On the Accuracy of Wave Functions and Charge Form Factors
Obtained from ATMS Calculations

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(Received January 17, 1980)

A function $B(E)$ is introduced which measures the impurity of a trial wave function coming
from the admixture of eigenstates with energies equal to or larger than $E$. An upper bound of
$B(E)$ is derived from the gap between the Ritz and Temple bounds of the energy. A small
energy gap means a very small impurity at large values of $E$. Implications on form factor
calculations based on the ATMS method are discussed. Around and above the region of the
second maximum of the elastic charge form factor, in particular, the ATMS results are very
reliable.

§ 1. Introduction

There has been some essential progress in variational calculations on few-nucleon systems with realistic interactions. In an earlier attempt to reproduce
the binding energies by the use of hard core potentials, the Temple lower bounds
were rather far below the upper bounds. Recently, the ATMS method has been
applied to various realistic few-body systems and it has been reported that a very
small gap between the upper and lower bounds can be obtained.

We are thus in the stage that we can make an accurate estimate of the
energy. Little has been said in the literature, however, about the accuracy of
variationally obtained wave functions. When we construct a trial wave function
for a realistic few-particle system, its deviation from the eigenfunction generally
includes a series of excited components which extends into very large excitation
energies, due to the short-range repulsive part of the interaction. It is known
that such an impurity pushes the lower bound far below the exact value of the
energy, due to the fact that Temple’s formula involves the expectation value of
the squared Hamiltonian. Conversely, when the gap between upper and lower
bounds becomes small, we expect a possibility to show that the impurity of the
wave function is small, especially at high excitation energies. The first purpose
of the present study is to derive mathematical expressions which make it possible
to estimate the accuracy of the wave function.

In recent studies on the mesonic degrees of freedom in nuclei, the calculations

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of the charge and magnetic form factors have become important. In particular accurate calculations at high momentum transfer for the nucleonic part become essential, in comparison with the experimental values, to estimate mesonic and other contributions. It has been pointed out that a non-negligible discrepancy exists between calculations by variational and by integral equation methods around the region of the second maximum of the elastic charge form factors of the few-nucleon systems. The second purpose of the present study is to demonstrate the fact that the form factors calculated by the ATMS method are rather accurate, in particular at high momentum transfer.

The organization of this paper is as follows. In § 2, we introduce two quantities \( A \) and \( B(E) \). The number \( A \) gives the total impurity of a trial wave function \( \psi \), and the function \( B(E) \) gives the impurity of \( \psi \) at energies equal to and larger than \( E \). We then derive some mathematical expressions to bound these quantities from above. In § 3, we make an application to the ATMS wave function of the three \( \alpha \)-particle system interacting by an Ali-Bodmer phenomenological potential. From this, we discuss the accuracy of the elastic charge form factor calculation based on the ATMS method. In § 4, we give concluding remarks.

§ 2. Theory

We assume that \( H \) is a few-body Hamiltonian for which \( E_i \) and \( \varphi_i \) are the eigenvalues and the eigenfunctions, respectively:

\[
H\varphi_i = E_i \varphi_i ,
\]

\[
\langle \varphi_i | \varphi_i \rangle = \delta_{ij} ,
\]

and that \( \psi \) is a trial function, normalized to unity, to represent the lowest eigenfunction \( \varphi_0 \). We expand \( \psi \) on \( \varphi_i \):

\[
\psi = \frac{1}{\sqrt{1 - \sum |a_i|^2 \varphi_0 + \sum |a_i| \varphi_i}} .
\]

The first term on the right-hand side is the dominant part, while the second term may be called the impurity of \( \psi \). The expectation values of \( H \) and \( H^2 \) with respect to \( \psi \) are written as

\[
\langle H \rangle = E_0 + \sum |a_i|^2 (E_i - E_0) ,
\]

\[
\langle H^2 \rangle = E_0^2 + \sum |a_i|^2 (E_i^2 - E_0^2) .
\]

\(^{*1}\) We use a boundary condition that wave functions vanish at surfaces of a large box. In the limit of large box, the summation of Eq. (3) over continuum states should be read as an integration.
Upper and lower bounds for \( E_0 \) are defined by

\[
E_0 = \langle H \rangle, \\
E_L = \langle H \rangle - (\langle H^2 \rangle - \langle H \rangle^2)/\langle E_I - \langle H \rangle \rangle,
\]

where Eq. (7) is the Temple formula.\(^9\) It is assumed that \( \varphi \) is such a trial function that the condition

\[
E_0 < E_I
\]

is satisfied. We call \( E_I - E_0 \) the gap \( G \),

\[
G = E_0 - E_L.
\]

Also, we define \( \varepsilon \) and \( \mu \) by

\[
\varepsilon = \langle H \rangle - (\langle H^2 \rangle - \langle H \rangle^2)/\langle E_I - \langle H \rangle \rangle, \\
\mu = (E_0 - E_0)/(E_I - E_L).
\]

From Eqs. (4), (5) and (10) we get

\[
\varepsilon = \frac{\sum_{i=1}^{n} |a_i|^2 (E_i - E_0)E_i}{\sum_{i=1}^{n} |a_i|^2 (E_i - E_0)},
\]

and from Eqs. (6), (7), (10) and (11) we get

\[
\mu = (E_I - E_0)/(\varepsilon - E_0).
\]

To get an interpretation of \( \varepsilon \), we consider a trial function for which

\[
a_1 = 0, \quad a_2 = a_3 = \cdots = 0.
\]

In this case we get the smallest possible value of \( \varepsilon \) and the largest possible value of \( \mu \), namely \( \varepsilon = E_I \), \( \mu = 1 \) and, consequently, \( E_0 = E_L \). In realistic cases, \( \varepsilon \) is much larger than \( E_I \). Equation (12) may be interpreted as the definition of a certain special average which we denote by \( \cdot \), while we denote a normal average by \( \cdot \). The average energy \( \bar{E} \) contained in \( \sum_{i=1}^{n} a_i \varphi_i \) is

\[
\bar{E} = \frac{\sum_{i=1}^{n} |a_i|^2 E_i}{\sum_{i=1}^{n} |a_i|^2}.
\]

Here, \( |a_i|^2/\sum_{i=1}^{n} |a_i|^2 \) is interpreted as an excitation probability distribution \( p_i \), and \( E_i \) as weight \( w_i \), thus

\[
\bar{E} = \sum_{i=1}^{n} p_i w_i.
\]

The special average \( \varepsilon = \bar{E} \), in contrast, has probability distribution
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\[ P_i = \frac{|a_i|^2 (E_i - E_0)}{\sum_{j=1}^m |a_j|^2 (E_j - E_0)} \]  

(17)

The weight is again \( w_i = E_i \), so that

\[ \varepsilon = \bar{E} = \sum_{i=1}^m P_i w_i. \]  

(18)

This consideration emphasizes that \( \varepsilon \) is an average taken with a probability distribution in which high excitation energies are enhanced by the factor \( (E_i - E_0) \). This enhancement tends to make \( \varepsilon \) large, in practical calculations. As a consequence, \( \mu \) tends to become small, as seen from Eq. (13).

Clearly, we see from Eq. (3) that \( \psi \) is a good approximation to the ground state wave function when all \( |a_i|^2 \) are small and when also \( \sum_{i=1}^m |a_i|^2 \) is small. We formulate in the following a set of mathematical expressions which characterize the quality of \( \psi \).

Let us introduce two quantities \( A \) and \( B(E) \) by the definitions

\[ A = \sum_{i=1}^m |a_i|^2, \]  

(19)

\[ B(E) = \sum_{i=1}^m |a_i|^2 \theta(E_i - E). \]  

(20)

The \( \theta \)-function is zero for \( E_i < E \) and one for \( E_i \geq E \). The number \( A \) gives the total impurity which is present in \( \psi \), while the function \( B(E) \) gives the impurity of \( \psi \) coming from the admixture of eigenstates above a given energy \( E \).

The trial functions used in actual calculations are characterized by \( E_0 \) and \( E_L \) in the sense that we calculate these and no other. We denote by \( S(E_0, E_L) \) the set of all trial functions which are compatible with the particular values of \( E_0 \) and \( E_L \). Then, we ask how \( B(E) \) is bounded on \( S(E_0, E_L) \).

We define \( B_k \) and \( C_k \) by

\[ B_k = \sum_{i=1}^m |a_i|^2, \]  

(21a)

\[ C_k = \sum_{i=1}^m |a_i|^2 (E_i - E_0)^2 \]  

(21b)

for \( k \geq 1 \). We can extend these definitions to \( k = 0 \), if we introduce

\[ |a_0|^2 = 1 - \sum_{i=1}^m |a_i|^2. \]  

(22)

Then we see immediately that the following relations hold

\[ B_k \geq B_{k+1}, \]  

(23a)

\[ C_k \geq C_{k+1}. \]  

(23b)
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for \( k \geq 0 \), and

\[ B_k(E_k - E_0)^2 \leq C_k \]  \hspace{1cm} (24)

for \( k \geq 1 \). From Eqs. \((4), (5), (6)\) and \((22)\) we get

\[ \langle \dot{H}^2 \rangle - \langle \dot{H} \rangle^2 = \sum_{i=0}^\infty \| a_i \|^2 (E_i - E_0)^2 = C_0 \]  \hspace{1cm} (25)

Using Eqs. \((6), (7)\) and \((9)\) we rewrite the left-hand side and get

\[ G(E_1 - E_0) = C_0 \]  \hspace{1cm} (26)

Using the relation \((23b)\) we get

\[ G(E_1 - E_0) \geq C_1 \geq C_2 \geq \cdots \]  \hspace{1cm} (27)

Together with the relation \((24)\) we get bounds for \( A \) and \( B(E_k) \),

\[ A = B_1 \leq G/(E_1 - E_0) \equiv A_0 \]  \hspace{1cm} (28)

\[ B(E_k) \leq G(E_1 - E_0)/(E_k - E_0)^2 \equiv B_0(E_k) \]  \hspace{1cm} (29)

In the present derivation, we have assumed that the upper and lower bounds are calculated with the same function \( \phi \). One can reach an even smaller gap \( G' \) by carrying out the parameter variation independently for the upper bound and for the lower bound. Equation \((28)\), with \( A \) referring to the upper bound wave function, is also valid, when \( G \) is replaced by this new gap \( G' \). This can be seen directly from Eq. \((4)\). We write

\[ G' \geq \langle \dot{H} \rangle - E_0 = \sum_{i=1}^\infty \| a_i \|^2 (E_i - E_0) \geq \sum_{i=1}^\infty \| a_i \|^2 (E_i - E_0) \]  \hspace{1cm} (30)

and get, with Eq. \((19)\),

\[ A \leq G'/(E_1 - E_0) \leq G'/ (E_1 - E_0) \]  \hspace{1cm} (31)

Next, we are interested in the question: Which trial function \( \phi \) yields the maximum value of \( B(E_k) \), for given gap \( G \) and for a chosen value of \( E_k \)? The answer is that, when the gap is smaller than \((E_1 - E_0)/2\), a trial function which, in the eigenstate representation of Eq. \((3)\), has the structure

\[ a_1 = a_2 = \cdots = a_{k-1} = a_{k+1} = a_{k+2} = \cdots = 0 \]

\[ a_k \neq 0 \]  \hspace{1cm} (32)

yields the maximum of \( B(E_k) \), and this maximum is given by

\[ B_{\text{max}}(E_k) = G(E_1 - E_0) / [(E_k - E_0)(E_k - E_0)] \]  \hspace{1cm} (33)

By this equation we are getting the smallest upper bound for \( B(E_k) \). Since \( E_0 \), however, is not known, the practical bound is given by Eq. \((29)\).
The derivation of Eqs. (32) and (33) is given in the Appendix. Let us only consider some plausibility arguments, in the present section. Suppose that we change in Eq. (3) the coefficient $a_i$ in such a way that, with $\delta |a_i|^2 > 0$,

$$|a_{i-1}|^2 - |a_i|^2 + \delta |a_i|^2$$

for a certain $i \geq 1$. This change leads to a change in $E_0$ and $E_1$. It can be shown that the latter change in turn leads to an increased gap $G$. Since $a_i$, for $i < k$, does not contribute to $B(E_k)$, a maximum of $B(E_k)$ for a given gap implies

$$a_1 = a_2 = \cdots = a_{k-1} = 0.$$  

(35)

Next, we change in Eq. (3) the coefficients $a_s$ and $a_i$ in such a way that, for $i > k$,

$$|a_{s-1}|^2 - |a_s|^2 + \delta |a_s|^2,$$

$$|a_{i-1}|^2 - |a_i|^2 - \delta |a_i|^2.$$ 

(36)

This change of the coefficients again leads to a change of $E_0$ and $E_1$ which in turn leads to an increased gap $G$. Thus, we see that for a fixed $B(E_k)$ the configuration

$$a_{k+1} = a_{k+2} = \cdots = 0$$

(37)

gives the smallest gap. This means that for a fixed gap the same configuration gives the largest $B(E_k)$.

It should be noted that $B_0(E)$ has a remarkable property: As $E$ becomes larger, $B_0(E)$ decreases drastically due to the denominator $(E - E_0)^2$. If the gap $G$ is small compared to $E_1 - E_0$, then one can say not only that $\sum |a_i|^2$ is small. One can say also that almost no contribution to this sum can come from high values of $i$.

Equations (28) and (29) give valuable information on the accuracy of wave functions obtained from variational calculations, provided that the gap between upper and lower bounds for the energy is small. We illustrate this in the next section for an ATMS wave function of three-body system with realistic interaction.

§ 3. Accuracy of the form factor calculation based on ATMS

ATMS$^g$ (Amalgamation of Two-body correlations into the Multiple Scattering process) is a method which constructs the wave function of a few-particle system on the basis of the multiple scattering theory. In its construction, the method solves the significant short-range correlations by a two-body scattering equation, and considers them in terms of two-body correlation functions.
It has been reported that the Ritz and Temple bounds calculated from the ATMS wave functions come very close to each other.3) There, the three \(a\)-particle system was treated in its ground state where the \(a\)-particles interact pairwise via a local potential

\[
V(r) = V_R \exp\left[-(\mu_R r)^2\right] - V_A \exp\left[-(\mu_A r)^2\right],
\]

(38)

where \(V_R = 500\text{ MeV}, V_A = 130\text{ MeV}, \mu_R = 0.7\text{ fm}^{-1}\) and \(\mu_A = 0.475\text{ fm}^{-1}\). This potential has a repulsive core of height 370 MeV, as shown in Fig. 1. Equation (38) is the potential of Ali and Bodmer proposed for the \(S\)-wave interaction,3) but we use this in all partial waves. The Coulomb interaction is neglected.

The ATMS wave function for this ground state assumes a form

\[
\psi = \mathcal{S}[u(r_{12})u(r_{23})u(r_{31}) + y(r_{12})v(r_{23})v(r_{31})P(123)],
\]

\[
P(123) = \frac{1}{4} r_{12}^2 + \frac{3}{4} (r_{23}^2 + r_{31}^2) - \frac{1}{2} r_{13}^2 r_{23} + \frac{3}{2} r_{23} r_{31}^2,
\]

(39)

where \(r_{ij}\) is the distance between the \(i\)-th and the \(j\)-th particle, and \(\mathcal{S}\) is the symmetrization operator. The first term in the square bracket takes account mainly of the \(S\)-wave two-body correlations while the second term mainly contains the \(D\)-wave correlations.

The system has no stable \(L = 0\) excited state, so the threshold \(-1.37\text{ MeV}\) of the \(a + 2a\) configuration was taken for \(E_c\). As a result, \(E_U = -5.18\text{ MeV}\) and \(E_L = -5.31\text{ MeV}\) were obtained for the Ritz and Temple bounds, respectively.

We apply Eqs. (28) and (29) to this case. We get, with \(E\) in MeV,

\[
A \leq A_U = 0.0341,
\]

(40)

\[
B(E) \leq B_c(E) = \frac{0.495}{(E + 5.18)^3}.
\]

(41)

Thus, this wave function has a total impurity smaller than 3.4\%. We note that our upper bounds for the impurity are practical only when the gap \(G \) is small. For example, in another calculation with an ordinary variational method, \(E_U = -3.3\text{ MeV}\) and \(E_L = -79.3\text{ MeV}\) were obtained for the same system.3,3) For this trial
wave function, $A_0$ becomes equal to 39 which is bigger than the maximum value allowed by the normalization condition $\langle \psi | \psi \rangle = 1$.

We plot $B_0(E)$ in Fig. 2, where we see how drastically it decreases as $E$ increases. Thus, the contribution coming from all the excited eigenstates above 2 MeV is smaller than 0.01 already, and the contribution from above 17 MeV is smaller than 0.001. This feature suggests that we can neglect the impurity of the ATMS wave function above a certain value of excitation energy, and enables us to discuss the accuracy of the elastic charge form factor calculated from this wave function. In particular, high accuracy might be expected at high momentum transfers. In the following, we first try to derive an error bound for the charge form factor no matter how bad it will be, and then try to give a realistic estimate of the error.

The charge form factor between two $L=0$ eigenstates $i$ and $j$ of a few-particle system is written as

$$F_{ij}(q) = \langle \psi_i | \exp(iqr_N) | \psi_j \rangle = \langle \psi_i | j_0(qr_N) | \psi_j \rangle,$$  

(42)

where $j_0(x)$ is the spherical Bessel function, $q$ is the momentum transfer, and $r_N$ is the distance between the centre of mass and the $N$-th particle as chosen for a representative particle. We write $N$ to denote the number of particles of the system. $F_{00}(q)$ is the elastic charge form factor of the ground state which we approximate by

$$F(q) = \langle \psi | j_0(qr_N) | \psi \rangle,$$  

(43)

where $\psi$ is the ATMS wave function. We expand $F(q)$ on $F_{ij}(q)$ by Eq. (3),

$$F(q) = \sum_{i<j}^{m} \sum_{j>j}^{n} a_i^* a_j F_{ij}(q),$$  

(44)

where we use the convention of Eq. (22).

We want to get an upper bound for the error
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\[ \Delta(q) \equiv F_{0\ell}(q) - F(q), \]  

We divide this into three parts:

\[ \Delta(q) = \Delta_1(q) + \Delta_2(q) + \Delta_3(q), \]  

where

\[ \Delta_1(q) = \sum_{i=1}^{\infty} |a_i|^2 F_{0\ell}(q), \]  

\[ \Delta_2(q) = - \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} [a_i^* a_j F_{ij}(q) + a_j^* a_i F_{ji}(q)], \]  

\[ \Delta_3(q) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_i^* a_j F_{ij}(q). \]  

We call \( \Delta_1(q) \) a norm defect because it arises from the fact that \( a_0 \psi_0 \) is not normalized to unity but to \( 1 - \sum_{r=1}^{\infty} |a_i|^2 \). To bound this, we replace \( \sum_{r=1}^{\infty} |a_i|^2 \) by \( A_0 \), and \( F_{0\ell}(q) \) by the nearest maximum \( F_{\text{max}}(q) \) of \( F(q) \), in Eq. (47), so that

\[ |\Delta_1(q)| \leq |D_{\text{max}}(q)|, \]

\[ D_{\text{max}}(q) = A_0 F_{\text{max}}(q). \]  

The resulted maximum error bound coming from this norm defect is shown in Fig. 3 by the shaded area.

To bound \( \Delta_2(q) \) and \( \Delta_3(q) \), we introduce and calculate two quantities \( I(q) \) and \( J(q) \) defined by

\[ I(q)F(q) = \langle \psi | H_{0\ell} (q \psi_{\nu}) | \psi \rangle, \]  

\[ J(q)F(q) = \langle \psi | H_{0\ell} (q \psi_{\nu}) | H | \psi \rangle. \]  

If \( \psi \) is the exact ground state wave function, \( I(q) \) and \( J(q) = -\sqrt{J^2(q)} \) are constant and equal to \( E_0 \). The values of \( I(q) \) and \( J(q) \) calculated from the ATMS wave function are listed in Table I.

From Eqs. (43) and (51), we get

\[ 2[I(q) - E_0]F(q) = \langle \psi | (H - E_0) \psi_{\nu}(q \psi_{\nu}) | \psi \rangle \]

\[ = \sum_{i=1}^{\infty} (E_i - E_0) [\sum_{j=1}^{\infty} [a_i^* a_j F_{ij}(q) + a_j^* a_i F_{ji}(q)]]. \]  

Then, we replace the positive factor \( E_i - E_0 \) on the right-hand side by the smallest one \( E_i - E_0 \), taking into account the fact that the admixture in \( \psi \) coming from high energy eigenstates is rather strictly bounded according to Eq. (41), so that
Table I. The elastic charge form factor $F(q)$ of three point $\pi$-particles calculated from the ATMS wave function. $I(q)$ and $J(q)$ are defined in the text.

<table>
<thead>
<tr>
<th>$q^2$(fm$^{-2}$)</th>
<th>$F(q)$</th>
<th>$I(q)$ (MeV)</th>
<th>$J(q)$ (MeV)</th>
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<td>1</td>
<td>0.33861</td>
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<td>-5.0569</td>
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</tr>
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\[
|\Delta_2(q)| \leq |\Delta_{s}^{m\text{ax}}(q)|, \\
\Delta_{s}^{m\text{ax}}(q) = -2[I(q) - E_0]F(q)/(E_1 - E_0). \tag{54}
\]

This $|\Delta_{s}^{m\text{ax}}(q)|$ is the largest estimate among those obtained by dividing the right-hand side of Eq. (53) by $E_1 - E_0$. A bound for $\Delta_3(q)$ is obtained similarly. From Eqs. (44), (51) and (52), we get

\[
[J^2(q) - 2I(q)E_0 + E_0^2]F(q) \\
= \langle \phi |(H - E_0)\sum_{ij}(H - E_0)\langle \phi | \\
= \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} (E_i - E_0)(E_i - E_0)\{a_i^* a_j F_\alpha(q)\}, \tag{55}
\]

so that we can safely bound $\Delta_3(q)$ by

\[
|\Delta_3(q)| \leq |\Delta_{s}^{m\text{ax}}(q)|, \\
\Delta_{s}^{m\text{ax}}(q) = [J^2(q) - 2I(q)E_0 + E_0^2]F(q)/(E_1 - E_0)^2. \tag{56}
\]

We always pick such $E_0$ value from the range $E_0 \geq E_0 \geq E_1$ that the error from $\Delta_2(q)$ and $\Delta_3(q)$ takes the maximum value.

We derive a bound for the total error $\Delta(q)$ according to Eq. (46). The result
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is shown in Fig. 3, where the contributions from \( \Delta_s(q) \) and \( \Delta_l(q) \) are entered into the dotted area. This is a very safe bound for the error \( \Delta(q) \). The fact that we can give good bounds to the theoretical error is an extraordinary feature of the ATMS method.

Now, we go on to a realistic estimate of the error \( \Delta(q) \). We first note that when we go from the calculation of \( F(q) \) to the calculation of \( I(q) \), a higher energy region of the impurity is emphasized. When we go to the calculation of \( I(q) \), an even higher energy region is emphasized. From Table I, we see that the two functions \( I(q) \) and \( F(q) \) obtained from the ATMS wave function are almost constant and very near to \( E_0 \). Particularly, they show a very similar behaviour above the second maximum region \( (q^2 \geq 4 \text{ fm}^{-2}) \) which we call a high momentum region. These features indicate that, in Eq. (44), the excited eigenstates above a certain value of excitation energy make essentially no contribution to \( F(q) \).

On the other hand, the lowest excited state \( \phi \) describes a bound \( 2\alpha \) pair and an \( \alpha \)-particle in a relative motion of lowest energy, and hence of a very large rms radius. Such a function certainly does not occur in our \( \phi \). A realistic curve of \( |a_1|^2 \) versus \( E_r \) starts at zero for \( E_r - E_1 \), has maximum for some higher \( E_r \) and goes to zero for \( E_r \to \infty \). It follows that our upper bound Eq. (29) gets bad at low excitation energies, and \( A \) must be much smaller than \( A_0 = 3.4\% \). This leads to a drastic reduction of \( \Delta_l(q) \).

The ATMS wave function is constructed on the basis of the Bethe-Goldstone equation. It was pointed out that a singular potential can be divided into a short-range part and a long-range part. The short-range part excites the relative two-body states into a region of fairly large momentum values. The situation of such an excitation is essentially unaltered when we go from the ground state to the

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*If we think in terms of an oscillator model for three point \( \alpha \) particles with an oscillator width which gives the ground-state rms radius, first maximum of the curve cannot be at an excitation energy lower than \( 2\hbar \omega \approx 12 \text{ MeV} \).
excited states of a few-particle system, provided that the excitation energies are small.

Suppose that we divide the impurity of the ATMS wave function into a lower energy part which comes from low energy eigenstates and a higher energy part which comes from high energy eigenstates. From the above consideration, it is expected that the lower energy part of the impurity does not bring about an appreciable change in the higher part of the momentum distribution. In appreciably excited eigenstates, the momentum distribution becomes different, concentrating at certain high momentum values. As indicated by Eq. (41), however, $B(E)$ rapidly decreases for high values of $E$. Thus, we expect that the low energy impurity mainly cancels the norm defect error, and the higher energy part of the impurity is so small that it cannot do any harm. We may expect that charge form factor curves calculated from the ATMS wave function are very accurate at high momentum transfers.

These considerations lead us to set up a model configuration for the ATMS wave function to estimate the error $\Delta(q)$ at high values of $q$, i.e.,

$$\psi_{\text{model}} = \sqrt{1 - |a_n|^2} \varphi_n + a_n \varphi_n.$$  \hspace{1cm} (57)

$\varphi_n$ is an excited eigenstate which has an appreciably large excitation energy and is properly chosen. We have seen in §2 that this configuration gives the maximum impurity $B(E)$ for $E = E_n$ for the obtained energy gap $G$.

We divide $\Delta(q)$ according to Eqs. (46) through (49). Now,

$$|J_1(q)| = |a_n|^2 F_0(q) \leq B_0(E_n) F(q),$$ \hspace{1cm} (58)

$$\Delta_2(q) = -2[I(q) - E_0] F(q)/(E_n - E_0),$$ \hspace{1cm} (59)

$$\Delta_3(q) = [I(q) - 2I(q) E_0 + E_n^2] F(q)/(E_n - E_0)^2.$$ \hspace{1cm} (60)

It should be noted that here Eqs. (59) and (60) are exact relations.

For the choice of $E_n$, we refer to a commutation relation

$$[H, \exp(iqr_n)] = \frac{\hbar^2}{2M} \frac{N-1}{N} \exp(iqr_n)\left(q^2 - i2q\frac{\beta}{\sigma^2}\right).$$ \hspace{1cm} (61)

Then, we get

$$\langle \varphi_n | \exp(-iqr_n) H \exp(iqr_n) | \varphi_n \rangle = E_0 + \frac{N-1}{2N} \frac{\hbar^2}{M} q^2.$$ \hspace{1cm} (62)

We may consider that $\exp(iqr_n)\varphi_n$ is a state which is excited by the momentum transfer with an average excitation energy $(N-1)/(2N)(\hbar^2/M)q^2$. Thus, we take as

$$E_n - E_0 \sim \frac{N-1}{2N} \frac{\hbar^2}{M} q^2 = 3.46q^2.$$ \hspace{1cm} (63)
with \( q \) in fm\(^{-1}\).

The resulted error is very small. It is 1.5% in the second maximum region and 0.9% in the third maximum region. It almost disappears in the line drawn for \( F(q) \) in the second and third maximum regions. This illustrates high accuracy of the form factor calculation based on the ATMS method.

§ 4. Concluding remarks

We have introduced two quantities \( A \) and \( B(E) \) which are a measure of the impurity of a trial wave function, and we have derived some mathematical relations to estimate their maximum values. These relations become very useful in the ATMS method, due to the very small gap between the upper and lower bounds for the energy. The ATMS wave function, which has been obtained in the case of the three \( \alpha \)-particles interacting by phenomenological \( \alpha\alpha \) potential with repulsive core, has a total impurity smaller than 3.4%, and an impurity smaller than 0.1% above an excitation energy of 17 MeV. This means that the accuracy in the form factor calculation based on the ATMS method is very high, in particular around and above the second maximum of the elastic charge form factor. It should be noted that such an accuracy is a specific feature of the ATMS method and is not typical for other variational calculations.

Acknowledgements

One of us (E. S.) wants to thank Professor H. Tanaka and Professor S. Oryu for their hospitality and the Science University of Tokyo for its generous support.

Appendix

--- The Proof of Relations (32) and (33) ---

We want to prove that, among all possible trial functions which yields the same gap \( G \), the one which has \( a_{k} \neq 0 \), all other \( a_{i} = 0 \), has the largest value of \( B(E_{k}) \).

Proof

1) We show that the gap increases by \( \delta G > 0 \) if we change the coefficients in Eq. (3) in such a way that, with \( \delta|a_{i}|^{2} > 0 \),

\[ |a_{i}|^{2} \rightarrow |a_{i}|^{2} + \delta|a_{i}|^{2}. \quad (A \cdot 1) \]

An increase of the gap caused by the change \( (A \cdot 1) \) for \( i < k \) means that we have to decrease \( B(E_{k}) \) in order to go back to the given gap \( G \). Let us introduce the abbreviations:

\[ \langle \phi|H^{2}|\phi\rangle = Z_{1}, \quad \langle \phi|H|\phi\rangle = Z_{2}, \quad (A \cdot 2) \]
when taken with the coefficients of Eq. (3), and
\[ E_i - Z_k = N, \] (A·3)
\[ \delta |a_i|^2 (E_i - E_0) = X. \] (A·4)

Then, we can write
\[ \delta G = \frac{Z_i + \delta |a_i|^2 (E_i^2 - E_0^2) - [Z_i + \delta |a_i|^2 (E_i - E_0)]^2}{N - \delta |a_i|^2 (E_i - E_0)} \frac{Z_i - Z_k^2}{N} \]
\[ = \frac{Z_i + X(E_i + E_0) - [Z_i + X]^2}{N - X} \frac{Z_i - Z_k^2}{N}. \] (A·5)

We want to show that \( \delta G > 0 \) and proceed as follows. Since \( X > 0 \),
\[ \delta G \geq \frac{Z_i + X(E_i + E_0) - [Z_i + X]^2}{N} \left( \frac{Z_i - Z_k^2}{N} \right), \]
\[ N \delta G \geq Z_i + X(E_i + E_0) - [Z_i + X]^2 - Z_i + Z_k^2 \]
\[ = X(E_i + E_0 - 2Z_k - X) \geq X(E_i + E_0 - 2Z_k - X). \] (A·6)

The second \( X \) on the right-hand side can be dropped because \( X^2 \) is of order \( \delta^2 \).

We know from Eq. (A·2) that \( Z_k \) is the upper bound obtained from the ATMS calculation. If we now introduce the condition that
\[ G < \frac{1}{2} (E_i - E_0) \] (A·7)
which is easily fulfilled in ATMS, then the right-hand side of Eq. (A·6) is positive and we have
\[ \delta G > 0. \quad \text{q. e. d.} \] (A·8)

If any increase of \( |a_i|^2 \) (\( i < k \)) increases \( G \), then it follows that
\[ B(E_k) = B_{\text{max}}(E_k) \]
implies
\[ a_i = 0 \quad \text{for} \quad i < k. \] (A·9)

2) We want to show that
\[ B(E_k) = B_{\text{max}}(E_k) \] (A·10a)
also implies
\[ a_i = 0 \quad \text{for} \quad i > k. \] (A·10b)

In order to show this, we investigate the following variation of the coefficients of
Eq. (3):
\[ |a_i|^2 - |a_i|^2 + \delta|a_k|^2, \quad (A\cdot11a) \]
\[ |a_k|^2 - |a_k|^2 - \delta|a_k|^2, \quad (A\cdot11b) \]
where \( \delta|a_k|^2 \) is a positive quantity. For the sake of simplicity, we assume that redundancies other than those arising from (exactly treated) symmetry are removed by a small perturbation. We then have
\[ E_i > E_k. \quad (A\cdot12) \]
We use the abbreviations \((A\cdot2)\sim(A\cdot4)\), and introduce the abbreviation
\[ \delta|a_k|^2(E_i-E_k) \equiv Y. \quad (A\cdot13) \]
We then have
\[ \delta G = \frac{Z_i + Y(E_i + E_k) - [Z_i + Y]^2}{N-Y} - \frac{Z_i - Z_i^2}{N}, \]
\[ N \delta G > Y(E_i + E_k) - 2Z_i Y - Y^2. \quad (A\cdot14) \]
We drop \( Y^2 \) because it is of order \( \delta^2 \) and have
\[ N \delta G > Y[(E_i + E_k) - 2Z_i]. \quad (A\cdot15) \]
Again, we have to remember that \( Z_i \) is the ATMS upper bound and that
\[ E_i + E_k > 2E_i. \quad (A\cdot16) \]
Then, because of \((A\cdot7)\), we find
\[ \delta G > 0. \quad (A\cdot17) \]
Now, according to its definition, \( B(E_k) \) is invariant under the variation \((A\cdot11)\). But the variation \((A\cdot11) \) has increased the gap \( G \). Therefore, we get the smallest gap for fixed \( B(E_k) \) and consequently, the largest \( B(E_k) \) for fixed \( G \), when
\[ a_i = 0 \quad \text{for} \quad i > k \quad (A\cdot18) \]
is valid. This proves the relation \((A\cdot10a, b)\).
We have shown now that \( B(E_k) \) assumes its maximum value \( B_{\text{max}}(E_k) \) when \( a_i = 0 \) for \( i < k \) and \( a_i = 0 \) for \( i > k \), which means that the maximum is reached when only \( a_k \) is different from zero.

q. e. d.
Finally, we calculate $B_{\text{max}}(E_h)$. From Eqs. (12) and (A.10a, b) we get

$$\varepsilon = E_h,$$  \hspace{1cm} (A.19)

and from Eqs. (4), (9) and (11) we get

$$G_{\mu} = |a_h|^2 (E_h - E_0).$$  \hspace{1cm} (A.20)

Together with Eq. (13), we have

$$|a_h|^2 = B_{\text{max}}(E_h) = \frac{G(E_i - E_0)}{(E_h - E_0)(E_h - E_i)}.$$  \hspace{1cm} (A.21)

References