Variational Calculation of the $S$-Phase Shift for Neutron-Proton Scattering

Kenji Hasegawa,* Kohki Kimura*† and Junji Nanao*††

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The $S$-phase shifts for neutron-proton scattering up to about 200 Mev of the incident energy are calculated by a newly proposed variational method. A central force of exponential shape with a hard core is employed. The results are found to be very close to the exact solutions in view of the simple form of the trial function. These results are compared with those of a previous work obtained by the use of the usual variational method.

1 Introduction

In a previous paper†† (hereafter refered to as A), we have made a variational calculation of neutron-proton scattering assuming a central force of exponential shape with a hard core. In that work the results are very close to the exact solutions in view of the simple form of the trial function. The variational method used in A is essentially the same as the one proposed by Hulthén and Kohn for the phase shifts. In this method the basic role is played by the stationary expression for the phase shift which is stationary in the small variation of the trial function. The variational method used in A is essentially the same as the one proposed by Hulthén and Kohn for the phase shifts. In this method the basic role is played by the stationary expression for the phase shift which is stationary in the small variation of the trial function about the exact wave function. In a practical calculation the adjustable parameters in the trial function are determined by requiring them to give the stationary values of this expression. This requirement, however, forms only a necessary condition for the trial function to agree with the exact wave function. In other words, it remains an open question whether or not the result obtained by this method is really equal to or close to the exact solution, unless the latter is obtainable.

In fact, it is possible that the stationary expression has several stationary values, among which only one may be true while the rest are false. In such a case, there is in principle no criterion theoretically to rule out the false ones except those which are evidently inadequate. Some discussion is given by Kato on the upper and the lower limits of the stationary expression, but it is restricted to the case where the potential has a definite sign, and its extension to the general scattering problems seems to be very difficult.

Now, it is the purpose of the present paper to propose a new type of variational method in which the above-mentioned deficiencies are considerably improved. This

* Division of Applied Science.
† Graduate student. Present adress : Department of Physics, Hiroshima University.
†† Graduate student. Present adress : Department of Applied Physics, Fukui University.
new method is different from the usual one only in that it contains an additional quantity whose minimum determines the optimum values of the variational parameters. The usual stationary expression is then calculated for these values of the parameters. In sect. 2, the outline of the variational method used in A is described and the additional quantity to minimize is introduced. We shall confine ourselves to only the $S$ state. In sect. 3, we make as an example a numerical calculation of the $S$-phase shifts for neutron-proton scattering by the use of the new variational method. We use the same potential as well as the same type of the trial function as adopted in A, and the results are compared with those of A. Section 4 is devoted to the concluding remarks.

2 Formulation

2.1 Outline of the previous method

The variational method used in A is summarized as follows. We define an operator $L$ by

$$ L = -\left( \frac{d^2}{dr^2} + k^2 \right) + U(r) $$

(1)

with

$$ k^2 = \frac{8\pi^2 M}{\hbar^2} E, $$

(2)

$$ U(r) = \frac{8\pi^2 M}{\hbar^2} V(r), $$

(3)

where $M$ is the reduced mass, $E$ the energy in the center of mass system and $V(r)$ the interaction potential. Here we assume that the potential contains the repulsive core, namely

$$ V(r) = \begin{cases} V(r) & (r \leq r_c) \\ \infty & (r > r_c) \end{cases}. $$

(4)

The exact $S$-state wave function $u(r)$ then satisfies the Schrödinger equation

$$ L[u] = 0 $$

(5)

with the boundary condition:

$$ u(r) = 0 \quad \text{for} \quad r \leq r_c, $$

$$ u(r) \rightarrow \sin(kr + \delta), \quad (r \rightarrow \infty) $$

(6)

The trial function $u_t(r)$ is taken to satisfy the similar boundary condition:

$$ u_t(r) = 0 \quad \text{for} \quad r \leq r_c, $$

$$ u_t(r) \rightarrow \sin(kr + \eta), \quad (r \rightarrow \infty) $$

(7)

Then, it is shown in A that the expression

$$ \lambda = -\frac{1}{k} J $$

(8)

with

$$ J = \int_{r_c}^{\infty} u_t L[u_t] dr $$

(9)

should be stationary in variation of $\eta$ about the exact phase shift $\delta$, in order that $u_t$ may coincide with $u$.

This statement can be put into a more clear-cut form as follows. In the manner adopted by Kato\textsuperscript{6}, we set

$$ \delta u = u_t - u. $$

(10)
The quantity $J$ then can be rewritten by integration by parts as
\[
J = \int_{r_c}^{\infty} \partial u L[\partial u] dr - \left[ u - \frac{d}{dr} \partial u - \frac{d}{dr} \partial u \right]_{r_c}^{\infty},
\]
where the relation
\[
L[u_i] = L[\partial u]
\]
has been used. By the boundary conditions (6) and (7), the second term in the right-hand side of (11) becomes
\[
k \sin(\eta - \delta).
\]
We thus obtain
\[
\sin(\eta - \delta) = -\frac{1}{k} J + \varepsilon
\]
with
\[
\varepsilon = -\frac{1}{k} \int_{r_c}^{\infty} \partial u L[\partial u] dr.
\]
It is clearly seen that (12) agrees with (8) except the term of the order $(\eta - \delta)^2$ as well as the quantity $\varepsilon$, which depends on $\partial u$ quadratically. We are therefore led to the statement that the expression
\[
A = \eta - \sin^{-1} \frac{J}{k}
\]
agrees with the exact phase shift $\delta$ except the quantity $\varepsilon$, which may be regarded as the error in the approximate phase shift $A$.

Now, in the practical variational evaluation performed in A, we have taken the trial function of the form
\[
u_i(r) = \cos(\eta + kr_c) \sin(\eta + kr_c) + \sin(\eta + kr_c) \cos(\eta + kr_c)
\times \left[ 1 - e^{-r-r_c} \right] \left[ 1 + be^{-r-r_c} \right],
\]
where $\eta$ and $b$ are the variational parameters. One set of the conditions by which the optimum values of $\eta$ and $b$ are to be determined is proposed in A by
\[
\frac{\partial A}{\partial \eta} = 0, \quad J = 0,
\]
and the best approximation for $\delta$ is given by this value of $\eta$. These conditions are clearly equivalent to
\[
\frac{\partial A}{\partial \eta} = 0, \quad J = 0,
\]
so that we can adopt (17) instead of (16), obtaining the same results.

### 2.2 Additional condition

The conditions (16) or (17) are only necessary conditions which should be satisfied by those values of $\eta$ and $b$ at which $u_i$ agrees with $u$. Conversely, at any values of $\eta$ and $b$ which satisfy (16) or (17), $u_i$ does not necessarily agree with $u$, nor does $\eta$ coincide with $\delta$. In particular, if several values of $\eta$ and $b$ satisfied (16) or (17), it would be difficult theoretically to distinguish the optimum values of $\eta$ and $b$ from the rest.

Now, in order to remedy essentially such deficiencies in the previous variational method, it is of course necessary to find how to estimate the error $\varepsilon$ for any given values of $\eta$ and $b$. This is, however, usually very difficult as long as $\partial u$ is unknown, so that we must be here content only to obtain some way to find the values of $\eta$ and $b$
which probably minimize $\varepsilon$ (in magnitude). Then, since we know the value of the quantity $L[\delta u]$ through $L[u_i]$ for any given $u$, we first try to express $\delta u$ in terms of $L[u_i]$.

Defining Green's function $G_0(r, r')$ by

$$ \left( \frac{d^2}{dr^2} + k^2 \right) G_0(r, r') = \delta(r - r'), $$

we can convert the identity

$$ \left( \frac{d^2}{dr^2} + k^2 \right) \delta u = U \delta u - L[u_i] $$

into

$$ \delta u = \int_{r_c}^{\infty} G_0(r, r') U(r') \delta u(r') dr' - \int_{r_c}^{\infty} G_0(r, r') L[u_i(r')] dr'. $$

The relation (23) can most easily be proved by operating $\left( \frac{d^2}{dr^2} + k^2 \right)$ on both sides of (20).

It is to be noted here that the addition of any solution $\phi$ of the equation

$$ \left( \frac{d^2}{dr^2} + k^2 \right) \phi = 0 $$

to (20) equally leads to (19), but since $\delta u = 0$ when $L[u_i] = 0$, we should have $\phi = 0$. The explicit form of $G_0(r, r')$ is given by

$$ G_0(r, r') = -\frac{1}{k} \sin(kr) \cos(kr), $$

where $r <$ indicates the smaller of $r$ and $r'$, and $r >$ the larger. (See, for example, Chapter 11 of reference 5.)

If we then regard (20) as integral equation for $\delta u$, we can express the formal solution of (20) in the form

$$ \delta u = \int_{r_c}^{\infty} G(r, r') L[u_i(r')] dr', $$

where $G(r, r')$ satisfies the integral equation

$$ G(r, r') = G_0(r, r') + \int_{r_c}^{\infty} G_0(r, r'') U(r'') G(r'', r') dr''. $$

The proof is most easily given by substituting (20) into (20). If the potential $U(r)$ decreases sufficiently rapidly as $r$ becomes large, the upper limit of the integral in (20) can effectively be replaced by some finite value, say $R$. Then, the function $G_0(r, r')$ as well as the kernel $G_0(r, r') U(r')$ are clearly of a $L^2$ type in this finite range, i.e.

$$ \int_{r_c}^{R} \int_{r_c}^{R} |G_0(r, r')|^2 dr dr' < \infty, \quad \int_{r_c}^{R} \int_{r_c}^{R} |G_0(r, r') U(r')|^2 dr dr' < \infty, $$

so that (20) has a $L^2$ solution in this range of $r$ and $r'$. We then put

$$ m = \int_{r_c}^{R} \int_{r_c}^{R} |G(r, r')|^2 dr dr' < \infty. $$

We can therefore rewrite $\varepsilon$ in the form

$$ \varepsilon = \frac{1}{k} \int_{r_c}^{R} \int_{r_c}^{R} L[u_i(r)] G(r, r') L[u_i(r')] dr dr', $$

for $L[u_i(r)]$ also decreases sufficiently rapidly as $r$ becomes large. Now, for an integral of the form $I = \int |H(r)| K(r) dr$, we have

$$ |I|^2 \leq \int |H(r)|^2 dr \int |K(r)|^2 dr $$

by the Schwarz inequality, so that (27) leads to

$$ \varepsilon \leq \frac{m}{k^2} \left( \int_{r_c}^{\infty} |L[u_i]|^2 dr \right)^2. $$
We are thus led to the idea that an integral of the form
\[
\mathcal{J} = \int_{r_c}^{\infty} (L[u])^2 dr
\]
can be adopted as a convenient measure of the smallness of \( \varepsilon \). Of course, \( \mathcal{J} \) needs not necessarily be small in order that \( \varepsilon \) may be small, but conversely \( \varepsilon \) should necessarily be small, if \( \mathcal{J} \) is quite small. It is also to be remarked that \( \mathcal{J} \) must be zero and as well stationary at those values of the variational parameters for which \( u_t \) coincides with \( u \).

Consequently, we propose here the following type of variational procedure to determine an approximate S-phase shift:

**Determine the values of the variational parameters by requiring them to give the minimum of \( \mathcal{J} \). Then, evaluate \( \langle \psi | \mathcal{J} | \psi \rangle \) for these values of the parameters. In order to check the smallness of \( \mathcal{J} \) obtained in this way, we may compare the minimum of \( \mathcal{J} \) with a certain specific value of \( \mathcal{J} \) in which some simple approximate wave function, e.g. a plane wave, is substituted for \( u \).**

As an illustration we shall make a numerical evaluation of the S-phase shifts for neutron-proton scattering by the use of this method in the next section.

### 3 Numerical evaluation and the results

We take the same potential and the same trial function as used in A, namely the trial function of the form \( \langle \psi | \mathcal{J} | \psi \rangle \) and the potential
\[
V(r) = \begin{cases} \infty, & (r \leq r_c) \\ -V_0 \exp[-\alpha(r-r_c)], & (r > r_c) \end{cases}
\]
The potential parameters\(^7\) are listed in Table 1.

<table>
<thead>
<tr>
<th>State</th>
<th>( V_0 ) (in Mev)</th>
<th>( \alpha ) (in fm(^{-1}))</th>
<th>( r_c ) (in fm)</th>
</tr>
</thead>
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<tr>
<td>Singlet Even</td>
<td>330.794</td>
<td>2.4021</td>
<td>0.4</td>
</tr>
<tr>
<td>Triplet Even</td>
<td>474.43</td>
<td>2.5214</td>
<td>0.4</td>
</tr>
</tbody>
</table>

The quantity to minimize is taken to be
\[
\rho = \mathcal{J}/\mathcal{J}_0
\]
with
\[
\mathcal{J}_0 = \int_{r_c}^{\infty} (L[\phi])^2 dr,
\]
where \( \phi \) is a solution of the equation
\[
\left( \frac{d^2}{dr^2} + k^2 \right) \phi = 0 \quad \text{for} \quad r > r_c
\]
and satisfies
\[
\phi = 0 \quad \text{for} \quad r \leq r_c.
\]
The explicit form of \( \phi \) is
\[
\phi(r) = \sin(kr - kr_c).
\]
The numerical calculations have been made at the laboratory energies of 42, 90, 128, 156 and 215 Mev. The results for the S-phase shifts are shown in Table 2. Those
obtained in A are also shown for comparison.

Table 2. Results for the S-phase shifts (in radian). The results of the previous calculation, the exact solutions and the empirical values* are also shown for comparison.

(a) Singlet

<table>
<thead>
<tr>
<th>$E_{Lab}$ (in Mev)</th>
<th>Present calculation</th>
<th>Previous calculation</th>
<th>Exact solution</th>
<th>Empirical</th>
</tr>
</thead>
<tbody>
<tr>
<td>42</td>
<td>0.8454</td>
<td>0.7416</td>
<td>0.7511</td>
<td>0.720</td>
</tr>
<tr>
<td>90</td>
<td>0.4880</td>
<td>0.4719</td>
<td>0.4767</td>
<td>0.471</td>
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<tr>
<td>128</td>
<td>0.3254</td>
<td>0.3202</td>
<td>0.3235</td>
<td>0.324</td>
</tr>
<tr>
<td>156</td>
<td>0.2300</td>
<td>0.2275</td>
<td>0.2301</td>
<td>0.232</td>
</tr>
<tr>
<td>215</td>
<td>0.0658</td>
<td>0.0650</td>
<td>0.0668</td>
<td>0.066</td>
</tr>
</tbody>
</table>

(b) Triplet

<table>
<thead>
<tr>
<th>$E_{Lab}$ (in Mev)</th>
<th>Present calculation</th>
<th>Previous calculation</th>
<th>Exact solution</th>
<th>Empirical</th>
</tr>
</thead>
<tbody>
<tr>
<td>42</td>
<td>1.3406</td>
<td>1.1591</td>
<td>1.1713</td>
<td>1.192</td>
</tr>
<tr>
<td>90</td>
<td>0.8274</td>
<td>0.7877</td>
<td>0.7945</td>
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<tr>
<td>128</td>
<td>0.6132</td>
<td>0.6000</td>
<td>0.6049</td>
<td>0.625</td>
</tr>
<tr>
<td>156</td>
<td>0.4948</td>
<td>0.4894</td>
<td>0.4934</td>
<td>0.522</td>
</tr>
<tr>
<td>215</td>
<td>0.3003</td>
<td>0.3011</td>
<td>0.3037</td>
<td>0.335</td>
</tr>
</tbody>
</table>

* As the empirical values we list here the calculated phase shifts given by Hamada and Johnston using their detailed potential model.

The minima of $\rho$ as well as the corresponding values of the variational parameters $\eta$ and $b$ are shown in Table 3. The values of $\eta$ and $b$ used in A as well as the corresponding value of $\rho$ are also shown for comparison.

Table 3. Minima of the quantity $\rho$, the measure of the accuracy, as well as the corresponding values of the variational parameters $\eta$ and $b$. The values of $\eta$ and $b$ obtained in the previous calculation and the corresponding values of $\rho$ are also shown for comparison.

(a) Singlet

<table>
<thead>
<tr>
<th>$E_{Lab}$ (in Mev)</th>
<th>Present calculation</th>
<th>Previous calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\eta$</td>
<td>$b$</td>
<td>$\rho$</td>
</tr>
<tr>
<td>42</td>
<td>1.0200</td>
<td>-0.0560</td>
</tr>
<tr>
<td>90</td>
<td>0.6007</td>
<td>0.0830</td>
</tr>
<tr>
<td>128</td>
<td>0.4191</td>
<td>0.1595</td>
</tr>
<tr>
<td>156</td>
<td>0.3160</td>
<td>0.2040</td>
</tr>
<tr>
<td>215</td>
<td>0.1405</td>
<td>0.2895</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\eta$</th>
<th>$b$</th>
<th>$\rho$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7416</td>
<td>0.91</td>
<td>1.3426</td>
</tr>
<tr>
<td>0.4719</td>
<td>0.95</td>
<td>0.5753</td>
</tr>
<tr>
<td>0.3202</td>
<td>0.96</td>
<td>0.3750</td>
</tr>
<tr>
<td>0.2275</td>
<td>0.97</td>
<td>0.2961</td>
</tr>
<tr>
<td>0.0650</td>
<td>1.02</td>
<td>0.2135</td>
</tr>
</tbody>
</table>
4 Concluding remarks

By the use of the simple variational method proposed in 2.2, we have obtained the results which are very close to the exact solutions in view of the simple form of the trial function. The minima of the quantity $\rho$, the measure of the accuracy, are really quite small.

It seems rather striking that the optimum values of the variational parameters $\eta$ and $b$ in the present calculation are considerably different from those obtained in A. In particular, at 42 Mev for each spin state, the sign of $b$ in the present case is opposite to the one given in A. The values of $\rho$ are also considerably large for the values of $\eta$ and $b$ obtained in A, even larger than unity at 42 Mev. However, the results for the phase shifts in the present calculation are not so different from the previous ones.

These facts may be explained in the following way. In the previous calculation, the quantity $\delta u$ and/or $L(\delta u)$ probably not very small but the error $e$ will be fortunately very small. On the other hand, in the present calculation the quantities $e$, $\delta u$ and/or $L(\delta u)$ will all be quite small.

Now, the variational evaluation of the $S$-phase shift for two-body scattering itself is of little value from the practical point of view, since the exact phase shift can easily be evaluated in this case. Nevertheless, the method proposed in the present paper will be useful at least in its basic idea, if it is extended to a more complicated problem of scattering involving more than two particles. For such a problem no exact solution is obtainable and, moreover, we must use the stationary expression for the scattering amplitude$^{11,91}$, since its partial wave decomposition in a closed form is no more possible. This may cause some complication, but in principle there is no essential difficulty in extending the method proposed in the present paper to such a complicated problem as neutron-deuteron scattering.

Acknowledgement

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References