_n R_n+\eta_n)\,, \quad (17)$$

so that for $\Delta R\to 0$ and $n\to\infty$, we obtain

$$A'(r)=\{A(k,r)/2\kappa^2(r)\}U'(r)\cos^2[\kappa(r)r+\eta(k,r)]. \quad (18)$$

This has the boundary condition $A(k,\infty)=1$ (unit normalization), and solution

$$A(k,r)=\exp\left\{-\frac{1}{2}\int_r^\infty [U'(r)/\kappa^2(r)]\times\cos^2[\kappa(r)r+\eta(k,r)]dr\right\}. \quad (19)$$

III. PROPERTIES OF THE PHASE-AMPLITUDE FUNCTIONS, $l=0$

First we investigate the behavior of the solutions $\eta_0(k,r)$ of Eq. (14). The two main cases are

(a) *Nonsingular potentials*, $U(0)=-U_0$. A series expansion of $\eta_0(k,r)$ gives the leading term

$$\eta_0(k,r\to 0)\approx(1/12)\kappa(0)U'(0)r^4,\quad \kappa^2(0)=k^2+U_0. \quad (20)$$

(b) *Singular potentials*, $U(r\to 0)=-U_0r^{2\epsilon-2}$, $0<\epsilon<1$. One finds here, that

$$\eta_0(k,r\to 0)\approx\frac{2}{3}\left(\frac{1-\epsilon}{1+2\epsilon}\right)U_0{}^{3/2}r^{3\epsilon}. \quad (21)$$

For both (a) and (b), there is therefore no difficulty in numerically integrating Eq. (14) outwards to obtain $\eta_0(k)$. Note that $\eta_0'(r)$ changes sign when $U'(r)$ changes sign, with one unlikely exception.

The amplitude function (19) for $A(k,r)$ is finite everywhere in case (a) above; in (b) we find $A(k,r\to 0)\approx r^{1-\epsilon}$, with the wave function (8) giving $\psi(r\to 0)\propto r$ as usual.

If $U'(r\geq R)\geq 0$, Eq. (18) shows $A'(r\geq R)\geq 0$, so that from Eq. (19), $A(k,r\geq R)\leq 1$, and $|\Psi_0(k,r\geq R)|\leq 1$. Thus $|\Psi_0(k,r)|\leq 1$ for a monotonically decreasing attractive potential ($l=0$ only). If $U'(r\leq R)<0$, a reflection effect in the region $r\leq R$ may be sufficient to make $|\Psi_0(k,r\leqslant R)|>1$.

IV. COUNTING THE COMPOSITE BOUND STATES

At zero energy, one numerically integrates Eq. (14) for $\eta_0(0,r)$ out to $r=R$, where $U(r\geq R)\approx 0$, obtaining, for example $\eta_0(0,R)\approx\eta_0(0,\infty)=\eta_0(0)$.

Levinson's theorem for $\eta_l(k)$ is[13,14]

$$\eta_l(0)-\eta_l(\infty)=\eta_l\pi\,, \tag{22}$$

subject to the condition

$$\int_0^\infty r^j|U(r)|dr<\infty \quad (j=1,2)\,, \tag{23}$$

which also results in

$$\eta_l(\infty)=0. \tag{24}$$

The number of bound states follows from $\eta_l(0)=\eta_l\pi$, unless an $l=0$ resonant state occurs at zero energy, changing the result to

$$\eta_0(0)=(\eta_0+\tfrac{1}{2})\pi.$$

V. NEUTRAL-PARTICLE PHASE-AMPLITUDE EQUATIONS FOR ARBITRARY l VALUES

We again employ the step function (7) for the potential $U(r)$, but the wave function (8) in region N is replaced by

$$\Psi_{ln}(r)=A_{ln}[\mathcal{J}_l(\kappa_n r_n)\cos\eta_l(\kappa_n)-\mathfrak{N}_l(\kappa_n r_n)\sin\eta_l(\kappa_n)]\,, \tag{25}$$

where in terms of the spherical Bessel and Neumann functions of Schiff,[15]

$$\mathcal{J}_l(x)=xj_l(x)\,,\quad \mathfrak{N}_l(x)=xn_l(x). \tag{26}$$

Continuity of $\Psi_{ln}'(r)/\Psi_{ln}(r)$ at $r=r_n$ leads to

$$\kappa_n\left\{\frac{\mathcal{J}_l'(\kappa_n r_n)-\tan\eta_l(\kappa_n)\mathfrak{N}_l'(\kappa_n r_n)}{\mathcal{J}_l(\kappa_n r_n)-\tan\eta_l(\kappa_n)\mathfrak{N}_l(\kappa_n r_n)}\right\}=\kappa_{n+1}\left\{\frac{\mathcal{J}_l'(\kappa_{n+1}r_n)-\tan\eta_l(\kappa_{n+1})\mathfrak{N}_l'(\kappa_{n+1}r_n)}{\mathcal{J}_l(\kappa_{n+1}r_n)-\tan\eta_l(\kappa_{n+1})\mathfrak{N}_l(\kappa_{n+1}r_n)}\right\}, \tag{27}$$

where the prime stands for $d/d\rho=d/d(\kappa r)$.

From Eqs. (11) and (12), we have

$$\mathcal{J}_l(\kappa_{n+1}r_n)=\mathcal{J}_l(\kappa_n r_n)-(r_n/2\kappa_n)(\Delta U_n)\mathcal{J}_l'(\kappa_n r_n)\,, \tag{28}$$

$$\mathcal{J}_l'(\kappa_{n+1}r_n)=\mathcal{J}_l'(\kappa_n r_n)-(r_n/2\kappa_n)(\Delta U_n)\mathcal{J}_l''(\kappa_n r_n)\,, \tag{29}$$

with analogous relations holding for $\mathfrak{N}_l(\kappa_{n+1}r_n)$ and $\mathfrak{N}_l'(\kappa_{n+1}r_n)$. We substitute these into Eq. (27) and employ the identities

$$\mathcal{J}_l'(\kappa_n r_n)=[(l+1)/\kappa_n r_n]\mathcal{J}_l(\kappa_n r_n)-\mathcal{J}_{l+1}(\kappa_n r_n)\,, \tag{30}$$

$$\mathcal{J}_l''(\kappa_n r_n)=-\{1-[l(l+1)/\kappa_n^2 r_n^2]\}\mathcal{J}_l(\kappa_n r_n)\,, \tag{31}$$

$$\tan\eta_l(\kappa_{n+1})=\tan\eta_l(\kappa_n)+\Delta\eta_l(\kappa_n)\sec^2\eta_l(\kappa_n)\,. \tag{32}$$

Finally, one obtains

$$\Delta\eta_l(\kappa_n)=\frac{r_n}{2\kappa_n}\left\{\psi_l^2(\kappa_n r_n)-\frac{(2l+1)}{\kappa_n r_n}\psi_l(\kappa_n r_n)\phi_{l+1}(\kappa_n r_n)+\phi_{l+1}^2(\kappa_n r_n)\right\}\Delta U_n\,, \tag{33}$$

and then

$$\eta_l'(r)=\frac{r}{2\kappa(r)}\left[\psi_l^2(r)-\frac{(2l+1)}{\kappa(r)r}\psi_l(r)\phi_{l+1}(r)+\phi_{l+1}^2(r)\right]U'(r)\,, \tag{34}$$

where $\eta_l'(r)=d\eta_l(r)/dr$, $\kappa=\kappa(r)$, and

$$\psi_l(r)=\mathcal{J}_l(\kappa r)\cos\eta_l(r)-\mathfrak{N}_l(\kappa r)\sin\eta_l(r)\,, \tag{35}$$

$$\phi_{l+1}(r)=\mathcal{J}_{l+1}(\kappa r)\cos\eta_l(r)-\mathfrak{N}_{l+1}(\kappa r)\sin\eta_l(r). \tag{36}$$

Equation (34) is a first-order differential equation, which may be integrated outwards from $r=0$ to find the phase shift, via $\eta_l(k,r\geq R)\approx\eta_l(k,\infty)=\eta_l(k)$, where $U(r\geq R)\approx 0$. It is first necessary to know the behavior of $\psi_l(r\to 0)$, the two main cases being

(a) *Nonsingular potentials*, $U(0)=-U_0$. A series expansion of $\eta_l(k,r)$ leads to

$$\eta_l(k,r\to 0)\approx\frac{\kappa^{2l+1}(0)U'(0)r^{2l+4}}{(2l+1)!!(2l+3)!!(2l+4)}. \tag{37}$$

(b) *Singular potentials*, $U(r\to 0)=-U_0 r^{2\epsilon-2}$, $0<\epsilon<1$. One finds here that

$$\eta_l(k,r\to 0)\approx\frac{2(1-\epsilon)}{(2l+1+2\epsilon)}\frac{U_0^{l+3/2}r^{(2l+3)\epsilon}}{(2l+1)!!(2l+3)!!}. \tag{38}$$

The number of bound states η_l follows as in Sec. IV, $\eta_l(0,r)$ being integrated out via Eq. (34) to give $\eta_l(0,\infty)=\eta_l(0)$, say. Levinson's theorem [Eqs. (22)–(24)] then gives η_l via $\eta_l(0)=\eta_l\pi$.

An amplitude equation may be obtained using the continuity of $\Psi_{ln}(r)$ at $r=r_n$. Thus

$$A_{ln}[\mathcal{J}_l(\kappa_n r_n)\cos\eta_l(\kappa_n)-\mathfrak{N}_l(\kappa_n r_n)\sin\eta_l(\kappa_n)]=A_{l,n+1}[\mathcal{J}_l(\kappa_{n+1}r_n)\cos\eta_l(\kappa_{n+1})-\mathfrak{N}_l(\kappa_{n+1}r_n)\sin\eta_l(\kappa_{n+1})]; \tag{39}$$

leading via Eq. (11) for ΔA_n to

$$\Delta A_{ln}/A_{ln}=-\Delta\psi_l(\kappa_n,r_n)/\psi_l(\kappa_n,r_n). \tag{40}$$

On evaluating $\Delta\psi_l$ from Eqs. (35) and (33), Eq. (40) leads to

$$\Delta A_{ln}=\frac{r_n}{2\kappa_n}A_{ln}\left[\frac{(l+1)}{\kappa_n r_n}\frac{\phi_{l+1}(\kappa_n,r_n)}{\psi_l(\kappa_n,r_n)}-\chi_l(\kappa_n,r_n)\left\{\psi_l(\kappa_n,r_n)-\frac{(2l+1)}{\kappa_n r_n}\phi_{l+1}(\kappa_n,r_n)+\frac{\phi_{l+1}^2(\kappa_n,r_n)}{\psi_l(\kappa_n,r_n)}\right\}\right]. \tag{41}$$

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[13] N. Levinson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **25**, 9 (1949).
[14] P. Swan, Nucl. Phys. **46**, 669 (1963).
[15] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949).

Thus one obtains

$$A_l'(r)=\frac{r}{2\kappa(r)}A_l(r)\left[\frac{(l+1)}{\kappa(r)r}\frac{\phi_{l+1}}{\psi_l}-\chi_l\left\{\psi_l-\frac{(2l+1)}{\kappa(r)r}\phi_{l+1}+\phi_{l+1}^2/\psi_l\right\}\right]U'(r), \quad (42)$$

where

$$\chi_l(r)=-\mathcal{J}_l(\kappa r)\sin\eta_l(r)-\mathfrak{N}_l(\kappa r)\cos\eta_l(r) \quad (43)$$

and $\kappa=\kappa(r)=[k^2-U(r)]^{1/2}$.

Equation (42) is easily integrated to give

$$A_l(r)=\exp\left\{-\frac{1}{2}\int_r^\infty\frac{r}{\kappa(r)}U'(r)\left[\frac{(l+1)}{\kappa(r)r}\frac{\phi_{l+1}}{\psi_l}-\chi_l(r)\left(\psi_l-\frac{(2l+1)}{\kappa(r)r}\phi_l+\frac{\phi_{l+1}^2}{\psi_l}\right)\right]dr\right\}, \quad (44)$$

where we have used the boundary condition $A_l(\infty)=1$.

Comparison of Eq. (44) with its $l=0$ form [Eq. (18)] shows that the property $|\psi_0(k,r\geq R)|\leq 1$ for $U'(r\geq R)\geq 0$ does not extend to $\psi_{l\geq 1}(k,r)$. The reason is the existence of the centrifugal barrier, the true potential seen by the particles being $U(r)+l(l+1)/r^2$. This is not a monotonically decreasing attractive potential obeying condition (23), so that $|\psi_{l\geq 1}(k,r)|$ may exceed 1.

An example is that of zero potential, where $\mathcal{J}_{l\geq 1}(x)>1$ for some x values in an intermediate range.

VI. CHARGED-PARTICLE PHASE-AMPLITUDE EQUATIONS AND BOUND STATES

In the region N of the step function of Fig. 1, we write the charged particle wave function as

$$\Psi_{ln}(r)=A_{ln}[F_l(\kappa_n,r_n)\cos\eta_l(\kappa_n)+G_l(\kappa_n,r_n)\sin\eta_l(\kappa_n)], \quad (45)$$

where $F_l(\kappa_n,r_n)$ and $G_l(\kappa_n,r_n)$ are the regular and irregular Coulomb wave functions.

We again employ the continuity of $\Psi_{ln}'(r)/\Psi_{ln}(r)$ at $r=r_n$, with relations corresponding to Eqs. (27)–(29) obtained via the substitutions

$$\mathcal{J}_l(\kappa r)\rightarrow F_l(\kappa,r), \quad \mathfrak{N}_l(\kappa r)\rightarrow -G_l(\kappa,r).$$

However, Eq. (30) is replaced by the new form[16]

$$(l+1)F_l'(\rho_n)=\{(l+1)^2/\rho_n+\alpha_n\}F_l(\alpha_n,\rho_n)-\{(l+1)^2+\alpha_n^2\}^{1/2}F_{l+1}(\alpha_n,\rho_n), \quad (46)$$

where $\kappa(r)$ is defined in Eq. (15), and

$$\rho(r)=\kappa(r)r, \quad \alpha(r)=\beta/2\kappa(r), \quad \beta=(2\mu/\hbar^2)ZZ'e^2. \quad (47)$$

An identical relation holds for $G_l'(\rho)$, but Eq. (31) is replaced by

$$F_l''(\rho_n)=\{1-2\alpha_n/\rho_n-l(l+1)/\rho_n^2\}F_l(\rho_n), \quad (48)$$

the same form holding for $G_l''(\rho_n)$, and Eq. (32) is unaltered.

The procedure of Sec. V leads to the result

$$\Delta\eta_l(\kappa_n)=\frac{r_n}{2\kappa_n}\left\{\left[1-\frac{\alpha_n}{\rho_n}\left(2+\frac{1}{(l+1)}\right)+\alpha_n^2/(l+1)^2\right]\psi_l^2(\kappa_n,r_n)-[(2l+1)/\rho_n+2\alpha_n/(l+1)]\psi_l(\kappa_n,r_n)\phi_l(\kappa_n,r_n)+[1+\alpha^2/(l+1)^2]\phi_{l+1}^2(\kappa_n,r_n)\right\}\Delta U_n, \quad (49)$$

and hence

$$\eta_l'(r)=\frac{r}{2\kappa(r)}\left\{\left[1-\frac{\beta}{2\kappa^2(r)r}\left(2+\frac{1}{(l+1)}\right)+\frac{\beta^2}{4(l+1)^2\kappa^2(r)}\right]\psi_l^2(r)-\frac{1}{\kappa(r)}\left[\frac{(2l+1)}{r}+\frac{\beta}{(l+1)}\right]\psi_l(r)\phi_{l+1}(r)+\left[1+\frac{\beta^2}{4(l+1)^2\kappa^2(r)}\right]\phi_{l+1}^2(r)\right\}U'(r), \quad (50)$$

where

$$\psi_l(r)=F_l(\kappa r)\cos\eta_l(r)+G_l(\kappa r)\sin\eta_l(r), \quad (51)$$

$$\phi_{l+1}(r)=F_{l+1}(\kappa r)\cos\eta_l(r)+G_{l+1}(\kappa r)\sin\eta_l(r). \quad (52)$$

As for neutral particles, Eq. (50) may be integrated outwards from $r=0$ to give $\eta_l(k,R)\approx\eta_l(k,\infty)=\eta_l(k)$ say, where $U(r\geq R)\approx 0$. In particular, $\eta_l(0,r)$ yields $\eta_l(0,R)\approx\eta_l(0,\infty)=\eta_l(0)=\eta_{l}\pi$ via Levinson's theorem [Eqs. (22)–(24)], thus fixing the number of states bound in the short-range potential field $U(r)$ (with Coulomb modifications).

[16] *Handbook of Mathematical Functions*, edited by M. Abamowitz and I. A. Stegun (U. S. Department of Commerce, National Bureau of Standards, Washington, D. C., 1964), Appl. Math. Ser. 55, p. 539.

The integration requires knowledge of $\eta_l(k, r\to 0)$, obtained via series expansions. The two main cases are

(a) *Nonsingular potential* $U(0)=-U_0$. We find that

$$\eta_l(k, r\to 0)\approx -\beta\frac{U'(0)}{4(l+1)}C_l^2(\kappa(0))\kappa^{2l-1}(0)r^{2l+3}+\frac{U'(0)C_l^2(\kappa(0))\kappa^{2l+1}(0)}{2(2l+4)}$$
$$\times\left\{1-(2l+1)\frac{C_{l+1}(\kappa(0))}{C_l(\kappa(0))}+\frac{\beta}{4(l+1)\kappa^2(0)}\left[\left(\frac{2l+1}{2l+3}\right)\frac{C_l(\kappa(0))}{C_{l+1}(\kappa(0))}\frac{U'(0)}{\kappa^2(0)}-2\left(\frac{2l+3}{l+1}\right)\right]+\frac{\beta^2}{4(l+1)^2\kappa^2(0)}\right\}r^{2l+4}, \quad (53)$$

where [cf. Eq. (47)]

$$C_l(\kappa(r))=[(2l+1)!]^{-1}2^l(2\pi\alpha)^{1/2}[\exp(2\pi\alpha)-1]^{-1/2}\prod_{\nu=1}^{l}(\nu^2+\alpha^2)^{1/2}. \quad (54)$$

For zero Coulomb field ($f=0$), Eq. (53) reduces to the neutral particle value (37).

(b) *Singular potential*, $U(r\to 0)\to -U_0r^{2\epsilon-2}$. For $0<\epsilon\leq\frac{1}{2}$, one obtains

$$\eta_l(k, r\to 0)\approx\frac{2U_0^{l+3/2}(1-\epsilon)}{(2l+1)!!(2l+3)!!(2l+1+2\epsilon)}r^{(2l+3)\epsilon}. \quad (55)$$

For $\frac{1}{2}\leq\epsilon<1$, the leading terms are

$$\eta_l(k, r\to 0)\approx\frac{U_0^{l+1/2}(1-\epsilon)}{(2l+1)!!}\left[-\beta\frac{(2l+3)}{2(l+1)^2}r^{(2l+1)\epsilon+1}+\frac{2U_0r^{(2l+3)\epsilon}}{(2l+3)!!(2l+1+2\epsilon)}\right]. \quad (56)$$

VII. EVALUATION OF BOUND-STATE ENERGIES

The eigenenergies may be evaluated approximately via the scattering phase shifts, avoiding the cumbersome consistency procedure outlined at the lead of Sec. I. The two cases involved are

(a) $\eta_l(0)=\pi$, $\eta_l(k>0)<\pi$. Note that $n_l=1$ implies $\eta_l(0)=\pi$ and vice versa, but *not* $\eta_l(k>0)<\pi$. Examples of $\eta_l(0)=\pi$, $\eta_l(k>0)\geq\pi$ may be seen for $l=0$ square well scattering in Fig. 2.

The scattering phases $\eta_l(k)$ obey the shape-dependent formula for neutral particles[17]:

$$[(2l+1)!!]^{-2}k^{2l+1}\cot\eta_l(k)\approx\sum_{m=0}^{N}(-1)^{m+1}C_{lm}k^{2m}, \quad (57)$$

or for charged particles[18]

$$C_l^2k^{2l+1}\cot\eta_l(k)+[(2l+1)!(2l+1)]^{-1}\sum_{n=0}^{2l}[(-1)^n\beta^n/n!][1-n/(2l-n+1)]\Psi_l^{(2l-n+1)}(0)$$
$$+(2l+1)^{-1}\{k^{2l+1}p_l(\alpha)[Q_l(\alpha)-\sum_{s=1}^{2l}1/s]+[(2l)!(2l+1)!]^{-1}\beta^{2l+1}\sum_{s=1}^{2l}1/s+k^{2l+1}r_l(\alpha)\}\approx\sum_{m=0}^{N}(-1)^{m+1}C_{lm}k^{2m}. \quad (58)$$

Here C_{lm} $(m=0,\cdots,N)$ are scattering coefficients, and the quantities $C_l(k)$, $\Psi_l(r)$, $p_l(\alpha)$, $Q_l(\alpha)$ and $r_l(\alpha)$ are well known in Coulomb scattering.[16,18]

The C_{lm} coefficients are found via the least-square fitting of calculated $\eta_l(k)$ curves (57) or (58) with an orthogonal series in powers of k^2 (Legendre or Tchebycheff polynomials are suitable). The coefficients $C_{l0}=1/a_l$ and $C_{l1}=r_l/2$ are constants, but for $m\geq 2$, $C_{lm}=C_{lm}(E_{\max})$ for an energy range $E=0-E_{\max}$ (except for very low energies, where the series for $N\to\infty$ is convergent),[17]

The wave function for large $x_l=kr-\frac{1}{2}l\pi$ has the asymptotic form

$$\phi_l(k, r\to\infty)=\exp(-ix_l)-S(k)\exp(ix_l), \quad (59)$$

so that a bound state requires $k=-i\alpha$ (α real, positive) and $S(k)=\exp[2i\eta_l(k)]=0$; equivalent to

$$k=-i\alpha,\quad \cot\eta_l(k)=-i. \quad (60)$$

Equations (57) and (60) become

$$[(2l+1)!!]^{-2}(-1)^{l+1}\alpha^{2l+1}\approx\sum_{m=0}^{N}C_{lm}\alpha^{2m}, \quad (61)$$

which may be solved numerically to find α, only real, positive solutions corresponding to bound states.

[17] P. Swan and W. A. Pearce, Nucl. Phys. **79**, 77 (1966).
[18] P. Swan, Nucl. Phys. (to be published).

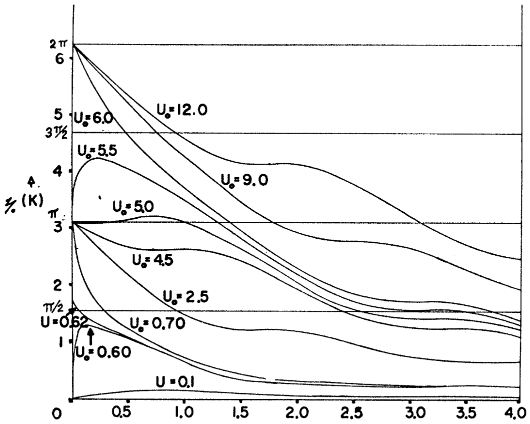

FIG. 2. Phase shifts $\eta_0(k)$ for a square well of width 2.0 F and depth $U_0=(2\mu/\hbar^2)V_0$ F^{-2}.

The binding energy $-W$ in each case is related to α by $\alpha^2=(2\mu/\hbar^2)W$ ($W\geq 0$). The charged particle case (58) follows similarly to (61).

(b) $\eta_l(0)=\eta_l\pi(\eta_l\geq 1)$. Relations (57) and (58) are invalid if $\eta_l(k>0)\geq\pi$. However, any empirical function with the right properties, and flexible enough to fit typical $\eta_l(k)$ curves, may be used instead. Figure 2 shows a number of $\eta_0(k)$ curves for a square well of width 2.0 F and variable depth $U_0=(2\mu/\hbar^2)V_0$ F^2.

A suitable empirical modification of Eq. (57) for neutral particles is

$$[(2l+1)!!]^{-2}k^{2l+1}\cot\eta_l(k)$$

$$=A_l^{-1}(k)\frac{\prod_{\gamma=1}^{q_l}(1-\mu_{l\nu}^2k^2)}{\prod_{\nu=1}^{p_l}(1-\lambda_{l\nu}^2k^2)}\sum_{m=0}^{N}(-1)^{m+1}D_{lm}k^2, \quad (62)$$

where

$$A_l(k)=\{1+[\prod_{\nu=1}^{p_l}(\lambda_{l\nu}/\mu_{l\nu})^2]^{-1}k^2\}(1+k^2)^{-1}, \quad p_l=q_l,$$

$$=\{1+(-1)^{p_l-q_l}[(\prod_{\nu=1}^{q_l}\mu_{l\nu}^2)/(\prod_{\nu=1}^{p_l}\lambda_{l\nu}^2)]\times k^{2(p_l-q_l)}\}^{-1}, \quad p_l>q_l. \quad (63)$$

Equation (62) allows explicitly for p_l values of $\eta_l(k)=s_l\pi$ (s_l=positive integer ≥ 1) at $k^2=\lambda_{l\nu}^{-2}(\nu=1\cdots p_l)$ and q_l values of $\eta_l(k)=(s_l+\frac{1}{2})\pi)$ at $k^2=\mu_{l\nu}^{-2}$ $(\nu=1\cdots q_l)$.

The charged-particle expression (58) has the same modification on the right as Eq. (62), but q_l is here the number of zeros from the left of Eq. (58).

Equations (60) and (62) give

$$[(2l+1)!!]^{-2}(-1)^{l+1}\alpha^{2l+1}\approx A_l^{-1}(-i\alpha)$$
$$\times[\prod_{\nu=1}^{q_l}(1+\mu_{l\nu}^2\alpha^2)/\prod_{\nu=1}^{p_l}(1+\lambda_{l\nu}^2\alpha^2)]\sum_{m=0}^{N}D_{lm}\alpha^{2m}, \quad (64)$$

which may be solved numerically in the same way as Eq. (61), only real, positive α values giving bound-state energies.

The phase shifts $\eta_l(k)$ can be calculated via the method used in this paper, but it is simpler to solve the Schrödinger wave equation directly, as no spherical Bessel, Neumann, or Coulomb wave functions are then involved.

The best method is to solve an alternative phase equation due to Drukarev and others,[19] obtained by writing

$$\psi_l'(r)/\psi_l(r)=u_l(r)=k\cot[kr+\delta_l(r)]. \quad (65)$$

This leads to the equation

$$\delta_l'(r)+k^{-1}[U(r)+l(l+1)/r^2]\sin^2[kr+\delta_l(r)]=0, \quad (66)$$

where $\delta_l(k,r)$ is unrelated to $\eta_l(k,r)$ above, but

$$\delta_l(k,\infty)=\delta_l(k)=\eta_l(k)-\tfrac{1}{2}l\pi.$$

The modification to Coulomb fields gives

$$\delta_l'(r)+k^{-1}[U(r)+\beta/r+l(l+1)/r^2]$$
$$\times\sin^2[kr-\alpha\ln 2kr+\sigma_l+\delta_l(r)]=0, \quad (67)$$

where $\sigma_l=\arg\Gamma(i\alpha+l+1)$.

For a given potential $U(r)$, a series solution for $\eta_l(r\rightarrow 0)$ is employed to start the numerical integration off for small r, $\eta_l(k)$ being found for $r\geq R(U(r\geq R)\approx 0)$.

It should be noted that Eqs. (66), (67), and their variants[19] (which also involve spherical Bessel, Neumann, and Coulomb wave functions) are quite unrelated to Eqs. (34) and (50) of this paper. In particular, as they involve k rather than $\kappa(r)=[k^2-U(r)]^{1/2}$, they determine only the scattering length [via an equation for $a_l(r)$] at zero energy,[8] and not the number of bound states n_l.

[19] P. M. Morse and W. P. Allis, Phys. Rev. 44, 269 (1933); G. F. Drukarev, Zh. Eksperim. i Teor. Fiz. 19, 247 (1949); G. T. Kynch, Proc. Phys. Soc. (London) 65, 83 (1952); S. Franchetti, Nuovo Cimento 6, 601 (1957); F. Calogero, *ibid.* 17, 261 (1963).