ON THE ACCURACY OF THE TAN η_l DISTORTED WAVE APPROXIMATION FOR SCATTERING PHASE-SHIFTS

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Summary

The distorted wave approximation for $\tan \eta_l$ involves a wave function distorted from its asymptotic form at $r \to \infty$ by a form factor $g_l(r)$. Schwinger's variational principle is adapted to show that increasing the number of variable parameters in $g_l(r)$ does not necessarily improve the first-order fit to the scattering parameters. Results are given for ^{3}S and ^{1}S neutron-proton scattering for several potential well shapes, including the effective range r_0 and first shape parameter P_0.

It is concluded that the distorted wave method gives maximum accuracy with a simple form factor with only one variable parameter λ_l, adjusted to fit the zero-energy scattering length a_l. The use of additional parameters is not in general justified by the results.

I. Introduction

The distorted wave approximation for elastic scattering phases is given by (Swan 1960*a*, 1960*b*, 1960*c*, 1961)

$$\tan \eta_l \approx B_{1l}/(1-B_{2l}), \tag{1}$$

where

$$B_{1l} = -\frac{1}{k}\int_0^\infty \mathrm{d}r\, U(r)\mathscr{J}_l^2(kr) = \eta_l(B.O.),$$

$$B_{2l} = \frac{1}{k}\int_0^\infty \mathrm{d}r\, U(r) g_l(r)\mathscr{J}_l(kr)\mathscr{N}_l(kr). \tag{2}$$

Here $U(r) = (2\mu/\hbar^2)V(r)$, μ being the reduced mass of the two-body system, and $V(r)$ the interaction potential. The modified spherical Bessel and Neumann functions $\mathscr{J}_l(x)$ and $\mathscr{N}_l(x)$ are

$$\mathscr{J}_l(x) = x j_l(x), \qquad \mathscr{N}_l(x) = x n_l(x),$$

where $j_l(x)$ and $n_l(x)$ are the spherical Bessel and Neumann functions as defined by Schiff (1949).

The form factor $g_l(r)$ must satisfy the boundary conditions

$$g_l(r \to 0) \approx r^{2l+1}, \qquad g_l(r \to \infty) = 1.$$

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For tailed potentials, a suitable form for $g_l(r)$ has been found to be (Swan 1960c) the two-parameter function

$$g_l(r) = A_l r^{2l+1}\phi_l(\lambda_l,r)+[1-\phi_l(\lambda_l,r)]^{2l+1}, \tag{3}$$

where $\phi_l(\lambda_l,r)$ is taken with a similar form to the potential $V(r)$ (or as nearly as is practicable). In particular, $\phi_l(\lambda_l,r)$ must satisfy the conditions

$$\phi_l(\lambda_l,0) = 1, \qquad \phi_l(\lambda_l,\infty) = 0.$$

Earlier calculations for $l = 0$ took $\phi_l(\lambda_l,r)$ with the same range parameter as $V(r)$, corresponding to $\lambda_0 = 1$, with A_0 determined to give the correct zero energy scattering length a_0 (Swan 1960c). Computed results for the phase-shift η_0 and effective range r_0 were in good agreement with exact figures, except for singular potentials such as the Yukawa interaction, where the agreement was fair.

The purpose of the present paper is to show that it is in general not practicable to fit exactly higher parameters in the shape-independent expansion for $k \cot \eta_l$ by increasing the number of adjustable parameters in equation (3) for $g_l(r)$. For example, the effective range r_l cannot in general be fitted exactly by adjusting λ_l. This means that equation (1) for $\tan \eta_l$ cannot be made as accurate as one likes by putting more parameters in $g_l(r)$, results being characteristically insensitive to minor adjustments of $g_l(r)$.

It is possible, however, to use a variational principle for $k \cot \eta_l$ to improve somewhat the fit for η_l, the parameter λ_l in equation (3) being taken as adjustable. The improvement in accuracy is appreciable in those cases where the error is largest, such as the Yukawa potential, but is negligible where η_l is already fitted to 2–3% accuracy.

If the one-parameter form factor for $A_l = 0$,

$$g_l(r) = [1-\phi_l(\lambda_l,r)]^{2l+1}, \tag{4}$$

is used instead of equation (3), and λ_l is varied to fit a_l, results of equivalent accuracy are attained for η_l. In some cases, viz. $\phi_0(\lambda_0,r) = \exp(-\lambda_0 r/b)$, the variational method above gives $A_0 = 0$, and hence relation (4) for $g_l(r)$. In general, however, equation (4) gives as good an accuracy for η_l as is attainable, and the use of extra parameters, as in (3), does not give better fits to the effective range and shape parameters.

II. The Shape-independent Formula for Arbitrary l

If we expand $\mathscr{J}_l(kr)$ and $\mathscr{N}_l(kr)$ in power series, we find from (2) the expansions (Swan 1963)

$$\left.\begin{aligned} B_{1l} &= \frac{k^{2l+1}}{[(2l+1)!!]^2}\left[M_{2l+2}-\frac{1}{(2l+3)}M_{2l+4}k^2+\frac{(l+2)}{(2l+3)^2(2l+5)}M_{2l+6}k^4+\ldots\right], \\ B_{2l} &= \frac{1}{(2l+1)}\left[P_{l1}+\frac{2P_{l3}}{(2l-1)(2l+3)}k^2+\frac{6P_{l5}}{(2l-1)(4l^2-9)(2l+5)}k^4+\ldots\right], \end{aligned}\right\} \tag{5}$$

where

$$M_n = -\int_0^\infty \mathrm{d}r\, U(r)r^n, \qquad P_{ln} = -\int_0^\infty \mathrm{d}r\, g_l(r)U(r)r^n. \tag{6}$$

Equations (1) and (5) lead to the result

$$[(2l+1)!!]^{-2}k^{2l+1}\cot\eta_l(k) = -1/a_l+\tfrac{1}{2}r_l k^2 - P_l r_l^3 k^4 + \ldots, \tag{7}$$

where

$$-1/a_l \approx \frac{1}{M_{2l+2}}[1-P_{l1}/(2l+1)], \tag{8}$$

$$r_l \approx \frac{2}{(2l+3)M_{2l+2}}\left[\frac{2}{(1-4l^2)}P_{l3}-M_{2l+4}/a_l\right], \tag{9}$$

$$-P_l r_l^3 \approx \frac{1}{2(2l+3)M_{2l+2}}\left[M_{2l+4}r_l+\frac{2}{(2l+5)}\left\{\left(\frac{l+2}{2l+3}\right)\frac{M_{2l+6}}{a_l}-\frac{6P_{l5}}{(2l-3)(4l^2-1)}\right\}\right]. \tag{10}$$

Equation (7) for small kr_l is the shape-independent formula for scattering, generalized to arbitrary l values (Blatt and Jackson 1949; Chew and Goldberger 1949), so that a_l, r_l, and P_l in equations (8)–(10) are interpreted as approximate forms of the zero energy scattering length, effective range, and first shape parameter respectively. The shape parameter P_0 has been previously misquoted (Swan 1960*b*).

It is well known that the convergence of relation (7) becomes rapidly poorer as l increases, so that its practical usefulness has been largely restricted to the $l = 0$ case (Chew and Goldberger 1949). However, it may readily be treated by a variational principle for $k\cot\eta_l$.

III. Schwinger's Variational Principle for Arbitrary l

Blatt and Jackson (1949) have given Schwinger's variational principle for S-wave scattering. An extension to arbitrary l-values involves rewriting the wave equation in the integral equation form (Swan 1961)

$$\psi_l(r) = \mathscr{J}_l(kr)\cos\eta_l - \int_0^\infty \mathrm{d}r'\, G_l(r,r')U(r')\psi_l(r'), \tag{11}$$

where the Green's function is

$$G_l(r,r') = -(1/k)\mathscr{J}_l(kr_<)\mathscr{N}_l(kr_>), \tag{12}$$

$r_<$ and $r_>$ being the smaller and larger of r, r' respectively.

The asymptotic wave function is taken as

$$\psi_l(r\to\infty) = \mathscr{J}_l(kr)\cos\eta_l - \mathscr{N}_l(kr)\sin\eta_l, \tag{13}$$

whereas equations (11) and (12) give the result

$$\psi_l(r\to\infty) = \mathscr{J}_l(kr)\cos\eta_l + \frac{1}{k}\mathscr{N}_l(kr)\int_0^\infty \mathrm{d}r'\,\mathscr{J}_l(kr')U(r')\psi_l(r'). \tag{14}$$

Comparison of equations (13) and (14) leads to the integral equation for the phase

$$\sin\eta_l = -\frac{1}{k}\int_0^\infty \mathrm{d}r'\,\mathscr{J}_l(kr')U(r')\psi_l(r'). \tag{15}$$

We multiply relation (11) by $U(r)\psi_l(r)$, integrate between the limits 0 and ∞, and employ equation (15) to find

$$-k\cot\eta_l = \frac{\int_0^\infty U(r)\psi_l^2(r)\,\mathrm{d}r + \int_0^\infty \mathrm{d}r\int_0^\infty \mathrm{d}r'\,U(r)\psi_l(r)G_l(r,r')U(r')\psi_l(r')}{\left[\frac{1}{k}\int_0^\infty \mathrm{d}r'\,\mathscr{J}_l(kr')U(r')\psi_l(r')\right]^2}. \tag{16}$$

One may consider (15) as a variational principle for $k\cot\eta_l$, as it is stationary for small increments $\delta\psi_l$ and $\delta\eta_l$ in wave function ψ_l and phase η_l respectively. This means

$$\delta(k\cot\eta_l) = 0,$$

under the operation

$$\psi_l \to \psi_l+\delta\psi_l, \qquad \eta_l \to \eta_l+\delta\eta_l,$$

as is easily verified by substitution in equation (16).

IV. Variation Method for the Form Factor $g_l(\lambda_l,r)$

We may apply Schwinger's variational principle to the approximate expansion (7), where equations (8)–(10) give us a_l, r_l, P_l, . . . as functions of the two parameters A_l and λ_l, via the form factor $g_l(\lambda_l,r)$ of equation (3). If the zero-energy scattering length a_l is kept constant at the correct value, then A_l is no longer an independent parameter, so that $A_l = A_l(\lambda_l)$. Subject to this restriction, we take $\psi_l \to \psi_l+\delta\psi_l$ as equivalent to $\lambda_l \to \lambda_l+\delta\lambda_l$, leading to

$$\delta(k\cot\eta_l) = 0.$$

The constancy of a_l gives us

$$\partial a_l/\partial\lambda_l = 0, \tag{17}$$

and the stationary property of $k\cot\eta_l$ leads to

$$\partial r_l/\partial\lambda_l = 0, \tag{18}$$

the latter equation being valid for η_l at low energies ($kr_l \leqslant 1$), where the shape-dependent terms in the expansion (7) are negligible.

On employing equations (8) and (9), relations (17) and (18) become

$$\partial P_{l1}/\partial\lambda_l = \partial P_{l3}/\partial\lambda_l = 0. \tag{19}$$

From equations (19), (6) and (3), we define the integrals

$$\left.\begin{aligned} I_{nl} &= -\int_0^\infty \mathrm{d}r.r^n U(r)\phi_l(\lambda_l,r), \\ J_{nl} &= \int_0^\infty \mathrm{d}r.r^n U(r)\frac{\partial\phi_l}{\partial\lambda_l}, \\ K_{nl} &= \int_0^\infty \mathrm{d}r.r^n U(r)\frac{\partial\phi_l}{\partial\lambda_l}[1-\phi_l(\lambda_l,r)]^{2l}, \end{aligned}\right\} \tag{20}$$

so that equation (19) becomes

$$\left.\begin{aligned} -I_{2l+4,l}\partial A_l/\partial\lambda_l + J_{2l+4,l}A_l &= (2l+1)K_{3,l}, \\ -I_{2l+2,l}\partial A_l/\partial\lambda_l + J_{2l+2,l}A_l &= (2l+1)K_{1,l}, \end{aligned}\right\} \tag{21}$$

with solution

$$\left.\begin{aligned} A_l &= (2l+1)(I_{2l+2,l}K_{3,l}-I_{2l+4,l}K_{1,l})/(I_{2l+2,l}J_{2l+4,l}-I_{2l+4,l}J_{2l+2,l}), \\ \partial A_l/\partial\lambda_l &= (2l+1)(J_{2l+2,l}K_{3,l}-J_{2l+4,l}K_{1,l})/(I_{2l+2,l}J_{2l+4,l}-I_{2l+4,l}J_{2l+2,l}). \end{aligned}\right\} \tag{22}$$

We see that, given the correct value of a_l, equation (8) leads to λ_l, and equation (9) to r_l.

S-wave Scattering

For $l = 0$, the definition (20) shows that

$$K_{n,0} = J_{n,0}$$

while equation (8) becomes

$$A_0 I_{2,0} - I_{1,0} = 1 + M_{2,0}/a_0 - M_{1,0}. \tag{23}$$

This may be solved numerically for λ_0, and equations (9) and (10) give one

$$r_0 = (2/3M_{2,0})[2(A_{4,0}I_{4,0}+M_{3,0}-I_{3,0})-M_{4,0}/a_0], \tag{24}$$

$$-P_0 r_0^3 = [\tfrac{1}{6}M_{4,0}r_0 + (2/45)M_{6,0}/a_0 - (2/15)(A_{6,0}I_{6,0}+M_{5,0}-I_{5,0})]. \tag{25}$$

A particularly simple and important case occurs for

$$\phi_0(\lambda_0,r) = \exp(-\lambda_0 r/r_P), \tag{26}$$

where r_P is the potential range parameter. Equation (21) becomes

$$r_P I_{4,0}\partial A_0/\partial\lambda_0 = A_0 I_{5,0} - I_{4,0}, \qquad r_P I_{2,0}\partial A_0/\partial\lambda_0 = A_0 I_{3,0} - I_{2,0},$$

with solution

$$A_0 = 0, \qquad \partial A_0/\partial\lambda_0 = -1/r_P, \tag{27}$$

equations (23) and (24) for λ_0 and r_0 still applying.

V. Application to Neutron-Proton Scattering

We take as basis parameters derived from the liquid mirror reflection of subthermal neutrons (Hughes, Burgy, and Ringo 1950; Ringo, Burgy, and Hughes 1951; Salpeter 1951; Mather and Swan 1958). These values of a_0 and r_0 are given in Table 1, together with approximate values of the shape parameter P_0 and the shape correction term $P_0 r_0^3$ for several simple well shapes, P_0 being taken from Figure 10 of Blatt and Jackson (1949).

Table 1

Scattering parameters for neutron-proton scattering

Potential	^{3}S n-p $a_0 = 5\cdot38$ fm, $r_0 = 1\cdot70$ fm		^{1}S n-p $a_0 = -23\cdot69$ fm, $r_0 = 2\cdot7$ fm	
	P_0	$P_0 r_0^3$	P_0	$P_0 r_0^3$
Gaussian	$-0\cdot018$	$-0\cdot088$	$-0\cdot016$	$-0\cdot315$
Exponential	$0\cdot030$	$0\cdot147$	$0\cdot008$	$0\cdot158$
Yukawa	$0\cdot145$	$0\cdot712$	$0\cdot046$	$0\cdot905$

In subsequent calculations, we use the form factor (3) for $l = 0$. Expressions used for $\phi_0(\lambda_0,r)$ in $g_0(r)$ are given in Table 2 for ^{3}S and ^{1}S n-p scattering for several well shapes, together with the corresponding well depths V_0 and parametric ranges r_P. The latter quantities were derived from interpolation formulae of Blatt and Jackson (1949), assuming a_0 and r_0.

Table 2

Potential parameters for neutron-proton scattering

$V(r)$	$\phi_0(r)$	^{3}S n-p		^{1}S n-p	
		V_0 (MeV)	r_P (fm)	V_0 (MeV)	r_P (fm)
$-V_0 \exp(-r^2/r_P^2)$	$\exp(-\lambda r^2/r_P^2)$	$72\cdot117$	$1\cdot4837$	$32\cdot194$	$1\cdot7850$
$-V_0 \exp(-r/r_P)$	$\exp(-\lambda r/r_P)$	$216\cdot718$	$0\cdot62798$	$109\cdot467$	$0\cdot71233$
$-V_0 \exp(-r/r_P)/(r/r_P)$	$\exp(-\lambda r/r_P)$	$42\cdot237$	$1\cdot5636$	$47\cdot701$	$1\cdot1706$

In Table 3, we give results based on the form factor (3) for $l = 0$ and the potentials of Table 2, using several alternative procedures (*a*), (*b*), (*c*):

(*a*) We put $\lambda_0 = 1$ in $\phi_0(\lambda_0,r)$, with A_0 chosen to give a_0 correctly in (23), r_0 and P_0 coming from equations (24) and (25).

(*b*) This procedure uses the stationary property of $k \cot \eta_0$, so that equations (22) and (23) give A_0 and λ_0, the latter parameters being chosen to make r_0 stationary and to give a_0 correctly, respectively.

(*c*) We put $A_0 = 0$, thus using (4) instead of (3) for the form factor $g_0(r)$. Equation (23) is solved for λ_0, assuming the correct value of a_0, and r_0 and P_0 are evaluated from (24) and (25).

Numerical results for ^{3}S and ^{1}S n-p scattering, using Gaussian, exponential, and Yukawa interactions, are given in Table 3. For exponential and Yukawa potentials, we use (26) for $\phi_0(r)$, so that cases (*b*) and (*c*) above are the same, as $A_0 = 0$ in each.

TABLE 3

SCATTERING PARAMETERS IN THE DISTORTED WAVE APPROXIMATION

(*a*) $\lambda_0 = 1 \cdot 0$, (*b*) λ_0 for $\delta(k \cot \eta_0) = 0$, (*c*) λ_0 for $A_0 = 0$

Potential		^{3}S n-p				
		λ_0	A_0	r_0 (fm)	P_0	$P_0 r_0^3$
Gaussian	(*a*)	1·0	0·5734	1·7113	−0·0264	−0·1323
	(*b*)	1·3624	0·4284	1·6862	−0·0226	−0·1084
	(*c*)	1·8122	0	1·7014	−0·0236	−0·1162
Exponential	(*a*)	1·0	−0·2009	1·7289	0·0385	0·1990
	(*b*), (*c*)	0·8846	0	1·7264	0·0387	0·1991
Yukawa	(*a*)	1·0	0·4913	2·4312	0·0498	0·7156
	(*b*), (*c*)	2·2471	0	2·2301	0·0768	0·8518
		^{1}S n-p				
Gaussian	(*a*)	1·0	0·4317	2·6349	−0·0186	−0·3403
	(*b*)	1·2563	0·4071	2·6180	−0·0198	−0·3553
	(*c*)	1·6933	0	2·6405	−0·0190	−0·3501
Exponential	(*a*)	1·0	−0·2009	2·7516	0·0066	0·1375
	(*b*), (*c*)	0·7733	0	2·7325	0·0098	0·1999
Yukawa	(*a*)	1·0	0·2895	3·1611	0·0380	1·2003
	(*b*), (*c*)	1·4080	0	3·1294	0·0405	1·2412

When a_0 is given correctly, low energy scattering ($kr_0 \leqslant 1$) is governed almost entirely by the value of r_0, via the shape-independent formula (7). The variational procedure (*b*) implicitly neglects the shape-dependent term $P_0 r_0^3 k^4$, so that only r_0 can be hoped to be improved by procedure (*b*), as contrasted with (*a*). Actually, the only significant improvements in the value of r_0 occur for the Yukawa potential, where r_0 has a large error via (*a*), the change being considerable in the ^{3}S state. In other cases, the improvement is either very small, or the error in r_0 is even increased slightly. The reason for the latter occurrence is that Schwinger's variational principle for $k \cot \eta_l$ merely makes the latter stationary for small first-order changes $\delta\psi_l$ in ψ_l, but does not subject it to either an upper or lower bound. More parameters in ψ_l do not necessarily improve the second-order accuracy in η_l and therefore r_l, as the variational principle holds only to first order.

The result indicates that the distorted wave formula (1) for $\tan \eta_l$ already makes $k \cot \eta_l$ stationary correct to first order. Values obtained for the shape parameter P_0 and for $P_0 r_0^3$ are also quite good, so that phases η_l at higher energies are correctly described.

Case (*c*) in Table 3 gives the best results for r_0 obtained, although only for the Gaussian potential are they different from (*b*). We conclude that the one-parameter form factor (4) has the advantage of both simplicity and accuracy, the latter being equivalent to first order to that attained by a variational calculation with two parameters in $g_l(r)$. Any differences are second order, but for simplicity, (4) with a variable λ_l is preferable.

VI. References

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