A Symbolic Calculation Code for Nuclear Three-Body Problem

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A computational method is described for the Rayleigh–Ritz variational method in solving nuclear three-body problem where the hard core is included in the two-body potentials. Formula manipulation techniques have been developed to carry out all the required differentiation and complicated integrations analytically and these have been proved to be useful on a high-speed computer.

1. INTRODUCTION

The nuclear three-body data (in particular, those of the ground states of H^3 and He^3) have been regarded as potentially important sources of information on the nuclear forces. In 1935 Thomas [1] showed that the zero range two-body nuclear forces would give an infinite triton binding energy. Since then a large number of calculations have been carried out on the binding energies of H^3 and He^3. The most extensive calculations have been performed [2] in Australia by Blatt, Derrick, Delves, Davies among others by using some 'realistic' two-body nuclear potentials, which include hard cores.

The recent electron scattering experiments [3] have added useful information on the electromagnetic form factors of the ground states of three-body nuclei. This has stimulated active research in the field.

The problem is also of interest in that it is next in simplicity to the deuteron problem, but as yet it is not solvable by any analytical method in general, just as the helium atom is to the hydrogen atom. Although there have been some attempts at direct numerical solution, it is still difficult to deal accurately with the differential equations of elliptic type involving three independent variables even with the help of high-speed digital computers.

* Passed away on March 3, 1969, shortly before the completion of the present paper.

Probably the best way of solving the Schrödinger equation for the three-body problem is to use the Rayleigh–Ritz variational method. In fact, the wavefunctions of the helium atom have been obtained with successive accuracies culminating in Pekeris' 1078 parameter wave function [4]. All the integrations can be carried out analytically by the methods due to Hylleraas [5], Kinoshita [6], and Pekeris, among others. Their methods, however, are not suited to our nuclear three-body problem, because the system is composed of three particles with (almost) equal masses so that the principal s-state is totally symmetric under interchange of any pair or particles. Furthermore, the direct application of their methods is impossible if the two-body nuclear potentials have hard cores.

Blatt and his collaborators [2] have adopted elaborate H^3 trial wavefunctions with three interparticle distances r_i ($i = 1, 2$ and 3) (see Fig. 1) as the independent variables, and carried out the required triple integrations numerically.
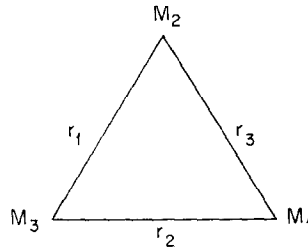

FIG. 1.   Coordinate system for H^3 and He^3. M_s is the mass of the odd nucleon (i.e., the proton in H^3 and the neutron in He^3.).

One of the authors (late T. Ohmura) has been studying [7] the isobaric-spin of H^3 and He^3, the effects of the difference between the wavefunction of H^3 and that of He^3, and so on. The present paper reports the computational details developed in the calculation. The trial wavefunctions are chosen along a line similar to that of Blatt's group and also that of Hylleraas. The exponential factor in Hylleraas' trial function must be replaced by a more elabolate correlation factor in order to take account of the hard core included in the two-body potentials. The factor is chosen after Ref. [8, Eq. (17)]. Apart from this factor the polynomial expansion in r_1, r_2 and r_3 is assumed for the trial functions. In principle, this type of wavefunctions allows us to carry out all the integrations analytically just as the Hylleraas or Pekeris functions do. However, the hard core requires the more complicated correlation factor and the triple integration in a very complicated domain.

For the severe demand on computational accuracy, some formula manipulation techniques should be used in performing the kinetic energy operations and the triple integrations analytically, because no numerical integration formula and no

numerical differentiation methods can avoid some inherent truncation and rounding errors which make the whole computations inaccurate to some extent [9]. Some general purpose formula manipulation systems such as FORMAC [10] and LISP 1.5 [11], have not turned out to be efficient for our problem, because they require too much computer storage and inhibitingly enormous computing time.

Therefore, a special purpose symbolic calculation code 'TRIPLE' is developed in FORTRAN. Our main ideas are matrix representation of polynomials and recurrence formula for the kinetic energy operations [12]. The code has proved to be useful for our nuclear three-body problem.

The present paper also complements Ref. [7], because the computational details were completely omitted there, although these technical problems are rather essential in the success of that calculation.

In Section 2 we give the Schrödinger equation for our problem and describe the trial wavefunctions and the variational procedure for the Schrödinger equation. The recurrence formula in constructing the necessary integrands is derived in Section 3, and explicit formulae for the integrals are given in Section 4. Various programming techniques including the details of matrix representation of polynomials are explained in Section 5, while the concluding discussions are given in Section 6.

2. VARIATIONAL METHOD

A. *Schrödinger Equation*

If the two-nucleon force is represented by central potentials, the ground state wavefunction of three-body nuclei has the form

$$\Psi = \Psi_s \chi_2 + \Psi_a \chi_1 \tag{1}$$

where both χ_1 and χ_2 are doublet spin functions, which are, respectively, symmetric and antisymmetric with respect to the like nucleons 1 and 2 (namely, two neutrons in H^3 and two protons in He^3)

$$\chi_1 = [\alpha(1)\,\beta(2) + \alpha(2)\,\beta(1)]\,\alpha(3)/\sqrt{6} - \sqrt{2/3}\alpha(1)\,\alpha(2)\,\alpha(3) \tag{2}$$

and

$$\chi_2 = [\alpha(1)\,\beta(2) - \alpha(2)\,\beta(1)]\,\alpha(3)/\sqrt{2}. \tag{3}$$

The Ψ_s and Ψ_a are the s-state spatial wavefunctions, symmetric and antisymmetric under the interchange of nucleon 1 and 2, respectively.

We will take r_1, r_2, and r_3 as the independent variables which describe the system (see Fig. 1).

The Schrödinger equation for He^3 is now reduced to the following coupled differential equations:

$$\{K + V_s^p(r_3) + V_s(r_1)/4 + V_s(r_2)/4 + 3V_t(r_1)/4 + 3V_t(r_2)/4 + V_c(r_3) - E\}\, \Psi_s$$

$$+ (\sqrt{3}/4)\{V_s(r_1) - V_s(r_2) - V_t(r_1) + V_t(r_2)\}\, \Psi_a = 0, \qquad (4\text{-}a)$$

and

$$\{K + V_t^p(r_3) + V_t(r_1)/4 + V_t(r_2)/4 + 3V_s(r_1)/4 + 3V_s(r_2)/4 + V_c(r_3) - E\}\, \Psi_a$$

$$+ (\sqrt{3}/4)\{V_s(r_1) - V_s(r_2) - V_t(r_1) + V_t(r_2)\}\, \Psi_s = 0, \qquad (4\text{-}b)$$

where

$$K = - \sum_{\text{cyclic}} \left\{ \frac{\hbar^2}{\mu_{23}} \frac{1}{r_1^2} \frac{\partial}{\partial r_1} \left(r_1^2 \frac{\partial}{\partial r_1} \right) + \frac{\hbar^2}{2M_1} \frac{(r_2^2 + r_3^2 - r_1^2)}{r_2 r_3} \frac{\partial^2}{\partial r_2 \, \partial r_3} \right\},$$

$$\mu_{j,k} = \frac{2M_j M_k}{M_j + M_k}. \qquad (4\text{-}c)$$

We take two-body nuclear potentials of a central type

$$V_{ij} = (3 + \sigma_i\sigma_j)\, V_t(r_{ij})/4 + (1 - \sigma_i\sigma_j)\, V_s(r_{ij})/4, \qquad (5)$$

where the triplet and singlet potentials are defined by

$$V_t(r) = \begin{cases} -A_t \exp[-\alpha_t(r - D)] & r \geqslant D \\ +\infty & 0 < r < D \end{cases} \qquad (6\text{-}a)$$

and

$$V_s(r) = \begin{cases} -A_s \exp[-\alpha_s(r - D)] & r \geqslant D \\ +\infty, & 0 < r < D. \end{cases} \qquad (6\text{-}b)$$

The force parameters A_t, A_s, α_t, and α_s for even parity states were adjusted so as to fit the low energy data of the neutron–proton system, and given in Table I of Ref. [7]. The parameters A_t and A_s for the odd parity states are the same as those for the even parity state for the Wigner force, but only the sign is changed for the Majorana force. If A_t and A_s vanish for odd parity states we call it "the even parity force," which is sometimes called as the Serber force also. We consider the above three types of nuclear forces.

The proton–proton potentials V_t^p and V_s^p (and also V_t^n and V_s^n) are taken to be the same as the neutron–proton potentials unless otherwise stated. The

Coulomb force between two protons in He^3 is modified in order to take account of the finite size of the proton with the exponential charge distribution of rms radius 0.8 fm.

The explicit form of $V_c(r)$ is

$$V_c(r) = \frac{e^2}{r} \left[1 - \left(1 + \frac{11}{16} \beta r + \frac{3}{16} (\beta r)^2 + \frac{1}{48} (\beta r)^3 \right) e^{-\beta r} \right] \qquad (7)$$

with $\beta = 4.33$ fm^{-1}.

The Schrödinger equation for H^3 is obtained if the Coulomb potential term is dropped and the role of the proton and that of the neutron are interchanged. Actual calculations are carried out with the constant $\hbar^2/\mu_i = \hbar^2/M_i = 41.47$ MeV · fm^2.

We shall decompose Ψ_s and Ψ_a into various classes of functions each of which has a distinct physical meaning.

$$\Psi_s = v_0 + v_1 + w_1, \qquad \Psi_a = v_2 - w_2 + v_3 \qquad (8)$$

The functions v_0 and v_2 are, respectively, completely symmetric and completely antisymmetric under interchange of any of nucleons. The functions v_1 and w_1 (v_2 and w_2) are symmetric (antisymmetric) with respect to like nucleons 1 and 2. They belong to intermediate symmetry classes of functions of three variables and satisfy the following relations,

$$v_2(12, 3) = [v_1(23, 1) - v_1(31, 2)]/\sqrt{3}, \qquad (9\text{-a})$$

$$v_1(12, 3) = -[v_2(23, 1) - v_2(31, 2)]/\sqrt{3}, \qquad (9\text{-b})$$

$$w_2(12, 3) = [w_1(23, 1) - w_1(31, 2)]/\sqrt{3}, \qquad (9\text{-c})$$

$$w_1(12, 3) = -[w_2(23, 1) - w_2(31, 2)]/\sqrt{3}, \qquad (9\text{-d})$$

where $v_1(12, 3) \equiv v_1$, $v_2(12, 3) \equiv v_2$, $w_1(12, 3) \equiv w_1$ and $w_2(12, 3) \equiv w_2$.

The principal s-state is represented by v_0, the s'-state by $v_1\chi_2 + v_2\chi_1$, the isospin $T = 3/2$ state by $w_1\chi_2 - w_2\chi_1$ and the completely antisymmetric s-state (called here as the s''-state) by v_3. All the s, s' and s''-states belong to the $T = 1/2$ state.

B. Variational Method

Let the Eqs. (4-a) and (4-b) be abbreviated by

$$(L_{ss} - E) \Psi_s + L_{sa}\Psi_a = 0, \qquad (10\text{-a})$$

and

$$(L_{aa} - E) \Psi_a + L_{as}\Psi_s = 0. \qquad (10\text{-b})$$

Multiplying $\Psi_s{}^*$ from the left to Eq. (10-a), and $\Psi_a{}^*$ from the left of Eq. (10-b), and integrating over the configuration space, we get

$$\int \left[\Psi_s{}^* L_{ss}\Psi_s + \Psi_s{}^* L_{sa}\Psi_a + \Psi_a{}^* L_{as}\Psi_s + \Psi_a{}^* L_{aa}\Psi_a\right] d\tau$$

$$= E \int \left[\Psi_s{}^*\Psi_s + \Psi_a\Psi_a{}^*\right] d\tau, \tag{11}$$

where

$$\int f \cdot d\tau \equiv \int_D^{\infty} r_1\, dr_1 \int_D^{\infty} r_2\, dr_2 \int_D^{\infty} r_3 \cdot f(r_1, r_2, r_3)\, dr_3$$

$$- \int_D^{\infty} r_2\, dr_2 \int_D^{\infty} r_3\, dr_3 \int_0^{\infty} (r_1 + r_2 + r_3) \cdot f(r_1 + r_2 + r_3, r_2, r_3)\, dr_1$$

$$- \int_D^{\infty} r_3\, dr_3 \int_D^{\infty} r_1\, dr_1 \int_0^{\infty} (r_1 + r_2 + r_3) \cdot f(r_1, r_1 + r_2 + r_3, r_3)\, dr_2$$

$$- \int_D^{\infty} r_1\, dr_1 \int_D^{\infty} r_2\, dr_2 \int_0^{\infty} (r_1 + r_2 + r_3) \cdot f(r_1, r_2, r_1 + r_2 + r_3)\, dr_3. \tag{12}$$

This triple integration will be called as τ-integration in the present paper.

Let the trial functions Ψ_s and Ψ_a be linear and homogeneous in the adjustable parameters η_i $(i = 1, 2,..., n)$, and let all the quantities be real in our calculation. Equation (11) now has the form

$$\sum_{i=1}^{n} \sum_{j=1}^{n} M_{ij}\eta_i\eta_j = E \sum_{i=1}^{n} \sum_{j=1}^{n} N_{ij}\eta_i\eta_j \tag{13}$$

with the hermiticity condition

$$M_{ij} = M_{ji}. \tag{14}$$

Since the energy E is stationary, partial differentiation of both sides of Eq. (13) with respect to η_k leads to the equation

$$\sum_{i=1}^{n} M_{ki}\eta_i = E \sum_{i=1}^{n} N_{ki}\eta_i \qquad (k = 1, 2,..., n), \tag{15}$$

where use has been made of Eq. (14). The homogeneous n simultaneous equation (15) determines the eigenvalue E and the ratios of η_k.

The assumed trial functions (see Eqs. (1 and 8)) for Ψ_s and Ψ_a are

$$v_0 = \mathscr{E} \cdot \{a_0 + a_1(r_1 + r_2 + r_3) + a_2(r_1^2 + r_2^2 + r_3^2) + a_3(r_2r_3 + r_3r_1 + r_1r_2)\},$$

$$v_2 = \sqrt{3}\,\mathscr{E} \cdot \{b_1(r_2 - r_1) + b_2(r_2^2 - r_1^2) + b_3(r_1r_3 - r_2r_3)\},$$

$$w_2 = \sqrt{3}\,\mathscr{E} \cdot \{c_1(r_2 - r_1) + c_2(r_2^2 - r_1^2) + c_3(r_1r_3 - r_2r_3)\},$$

$$v_3 = d_1 \cdot \mathscr{E} \cdot \{(r_1^2r_2 + r_2^2r_3 + r_3^2r_1 - r_1r_2^2 - r_2r_3^2 - r_3r_1^2)\},$$

(16)

where

$$\mathscr{E} = \begin{cases} \displaystyle\prod_{p=1}^{3} [e^{-\mu(r_p - D)} - e^{-\nu(r_p - D)}]; & \text{all} \quad r_p > D \\[2mm] 0; & \text{otherwise} \end{cases}$$

(17)

The functions v_1 and w_1 are obtained from Eqs. (9-b) and (9-d), respectively. The constants μ and ν in the correlation function $\mathscr{E}$ are taken from Table II of Ref. [8], and considered not to be subject to variation.

The linear parameters a_0, a_i, b_i, c_i ($i = 1, 2$ and 3) and d_1 are determined according to Eq. (15) so as to minimize the energy E of the system.

3. RECURRENCE FORMULA FOR $K\Psi$

Our trial wavefunctions are now expressed explicitly as follows:

$$\Psi_s = \mathscr{E} \cdot \{a_0 + [\alpha_1(r_1 + r_2) + \beta_1 r_3] + [\alpha_2(r_1^2 + r_2^2) + \beta_2 r_3^2]$$
$$+ [\alpha_3(r_2r_3 + r_3r_1) + \beta_3 r_1r_2]\}$$

(18)

and

$$\Psi_a = \mathscr{E} \cdot \{\gamma_1(r_2 - r_1) + \gamma_2(r_2^2 - r_1^2) + \gamma_3(r_3r_1 - r_2r_3)$$
$$+ d(r_1^2r_2 - r_1r_2^2 + r_2^2r_3 - r_2r_3^2 + r_3^2r_1 - r_3r_1^2)\},$$

(19)

where the parameters $(\alpha_i, \beta_i, \gamma_i)$ ($i = 1, 2$ and 3) are related to (a_i, b_i, c_i) ($i = 1, 2$ and 3) of Eq. (16) by

$$a_i + b_i + c_i = \alpha_i,$$

$$a_i - 2b_i - 2c_i = \beta_i,$$

$$\sqrt{3}(b_i - c_i) = \gamma_i \quad (i = 1, 2 \text{ and } 3).$$

(20)

These adjustable parameters a_0, $(\alpha_i, \beta_i, \gamma_i; i = 1, 2, 3)$, d are called 'state vector' and simply written $\eta = \{\eta_i\}$.

It is necessary for the variational procedure to evaluate the following quadratic forms, or matrix elements $N_{mm'}$, $K_{mm'}$ and U_{mm} :

$$\mathscr{N} = \int (\Psi_s^2 + \Psi_a^2) \, d\tau = \sum_m \sum_{m'} \eta_m \eta_{m'} \cdot N_{mm'} , \qquad (21)$$

$$\mathscr{K} = \int (\Psi_s K \Psi_s + \Psi_a K \Psi_a) \, d\tau = \sum_m \sum_{m'} \eta_m \eta_{m'} K_{mm'} , \qquad (22)$$

and

$$\mathscr{U} = \xi_s{}^W U_s{}^W + \xi_t{}^W U_t{}^W + \xi_s{}^M U_s{}^M + \xi_t{}^M U_t{}^M + \xi_s{}^e U_s{}^e + \xi^c C + \xi^p P$$

$$= \sum_m \sum_{m'} \eta_m \eta_{m'} U_{mm'} , \qquad (23)$$

where $\xi_s{}^W, \xi_t{}^W, \xi_s{}^M, \xi_t{}^M, \xi_s{}^e, \xi^c$, and ξ^p specify the two-body nuclear and Coulomb potentials, and $U_s{}^W$, $U_t{}^W$,... are all quadratic forms in η_i .

For example, $U_s{}^M$ has the form

$$U_s{}^M = \int [\Psi_s\{V_s(r_3) \, P_{12} + \tfrac{1}{4} V_s(r_1) \, P_{23} + \tfrac{1}{4} V_s(r_2) \, P_{31}\} \, \Psi_s$$

$$+ \frac{\sqrt{3}}{4} \Psi_s\{V_s(r_1) \, P_{23} - V_s(r_2) \, P_{31}\} \, \Psi_a$$

$$+ \frac{\sqrt{3}}{4} \Psi_a\{V_s(r_1) \, P_{23} - V_s(r_2) \, P_{31}\} \, \Psi_s$$

$$+ \Psi_a\{\tfrac{3}{4} V_s(r_1) \, P_{23} + \tfrac{3}{4} V_s(r_2) \, P_{31}\} \, \Psi_a] \, d\tau. \qquad (24)$$

Here P_{ij} are exchange operators, i.e.,

$$P_{ij}\Psi(r_i, r_j, r_k) = \Psi(r_j, r_i, r_k), \qquad (25)$$

and $U_s{}^W$ has the same form as $U_s{}^M$ if all the P_{ij} are omitted.

The quantities (potential energies in the triplet state) $U_t{}^M$ and $U_t{}^W$ are also similarly defined. The quadratic forms C and P correspond to the modified and the point Coulomb potentials, respectively,

$$C = \int V_c(r_3)(\Psi_s^2 + \Psi_a^2) \, d\tau \qquad (26)$$

and

$$P = \int r_3^{-1}(\Psi_s^2 + \Psi_a^2) \, d\tau, \qquad (27)$$

where, $V_c(r)$ is defined in Eq. (7).

The term U_s^e is added in Eq. (23) in order to take account of a small violation of charge hypothesis for nuclear forces.

All the triple integrations must be performed over the configuration space according to Eq. (12).

Before evaluating these quadratic forms, we must construct the functions $K\Psi_s$ and $K\Psi_a$, which are called kinetic energy derivatives, or simply k-derivatives, in the present paper.

As it is seen immediately, these derivatives lead to sums of enormous number of terms which are almost impossible to obtain by manual calculations. It is, therefore, desirable to derive some recurrence formula which performs these formal differentiations and which has a convenient form for use in a digital computer.

For this purpose, we shall first give a derivation of the recurrence relation.

The wavefunctions (18) and (19) can be represented in the form

$$\Psi_s = \mathscr{E} \cdot \sum_m \eta_m \varphi_s^{(m)}$$

and

$$\Psi_a = \mathscr{E} \cdot \sum_{m'} \eta_{m'} \varphi_a^{(m')}, \tag{28}$$

where

$$\varphi_{s(a)}^{(m)} = \sum_{n=1}^{N_{s(a)}^{(m)}} C_{s(a)}^{m,n} r_1^{l_1,n} r_2^{l_2,n} r_3^{l_3,n}. \tag{29}$$

In fact (see Eq. (18) and (19))

$$\varphi_s^{(1)} = 1$$
$$\varphi_s^{(2)} = r_1 + r_2$$
$$\cdots$$
$$\cdots$$
$$\varphi_s^{(7)} = r_1 r_2 \tag{30}$$
$$\varphi_a^{(1)} = r_2 - r_1$$
$$\cdots$$
$$\cdots .$$

The correlation function (17) can be expressed as a sum of simple exponential functions, i.e.,

$$\mathscr{E} = \sum_{k=1}^{8} \text{sn}(k) \cdot \exp[-\xi^{(k)} \cdot (\mathbf{r} - \mathbf{D})]$$

$$\equiv \sum_{k} \zeta(\xi^{(k)}) \equiv \sum_{k} \zeta^{(k)}, \tag{31}$$

where

$$(\mathbf{r} - \mathbf{D}) = (r_1 - D, r_2 - D, r_3 - D)^T,$$

$$\xi^{(1)} = (\mu, \mu, \mu), \qquad \text{sn}(1) = +1,$$

$$\xi^{(2)} = (\mu, \nu, \nu), \qquad \text{sn}(2) = -1,$$

$$\cdots \qquad\qquad \cdots \tag{32}$$

$$\cdots \qquad\qquad \cdots$$

$$\xi^{(8)} = (\nu, \nu, \nu), \qquad \text{sn}(8) = -1.$$

This decomposition of $\mathscr{E}$-function to $\zeta^{(k)}$-functions makes it a relatively simple matter to construct the recurrence formula for the kinetic energy operation $\mathbf{K}$ (4c). Really, $r_1 r_2 r_3 \mathbf{K} \Psi_s \equiv \kappa \Psi_s$ is reduced to

$$\kappa \cdot \Psi_s = \sum_m \eta_m \sum_k \kappa \varphi_s^{(m)} \cdot \zeta^{(k)},$$

and the simplest term among $\varphi_s^{(m)}$ and $\varphi_a^{(m)}$ being $\varphi_s^{(1)} = 1$, $\kappa \varphi_s^{(1)} \cdot \zeta^{(k)}$ can easily be obtained after some manipulations, i.e.,

$$\kappa \varphi_s^{(1)} \zeta^{(k)} = \kappa \cdot \zeta^{(k)}$$

$$= \tfrac{1}{2}(-\xi_2^{(k)} \xi_3^{(k)} r_1{}^3 - \xi_3^{(k)} \xi_1^{(k)} r_2{}^3 - \xi_1^{(k)} \xi_2^{(k)} r_3{}^3$$

$$+ \xi_1^{(k)} \xi_3^{(k)} r_1{}^2 r_2 + \xi_1^{(k)} \xi_2^{(k)} r_1{}^2 r_3 + \xi_1^{(k)} \xi_2^{(k)} r_2{}^2 r_3$$

$$+ \xi_2^{(k)} \xi_3^{(k)} r_1 r_2{}^2 + \xi_2^{(k)} \xi_3^{(k)} r_1 r_3{}^2 + \xi_1^{(k)} \xi_3^{(k)} r_2 r_3{}^2$$

$$+ 2(\xi_1^{(k)})^2 \, r_1 r_2 r_3 + 2(\xi_2^{(k)})^2 \, r_1 r_2 r_3 + 2(\xi_3^{(k)})^2 \, r_1 r_2 r_3$$

$$- 4\xi_1^{(k)} r_2 r_3 - 4\xi_2^{(k)} r_1 r_3 - 4\xi_3^{(k)} r_1 r_2) \cdot \zeta(\xi^{(k)}), \tag{33}$$

where

$$\kappa \equiv r_1 r_2 r_3 \mathbf{K}.$$

It must be noticed that the right side of this equation is not only a polynomial of r_1, r_2, and r_3, but also of $\xi_1^{(k)}$, $\xi_2^{(k)}$ and $\xi_3^{(k)}$. The fact also holds for higher order terms $\kappa \cdot \zeta^{(k)} \varphi_{S(a)}^{(m)}$ ($m = 1, 2,..., M$).

It will be shown that we can construct the k-derivatives of polynomials of higher degree in r_1, r_2, and r_3, with the help of a recurrence formula, in which the polynomial of Eq. (33) is the initial function of the recurrence procedure.

Let us assume that f be a function of the form

$$f = \sum_n \alpha_n r_1^{l_1,n} r_2^{l_2,n} r_3^{l_3,n}, \tag{34}$$

and ζ being

$$\zeta = \exp\left(-\sum_p \xi_p(r_p - D)\right),$$

and, furthermore, assume the function $g_{p,q}$ defined by

$$\zeta \cdot g_{p,q} = \frac{\partial^2}{\partial r_p \, \partial r_q} (\zeta \cdot f) \tag{35}$$

is already obtained. $g_{p,q}$ has the form

$$g_{p,q} = \sum_n \beta_n \xi_1^{i_1,n} \xi_2^{i_2,n} \xi_3^{i_3,n} r_1^{l_1,n} r_2^{l_2,n} r_3^{l_3,n}. \tag{36}$$

It can be shown that the following relation holds:

$$\frac{\partial^2}{\partial r_p \, \partial r_q} (\zeta \cdot r_s f) = \zeta \cdot \left(r_s - \delta_{qs} \frac{\partial}{\partial \xi_q} - \delta_{p,s} \frac{\partial}{\partial \xi_p}\right) g_{p,q}. \tag{37}$$

Here $\delta_{p,q}$ is the Kronecker's delta:

$$\delta_{p,q} = \begin{cases} 1 & p = q, \\ 0 & p \neq q, \end{cases} \tag{38}$$

for

$$\zeta \cdot g_{p,q} = \frac{\partial^2}{\partial r_p \, \partial r_q} (\zeta \cdot f)$$

$$= \zeta \cdot \left(\frac{\partial}{\partial r_p} - \xi_p\right)\left(\frac{\partial}{\partial r_q} - \xi_q\right) \cdot f \tag{a}$$

$$\zeta \cdot \frac{\partial}{\partial \xi_p} g_{p,q} = -\zeta \cdot \left(\frac{\partial}{\partial r_q} - \xi_q\right) \cdot f$$

$$= -\frac{\partial}{\partial r_q} (\zeta \cdot f) \tag{b}$$

$$\frac{\partial^2}{\partial r_p \, \partial r_q} (\zeta \cdot r_s \cdot f) = \left(r_s \frac{\partial^2}{\partial r_p \, \partial r_q} + \delta_{qs} \frac{\partial}{\partial \xi_q} + \delta_{ps} \frac{\partial}{\partial \xi_s}\right) \cdot (\zeta \cdot f) \tag{c}$$

Substituting (b) into (c) yields Eq. (37).

Since the operator κ has the form

$$\kappa = \sum_{p,q} Q_{p,q}(r_1, r_2, r_3) \frac{\partial^2}{\partial r_p \, \partial r_q} \qquad (39)$$

here, $Q_{p,q}(r_1, r_2, r_3)$ are polynomials of r_1, r_2, and r_3. Using Eq. (37), $\kappa(\zeta \cdot r_s \cdot f)$ can be reduced to

$$\kappa(\zeta \cdot r_s \cdot f) = \sum_{p,q} Q_{p,q} \frac{\partial^2}{\partial r_p \, \partial r_q} (\zeta \cdot r_s \cdot f),$$

$$= \sum_{p,q} Q_{p,q} \cdot \zeta \cdot \left(r_s - \delta_{qs} \frac{\partial}{\partial \xi_q} - \delta_{ps} \frac{\partial}{\partial \xi_p} \right) \cdot g_{p,q}, \qquad (40)$$

where

$$g_{p,q} = \zeta^{-1} \cdot \frac{\partial^2}{\partial r_p \, \partial r_q} (\zeta \cdot f). \qquad (35)$$

Because the function f has the form containing only r_1, r_2, and r_3 but not ξ_1, ξ_2, and ξ_3, there is no term in $g_{p,q}$ which contains ξ_s, so long as p and q are not equal to s, i.e.,

$$\frac{\partial}{\partial \xi_s} g_{p,q} = 0, \qquad \text{if} \quad s \neq p \quad \text{and} \quad s \neq q \qquad (41)$$

Equation (40) is now from Eq. (41):

$$\kappa(\zeta \cdot r_s \cdot f) = \zeta \cdot \left\{ \sum_{p,q} r_s Q_{p,q} g_{p,q} - \frac{\partial}{\partial \xi_s} \left(\sum_p Q_{p,s} g_{p,s} + \sum_q Q_{s,q} g_{s,q} \right) \right\},$$

$$= \zeta \cdot \left(r_s \sum_{p,q} Q_{p,q} g_{p,q} - \frac{\partial}{\partial \xi_s} \sum_{p,q} Q_{p,q} g_{p,q} \right),$$

$$= \zeta \cdot \left(r_s - \frac{\partial}{\partial \xi_s} \right) \cdot \sum_{p,q} Q_{p,q} g_{p,q}.$$

Then the following result holds:

$$\kappa(\zeta \cdot r_s \cdot f) = \zeta \cdot \left(r_s - \frac{\partial}{\partial \xi_s} \right) \cdot \zeta^{-1} \cdot \kappa(\zeta \cdot f) \qquad (42)$$

This means that from the function $\kappa(\zeta \cdot f)$, the k-derivatives of higher order functions $\zeta \cdot r_1^{l_1} r_2^{l_2} r_3^{l_3} f$ are obtained by recurrent use of Eq. (42).

For example, if we define $R_{l_1 l_2 l_3}$ by

$$\zeta \cdot R_{0,0,0} = \kappa \cdot \zeta,$$

$$\zeta \cdot R_{1,0,0} = \kappa \cdot r_1 \cdot \zeta,$$

$$\cdots \tag{43}$$

$$\zeta \cdot R_{l_1 l_2 l_3} = \kappa \cdot r_1^{l_1} r_2^{l_2} r_3^{l_3} \cdot \zeta,$$

then from Eq. (42), each $R_{l_1 l_2 l_3}$, which is, of course, a polynomial of both ξ_j and r_j ($j = 1, 2$ and 3), is obtained recurrently as follows:

$$R_{1,0,0} = \left(r_1 - \frac{\partial}{\partial \xi_1} \right) R_{0,0,0},$$

$$\cdots$$

$$R_{l_1 l_2 l_3} = \left(r_1 - \frac{\partial}{\partial \xi_1} \right) R_{l_1 - 1, l_2, l_3} \tag{44}$$

$$= \left(r_2 - \frac{\partial}{\partial \xi_2} \right) R_{l_1, l_2 - 1, l_3}$$

$$= \left(r_3 - \frac{\partial}{\partial \xi_3} \right) R_{l_1, l_2, l_3 - 1},$$

where $R_{0,0,0}$ is already obtained in Eq. (23).

Thus by the relation (42), one will be able to construct the k-derivatives of wavefunctions of any order, when they have the form shown in Eqs. (18) and (19).

Really, $\kappa \cdot \Psi_s$ (see Eq. (32)) turns out to be

$$\kappa \cdot \Psi_s = \sum_{m=1}^{M_s} \eta_m \sum_{k=1}^{8} \kappa \cdot \varphi_s^{(m)} \cdot \zeta^{(k)},$$

$$= \sum_m \eta_m \sum_k \sum_{n=1}^{N_s^m} c_{s,n}^{(m)} \kappa \cdot r_1^{l_1,n} r_2^{l_2,n} r_3^{l_3,n} \cdot \zeta^{(k)}, \tag{45}$$

$$= \sum_m \eta_m \sum_k \sum_n c_{s,n}^{(m)} R_{l_1,n l_2,n l_3,n} \cdot \zeta^{(k)},$$

and a similar result holds for $\kappa \cdot \Psi_a$ also.

4. τ-INTEGRATION

The k-derivatives of Ψ_s and Ψ_a are now obtained in the form

$$\kappa \cdot \Psi_{s(a)} = \sum_m \eta_m \sum_k \zeta(\xi^{(k)}) \sum_j \{ \mathbf{i}_j^{(m)}; k \mid \alpha_j^{(m)} \mid \mathbf{l}_j^{(m)} \},$$

where the symbols $\{\mathbf{i}_j^{(m)}; k \mid$ and $\mid \boldsymbol{l}_j^{(m)}\}$ are

$$\{\mathbf{i}_j^{(m)}; k \mid \equiv \{i_{1j}^{(m)}, i_{2j}^{(m)}, i_{3j}^{(m)}; k \mid$$

$$\equiv \xi_1(k)^{i_{1j}^{(m)}} \xi_2(k)^{i_{2j}^{(m)}} \xi_3(k)^{i_{3j}^{(m)}}$$

and

$$\mid \boldsymbol{l}_j^{(m)}\} \equiv \mid l_{1j}^{(m)}, l_{2j}^{(m)}, l_{3j}^{(m)}\}$$

$$\equiv r_1^{l_{1j}^{(m)}} r_2^{l_{2j}^{(m)}} r_3^{l_{3j}^{(m)}},$$

respectively, and $\alpha_j^{(m)}$ are scalar coefficients. $\{\eta_m\}$ is the state vector which is to be adjusted so that the energy is minimized. $\zeta(\boldsymbol{\xi}^{(k)})$ stands for an exponential function:

$$\zeta(\boldsymbol{\xi}^{(k)}) = \operatorname{sn}(k) \exp \left\{ - \sum_{p=1}^{3} \xi_p(k) \cdot (r_p - D) \right\}.$$

Here, $\operatorname{sn}(k)$ has a value $+1$ or -1, according to the index k, and $\xi_p^{(k)}$, μ or ν, according to the indices k and p (see Eq. (31)).

In the following, we shall consider τ-integration of integrands $\Psi_s \cdot \kappa \cdot \Psi_s$, $\Psi_a \cdot \kappa \cdot \Psi_a$, $\Psi_{s(a)} \cdot$ (function of r_p) $\cdot \Psi_{s(a)}$ and others. Since all of our integrands are now represented as sums of polynomials of r_1, r_2 and r_3 multiplied by the exponential functions $\zeta^{(k)}$, the analytical integration is possible using the integration-by-parts formula.

Following the line mentioned above, consider, e.g., $\int \Psi_s \cdot \kappa \cdot \Psi_s \, d\tau$ explicitly:

$$
\begin{aligned}
\int \Psi_s \cdot \kappa \cdot \Psi_s \, d\tau &= \sum_m \sum_{m'} \eta_m \eta_{m'} \sum_k \sum_{k'} \sum_j \sum_{j'} \alpha_j^{(m)} \beta_{j'}^{(m')} \\
&\quad \cdot \{\mathbf{i}_j^{(m)}; k \mid \int \zeta^{(k)} \cdot \zeta^{(k')} \cdot \mid \boldsymbol{l}_j^{(m)}\} \cdot \mid \boldsymbol{l}_{j'}^{(m')}\} \, d\tau \\
&= \sum_m \sum_{m'} \eta_m \eta_{m'} \sum_k \sum_{k'} \sum_j \sum_{j'} \alpha_j^{(m)} \beta_{j'}^{(m')} \\
&\quad \cdot \{\mathbf{i}_j^{(m)}; k \mid \cdot \int \zeta(\boldsymbol{\xi}^{(k)} + \boldsymbol{\xi}^{(k')}) \mid \boldsymbol{l}_j^{(m)} + \boldsymbol{l}_{j'}^{(m')}\} \cdot d\tau,
\end{aligned}
\tag{47}
$$

where we assumed that Ψ_s is represented as

$$\Psi_s = \sum_{m'} \eta_{m'} \sum_{k'} \zeta^{(k')} \sum_{j'} \beta_{j'}^{(m')} \mid \boldsymbol{l}_{j'}^{(m')}\}. \tag{48}$$

It can be seen that for our τ-integration only a formula (or a computer program) which calculates the integrals of the form

$$\int \zeta(\xi) \cdot \mid l\} \, d\tau = \int e^{-\Sigma_p \xi_p (r_p - D)} r_1^{l_1} r_2^{l_2} r_3^{l_3} \, d\tau \qquad (49)$$

is necessary.

Let the integrand in Eq. (49) be $\hbar$. The τ-integration of $\hbar$ is now, from the definition in Eq. (12),

$$J[\xi, l] \equiv \int \hbar(\xi, l; \mathbf{r}) \, d\tau$$

$$= e^{\Sigma_p \xi_p \cdot D} \left[\int_D^\infty \int_D^\infty \int_D^\infty e^{-\Sigma_p \xi_p r_p} \cdot r_1^{l_1 + 1} r_2^{l_2 + 1} r_3^{l_3 + 1} \, dr_1 \, dr_2 \, dr_3 \right.$$

$$- \sum_{\text{cyclic}} \int_D^\infty \int_D^\infty \int_D^\infty e^{-\{\xi_1 (r_1 + r_2 + r_3) + \xi_2 r_2 + \xi_3 r_3\}}$$

$$\left. \cdot (r_1 + r_2 + r_3)^{l_1 + 1} r_2^{l_2 + 1} r_3^{l_3 + 1} \, dr_1 \, dr_2 \, dr_3 \right]. \qquad (50)$$

The second term of the right side of the above equation can be expanded to

$$\sum_{i+j+k=l_1+1} \frac{(l_1 + 1)!}{i! \, j! \, k!} \int_D^\infty \int_D^\infty \int_0^\infty e^{-\xi_1 r_1} e^{-(\xi_1 + \xi_2) r_2} e^{-(\xi_1 + \xi_3) r_3} r_1^{i+1} r_2^{l_2 + j + 1} r_3^{l_3 + k + 1} \, dr_1 \, dr_2 \, dr_3. \qquad (51)$$

Defining $I_0(d, a, l)$ by

$$I_0(d, a, l) = \int_d^\infty e^{-ar} r^l \, dr \qquad (52)$$

with a recurrence relation,

$$I_0(d, a, l) = \frac{e^{-ad}}{a} + \frac{l}{a} I_0(d, a, l - 1), \qquad (53)$$

$$I_0(d, a, 0) = \frac{e^{-ad}}{a},$$

$J[\xi, l]$, then

$$J[\xi, l] = e^{\Sigma_p \xi_p D} \left[\prod_{p=1}^3 I_0(D, \xi_p, l_p + 1) \right.$$

$$- \sum_{\text{cyclic}} \sum_{i+j+k=l_1+1} \frac{(l_1 + 1)!}{i! \, j! \, k!} I_0(0, \xi_1, i + 1) I_0(D, \xi_1 + \xi_2, l_2 + j + 1)$$

$$\left. \cdot I_0(D, \xi_1 + \xi_3, l_3 + k + 1) \right]. \qquad (54)$$

By this function $J[\xi, l]$, $\int \Psi_s \cdot \kappa \cdot \Psi_s \, d\tau$ is found to be

$$\int \Psi_s \cdot \kappa \cdot \Psi_s \, d\tau = \sum_m \sum_{m'} \eta_m \eta_{m'} \sum_k \sum_{k'} \sum_j \sum_{j'} \alpha_j^{(m)} \beta_{j'}^{(m')}$$

$$\cdot \{l_j^{(m)}; k \mid \cdot J[\xi^{(k)} + \xi^{(k')}, l_j^{(m)} + l_{j'}^{(m')}]. \qquad (55)$$

The other quadratic forms can be obtained in a similar manner.

5. Program Descriptions

Following the formulations derived in the preceding chapters, a computer code 'TRIPLE' which computes three-body problems of both H^3 and He^3, was written in FORTRAN for an IBM7090 computer.

We shall outline some aspects of these programming techniques used here.

Expression of Polynomials $\varphi(r_1, r_2, r_3)$

Any polynomials which have the form

$$\varphi = \sum_{n=1}^{N} \beta_n r_1^{l_{1,n}} r_2^{l_{2,n}} r_3^{l_{3,n}}$$

may be completely specified by the quantities N and $(\beta_n, l_{1,n}, l_{2,n}, l_{3,n})$, $(n = 1, 2,..., N)$. These quantities are represented as 'arrays' in the following manner:

Example:

$$\varphi = r_1 r_2^2 - 3r_2^2 r_3 + 5r_1 - 2$$

Program:

INTEGER   LENGTH, POWER(3,4)
REAL   COEF(4)

Value of the Arrays:

LENGTH | 4 |

POWER

1	0	1	0
2	2	0	0
0	1	0	0

COEF | 1 | -3 | 5 | -2 |

Kinetic energy operation $\mathbf{K}\Psi$

A polynomial of the form

$$\chi = \sum_{n=1}^{N} \alpha_n \xi_1^{i_{1,n}} \xi_2^{i_{2,n}} \xi_3^{i_{3,n}} r_1^{l_{1,n}} r_2^{l_{2,n}} r_3^{l_{3,n}}$$

may be regarded as a polynomial of six independent variables, i.e., ξ_1, ξ_2, ξ_3, r_1, r_2 and r_3. It is completely specified by N and $(\alpha_n, i_{1,n} i_{2,n} i_{3,n}, l_{1,n}, l_{2,n}, l_{3,n})$, $(n = 1, 2,..., N)$. But at the same time, it may also be regarded as a polynomial of three independent variables r_1, r_2 and r_3, the coefficients of which are functions of ξ_1, ξ_2, and ξ_3. For the purpose of τ-integration, the latter is the better expression, while in kinetic energy operations (k-derivatives), we prefer the former. Also, it is convenient to express it in a six-dimensional array, where the values of the elements are those of α_n and the six indices of which correspond to the values $i_{1,n}$, $i_{2,n}$, $i_{3,n}$, $l_{1,n}$, $l_{2,n}$, $l_{3,n}$.

Example:

$$R_{0,0,0} = -\xi_2 \xi_3 r_1^3 - \xi_3 \xi_1 r_2^3 - \xi_1 \xi_2 r_3^3 + \xi_1 \xi_3 r_1^2 r_2 + \cdots$$
$$+ \xi_1^2 r_1 r_2 r_3 + \xi_2^2 r_1 r_2 r_3 + \xi_3^2 r_1 r_2 r_3 + \cdots$$
$$- 4\xi_3 r_1 r_2 .$$

Value of the corresponding array R000:

$$\text{All} \quad R000(i_1, i_2, i_3, l_1, l_2, l_3) = 0,$$

except for

$$R000(0, 1, 1, 3, 0, 0) = -1$$
$$R000(1, 0, 1, 0, 3, 0) = -1$$
$$R000(1, 1, 0, 0, 0, 3) = -1$$
$$R000(1, 0, 1, 2, 1, 0) = +1$$
$$\cdots$$
$$\cdots$$
$$R000(2, 0, 0, 1, 1, 1) = +1$$
$$R000(0, 2, 0, 1, 1, 1) = +1$$
$$R000(0, 0, 2, 1, 1, 1) = +1$$
$$\cdots$$
$$\cdots$$
$$R000(0, 0, 1, 1, 1, 0) = -4.$$

The recurrence formula (44) for k-derivatives can now be reduced to simple operations of the corresponding coefficient matrices. For example, the relation

$$R_{1,0,0} = \left(r_1 - \frac{\partial}{\partial \xi_1}\right) R_{0,0,0}$$

is interpreted as follows, representing the corresponding array of $R_{1,0,0}$ by $R100(i_1, i_2, i_3, l_1, l_2, l_3)$:

First, set all the $R100$'s zero. Then,

for $l_1, l_2, l_3 = 0, 1, 2,...$

       for $i_1, i_2, i_3 = 0, 1, 2$

           $R100(i_1, i_2, i_3, l_1 + 1, l_2, l_3)$
              $= R100(i_1, i_2, i_3, l_1 + 1, l_2, l_3) + R000(i_1, i_2, i_3, l_1, l_2, l_3)$

       for $i_1 = 1, 2;$ $i_2, i_3 = 0, 1, 2$

           $R100(i_1 - 1, i_2, i_3, l_1, l_2, l_3)$
              $= R100(i_1 - 1, i_2, i_3, l_1, l_2, l_3) - i_1 R000(i_1, i_2, i_3, l_1, l_2, l_3).$

The other $R_{i,j,k}$ functions are also obtained in a similar way, and any k-derivatives of wavefunctions $\chi = \kappa \cdot \varphi$ are obtained only by summing up the necessary $R_{i,j,k}$ functions.

Expression of Polynomials $\chi(\xi_1^{(k)}, \xi_2^{(k)}, \xi_3^{(k)}, r_1, r_2, r_3)$:

The k-derivative of a wavefunction $\chi = \kappa \cdot \varphi$

$$\chi = \sum_{n=1}^{N} \alpha_n (\xi_1^{(k)})^{i_{1,n}} (\xi_2^{(k)})^{i_{2,n}} (\xi_3^{(k)})^{i_{3,n}} r_1^{l_{1,n}} r_2^{l_{2,n}} r_3^{l_{3,n}}$$

has been obtained as a six-dimensional array. It is now reinterpreted as a polynomial of three independent variables r_1, r_2, and r_3 in order to perform the τ-integration $\int \varphi \cdot \chi \, d\tau$.

The coefficients of the polynomial are also functions of $\xi_2^{(k)}$, $\xi_2^{(k)}$, and $\xi_3^{(k)}$ and are in this time regarded as parameters of the computation. They are represented as computer functions, or 'SUBROUTINEs,' which compute their *values* when the values of $\xi_j^{(k)}$ are given. These coefficient subroutines are generated beforehand by a computer itself and are punched out in the form of standard FORTRAN statements.

We will illustrate this expression, taking again the example $R_{0,0,0}$.

Program for $R_{0,0,0}$:

INTEGER   LENGTH, POWER(3,13)

REAL   COEF(13)

Value of LENGTH $\boxed{13}$

POWER

3	0	0	2	2	0	1	1	0	1	0	1	1
0	3	0	1	0	2	2	0	1	1	1	0	1
0	0	3	0	1	1	0	2	2	1	1	1	0

Program of the coefficients:

SUBROUTINE COEFNT(COEF, $\xi_1^{(k)}$, $\xi_2^{(k)}$, $\xi_3^{(k)}$)

...

...

A000 $= +1.$

A100 $= \xi_1^{(k)}$

A010 $= \xi_2^{(k)}$

...

A111 $= \xi_1^{(k)} * \xi_2^{(k)} * \xi_3^{(k)}$

...

A002 $= (\xi_3^{(k)})^2$

COEF(1) $= -$A011

COEF(2) $= -$A101

...

COEF(9) $= +2. * $A002$ + 2. * $A020$ + 2. * $A200

...

COEF(13) $= -4. * $A001

RETURN

END

τ-Integration

A program which computes the triple definite integration

$$J[\xi, l] \equiv \int \zeta(\xi) \mid l\} \, d\tau = \int e^{-\sum_p \xi_p \cdot (r_p - D)} r_1^{l_1} r_2^{l_2} r_3^{l_3} \, d\tau$$

is written. This routine performs the decomposition of $(r_1 + r_2 + r_3)^{ip}$ according to Eq. (51), computes the triple integrations according to the formula (53), and sums them up numerically.

Then, accordingly to Eq. (55), the integration

$$\int \varphi^{(m)} \cdot \kappa \varphi^{(m')} \, d\tau$$

is obtained by summing up as many terms as is necessary.

More simple integrations such as

$$\int \varphi^{(m)} \cdot \varphi^{(m')} \, d\tau, \quad \text{or} \quad \int \varphi^{(m)} u_c(r_3) \, \varphi^{(m')} \, d\tau$$

are, of course, obtained in a similar way.

Eigenvalue problem

All the quadratic forms, or matrices N, K, and U, are now computed. The eigenvalue problem

$$(K + U)\eta = \lambda \cdot N\eta$$

is solved by the usual Jacobi method.

6. DISCUSSION

The idea of matrix representations of polynomials is, of course, classic [13], but, to the authors' knowledge, there are not so many that were well-applied to practical problems. The storage schemes of polynomials are very similar to the canonical form used in the ALPAK system [14], which has been developed as a general system of polynomial (and rational function) manipulation. The situation is, however, more complex in our problem, and we were forced to use three different storage schemes in the course of our calculations. In any event, there is an essential restriction in this method, i.e., the number of independent variables should be known beforehand. From our experiences, however, it is one of the most powerful tools of formula manipulation, so long as it can be applied to a particular problem. Really, in our three-body problem it has proved to be very useful. The method also makes it possible to write the whole program in FORTRAN, and, therefore, it keeps the computing time within an admissible range. This is the key to the success of the whole computation, for it was found that such general purpose systems of formula manipulation as LISP 1.5 [11] and FORMAC [10] consumed too much computing time and core storages for our

problems. The ALPAK system too, though we have not tried it, seems to be not so efficient because of the complexity of the problem.

It is interesting, from the physical point of view, to ask whether our methods can be applied when more realistic forces are introduced. As Delves and Blatt [15] have pointed out, it has not been found possible to integrate the kinetic and potential energies analytically when noncentral (tensor and LS) forces are introduced. Since the methods presented here are, in principle, analytic, they seem to be restricted to model forces which are purely central.

As is easily seen, our differentiation and integration methods can only be applied to trial wavefunctions of the form

$$\Psi = \mathscr{E} \cdot \text{polynomial of } (r_1, r_2, r_3),$$

but the degree of polynomials of r_1, r_2 and r_3 can, in principle, be arbitrarily high. This makes no physical restriction when the central forces are assumed. The only practical restriction is the computing time. In an actual calculation, in fact, the computing time would vastly increase as the degree of the polynomials increases. It is recommended for the saving of computing time to make a table of $J[\xi^{(k)}, l]$ beforehand, because the maximum number of the index k is 8, and the combination of l_1, l_2, and l_3 are finite. The computing time for fixed value of μ, ν, and D is about 20 min in IBM 7090. The details of such results is reported in Ref. [7].

The accuracy of the integrations could be checked, e.g., by a formula (see Ref. [7, Appendix])

$$\int v_i v_j \, d\tau = 0 \quad \text{for} \quad i \neq j, \quad (i, j = 0, 1 \text{ and } 2),$$

and, since only the rounding errors could contribute to the total errors of such integrations, the actual error was found to be negligibly small. This is, of course, the most advantageous point of our method in contrast to other numerical methods.

REFERENCES

1. L. H. THOMAS, *Phys. Rev.* **47** (1935), 903.
2. G. DERRICK AND J. M. BLATT, *Nucl. Phys.* **8** (1958), 310; *Nucl. Phys.* **17** (1960), 67. J. M. BLATT AND G. H. DERRICK, *Nucl. Phys.* **8** (1958), 602. G. DERRICK, *Nucl. Phys.* **16** (1960) 405; **18** (1960), 303. C. WERNTZ, *Phys. Rev.* **121** (1961), 849. G. DERRICK, D. MUSTARD, AND J. BLATT,

Phys. Rev. Lett. **6** (1961), 69. J. M. BLATT, G. H. DERRICK, AND J. N. LYNESS, *Phys. Rev. Lett.* **8** (1962), 323. L. M. DELVES AND G. H. DERRICK, *Ann. Phys.* **23** (1963), 133. L. M. DELVES, *Phys. Rev.* **135** (1964), B1316. T. KALOTAS AND L. M. DELVES, *Nucl. Phys.* **60** (1964), 363. J. M. BLATT AND L. M. DELVES, *Phys. Rev. Lett.* **12** (1964), 544. L. M. DELVES AND J. M. BLATT, *Nucl. Phys.* **A98** (1967), 503.

3. H. COLLARD, R. HOFSTADTWR, E. B. HUGHES, A. JOHANSSON, M. R. YEARIAN, R. B. DAY, AND R. T. WAGNER, *Phys. Rev.* **138** (1965).

4. C. L. PEKERIS, *Phys. Rev.* **115** (1959), 1216.

5. E. A. HYLLERAAS, *Z. Phys.* **54** (1929), 347.

6. T. KINOSHITA, *Phys. Rev.* **105** (1957), 1490.

7. T. OHMURA, Isobaric-Spin Impurity and Intermediate Symmetry States in Three-Body Nuclei, *Progr. Theor. Phys.* **41** (1969), 419.

8. T. OHMURA (formerly KIKUTA), M. MORITA, AND M. YAMADA, *Progr. Theor. Phys.* **15** (1956), 222.

9. D. MUSTARD, *et al., Computer J.* **6** (1963), 75.

10. FORMAC (operating and user's reference manual), No. 7090 R2.IBM0016, IBM Program Inf. Dept., New York, Aug. 1965.

11. J. MCCARTHY, *et al.,* "LISP 1.5 Programmer's Manual," M.I.T. Press, Cambridge, Mass., 1965.

12. T. KUROSAWA, E. MAEDA, H. FUJII, AND K. SHIMIZU, "Some Techniques of Formula Manipulation for the Solution of Nuclear Three-Body Problem," (Japanese), J.I.P.S. Symposium on Programming, 1968, C-35, Jan. 1968.

13. K. SPIELBERG, *J.A.C.M.* **8** (1961), 4. A. R. ROM, *Comm. A.C.M.* **9** (1961). J. E. SAMMET, *Comm. A.C.M.* **9** (1966), 8.

14. W. S. BROWN, *Bell Syst. Tech. J.* **42** (1963), 2081–2119. W. S. BROWN, J. P. HYDE, AND B. A. TAGUE, *Bell Syst. Tech. J.* **43** (1964), 795–804.

15. L. M. DELVES AND J. M. BLATT, *Nucl. Phys.* **A98** (1967), 503.