

## Separation of the Rotational Coordinates in the Three Body Problem

Yasuo MUNAKATA

Department of Physics, Shimane University, Matsue, Japan  
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### Abstract

For the quantum mechanical three body problem with central potentials, separation of the rotational coordinates is performed systematically. We treat two particles in a symmetric way to apply Pauli principle for the case of identical fermions. We construct a complete set of commuting observables,  $L^2$ , the total angular momentum,  $M$ , its  $z$ -component and  $N$ , the component around the normal through the third particle to the plane including three particles.  $K_1$ ,  $K_2$  and  $N$  form three components of  $\mathbf{L}$  in the body fixed moving frame. Single particle operators are expressed in compact forms by those operators. Thus, the separation procedure is simplified than hitherto known one. For the case of equal masses and  $L=0$ , a simple and symmetrical equation is derived.

### §1. Introduction and Summary

Nature has many three body systems in each different microscopic worlds. Examples are quite rich;  $H_2^+(p, p, e)$ ,  $H_e$ -atom ( ${}^4H_e, e, e$ ) and  $L_i$ -ion ( ${}^7L_i, e, e$ ) etc. in the molecular and atomic worlds,  ${}^3H(p, n, n)$  and  ${}^3H_e(p, p, n)$  in the nuclear world and finally  $p(u, u, d)$ ,  $n(u, d, d)$ ,  $\Lambda^0(u, d, s)$ ,  $\Delta^{++}(u, u, u)$  and  $\Lambda_c^+(u, d, c)$  etc. in the hadronic world. (We denote electron, proton, neutron, up-quark, down-quark, strange quark and charm quark as  $e, p, n, u, d, s$ , and  $c$ , respectively.) It should be noted that except for the hadronic world there exists only system with three particles in which two of them are identical fermions and the third one is different. The hadronic world has most varieties; three identical fermions, two identical fermions and three different fermions.

The first step to the dynamical study of the three body problem is the separation of the three translational coordinates and the three rotational ones from the total nine coordinates. The former is trivial because we can always choose the center of mass coordinate system. As was emphasized in Ref. [4], the latter is not so trivial because we must treat two identical fermions in a symmetrical way in order to apply the fermi statistics. To describe the rotational states of the system we must choose the eigenfunctions of the total angular momentum  $L$ . These functions are functions of the three Euler angles. These angles are not unique but the most natural one are those used in the classical papers by Hylleraas [1] about the helium atom; spherical angles

$\theta$  and  $\phi$  of one electron in the space-fixed coordinate system with the fixed nucleus at the origin and the azimuthal angle  $\psi$  of the second electron around the moving radial axis of the first one. Clearly these angles are quite unsymmetrical between two electrons. If one constructs the eigenfunctions of the total angular momentum with a specified eigenvalue around the body fixed symmetry axis, the symmetry between two electrons will be lost completely and the satisfaction of the Pauli principle becomes quite a complicated task. This would be the main reason that Hylleraas limited his study to total  $S$ -states which are independent of Euler angles. Also Breit's original work [2] was limited to  $P$ -states and work [3] thereafter had always been limited to specific angular momentum states.

For the case of two-electron with fixed nucleus general solution to this problem was achieved by Bhatia and Temkin [4]. They invented symmetric Euler angles and constructed explicitly eigenfunctions of the total angular momentum (vector spherical harmonics) in terms of those angles. The operations of parity and exchange become quite simple: the essential feature they achieved. In return for this merit they were obliged to work very hard to express the kinetic energy of each electron in terms of those variables. The procedure is quite complicated and not transparent.

In this paper we shall make two major improvements over their work. The first point is that we define a complete set of commuting observables  $L^2$ ,  $M$  and  $N$  which have *definite symmetry properties* with regard two (identical) particles.  $M$  is the  $z$  component of the total angular momentum  $L$  in the space fixed coordinate system with origin at the third particle (the coordinate system  $A$ ).  $N$ , which is antisymmetric with regard two particles, is the component of  $L$  around the normal through the origin to the instantaneous plane including three particles.  $N$  together with  $K_1$  and  $K_2$ , which will be defined in section 4, form the three orthogonal components of  $L$  in the body fixed moving coordinate system and satisfy the usual commutation relations for the angular momentum. Accordingly the simultaneous eigen ket of  $L$ ,  $M$  and  $N$  with eigenvalues  $l$ ,  $m$  and  $n$  can be constructed by the elementary knowledge of the angular momentum and need no explicit form in order to separate the angular variables. We can also express the kinetic energy of each particle in a rather compact and transparent way in terms of  $K$ ,  $K'$  and  $N$ .  $K$  and  $K'$  have more direct physical meanings than  $K_1$  and  $K_2$ , and the latter are expressed as linear combinations of the former. As the results of these analyses the radial equations are derived quite simply. In order to define  $K$ ,  $K'$  and  $N$  we have used three different coordinate systems or sets of variables  $A$ ,  $B$  and  $C$  freely.  $B$  is the above mentioned system used by Hylleraas.  $C$  is the system in which the role of particle 1 and 2 is exchanged. In short we define the symmetrical observables  $K_1$ ,  $K_2$  and  $N$  by using unsymmetrical variables.

The second point is that we take into account fully the recoil effects of the third particle. The analysis is done by using two relative coordinates, instead of by using usual center of mass and relative coordinates [8]. We confine ourselves to the central force potentials which are the functions of the relative coordinates. So our choice is

more convenient than the usual one. In the last section we demonstrate that, in the case of equal masses and  $L=0$ , our analysis leads to a symmetric equation between these three particles, in spite of our asymmetric treatment of third particle.

In Sec. 2 we express the components of the total angular momentum in various coordinate systems. Especially,  $K$ ,  $K'$  and  $N$  are expressed by using the set of variables  $B$ . In Sec. 3 single particle operators are expressed in terms of  $B$  and then in terms of  $K$ ,  $K'$  and  $N$  by using the results of Sec. 2. Sec. 4 is devoted to the construction of  $K_1$ ,  $K_2$  and  $N$  and the eigen ket of  $L$ ,  $M$  and  $N$ . Single particle operators in Sec. 3 are also rewritten in terms of  $K_1$ ,  $K_2$  and  $N$  in this section. In Sec. 5 we derive the radial equations and examine their symmetry properties. In Sec. 6 we derive a symmetrical equation between three particles as a consistency check of our treatment. Appendix a and b are devoted to mathematical preliminaries.

## §2. Total Angular Momentum in various Coordinate Systems

We consider three non-relativistic particles with mass  $m_i$ , Cartesian coordinates  $x_i$  and canonical momenta  $p_i \equiv -i\nabla_i$  ( $i=1, 2, 3$ ). If two of them are identical, we denote them  $i=1, 2$ . Define as usual the center of mass coordinates<sup>\*)</sup> and the relative coordinates together with their respective canonical momenta by

$$\left\{ \begin{array}{l} \xi = x_1 - x_3, \\ \eta = x_2 - \frac{m_3 x_3 + m_1 x_1}{m_3 + m_1}, \\ X = \frac{m_1 x_1 + m_2 x_2 + m_3 x_3}{m_1 + m_2 + m_3}, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} P = \frac{m_3 p_1 - m_1 p_3}{m_3 + m_1}, \\ k = \frac{(m_3 + m_1)p_2 - m_2(p_3 + p_1)}{m_1 + m_2 + m_3}, \\ P = p_1 + p_2 + p_3. \end{array} \right. \quad (1)$$

Because of the commutability of  $P$  with the total Hamiltonian, we can always choose the system  $P=0$  (the center of mass coordinates). In this system the kinetic energy  $T$  and the total angular momentum  $L$  are given by

$$T \equiv \sum_{i=1}^3 \frac{p_i^2}{2m_i} = \frac{P^2}{2\mu_{31}} + \frac{k^2}{2\mu_2}, \quad (2)$$

$$L \equiv \sum_{i=1}^3 x_i \times p_i = \xi \times p + \eta \times k \quad (3)$$

where  $\mu_{ij} = m_i m_j / (m_i + m_j)$  is the usual reduced mass and  $\mu_2 = (m_3 + m_1)m_2 / (m_1 + m_2 + m_3)$ .

We confine ourselves to the central force problem. Then the potentials are given in terms of the coordinates differences between three particles. Therefore, it is more

<sup>\*)</sup> For a general definition of the center of mass coordinates and the method of  $K$ -harmonics, see an interesting review article Ref. [5].

advantageous and intuitive to use

$$\left\{ \begin{array}{l} \mathbf{r}_1 \equiv \mathbf{x}_1 - \mathbf{x}_3 = \boldsymbol{\xi}, \\ \mathbf{r}_2 \equiv \mathbf{x}_2 - \mathbf{x}_3 = \boldsymbol{\eta} + \frac{m_1}{m_3 + m_1} \boldsymbol{\xi}, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} \mathbf{k}_1 \equiv -i \frac{\partial}{\partial \mathbf{r}_1} = \mathbf{p} - \frac{m_1}{m_3 + m_1} \mathbf{k}, \\ \mathbf{k}_2 \equiv -i \frac{\partial}{\partial \mathbf{r}_2} = \mathbf{k}, \end{array} \right. \quad (4)$$

than to use (1), [8]. In terms of (4),  $T$  and  $L$  are reexpressed as

$$T = \frac{\mathbf{k}_1^2}{2\mu_{31}} + \frac{\mathbf{k}_2^2}{2\mu_{23}} + \frac{\mathbf{k}_1 \mathbf{k}_2}{m_3} \equiv T_1 + T_2 + T_3, \quad (5)$$

and

$$\mathbf{L} = \mathbf{r}_1 \times \mathbf{k}_1 + \mathbf{r}_2 \times \mathbf{k}_2 \equiv \mathbf{l}_1 + \mathbf{l}_2. \quad (6)$$

We make two remarks;

- (i)  $L$  is invariant under the transformation (4).
- (ii) In the fixed nucleus case of the atomic problem,  $m_e/m_3 \rightarrow 0$ , ( $m_1 = m_2 = m_e$ ) so the third term of (5) can be neglected.

Eq's. (5) and (6) are our starting point of analysis.

As is stated in the introduction, we use three different coordinate systems  $A$ ,  $B$  and  $C$ .  $A$  is the space fixed polar coordinate system with the origin at the third particle. In this system  $\mathbf{r}_i: (r_i, \theta_i, \phi_i)$   $i=1, 2$ , so the set  $A$  of independent variables of the rotation are

$$(\theta_1, \phi_1, \theta_2, \phi_2): A$$

In  $B$ ,  $\mathbf{r}_1$  is described in the same way as in  $A$  but  $\mathbf{r}_2$  is described referring to the moving polar axis  $\mathbf{r}_1$  with the polar angle  $\Theta$  and the azimuthal angle  $\psi$  so the set  $B$  of independent variables are

$$(\theta = \theta_1, \phi = \phi_1, \Theta, \psi): B$$

In  $C$ , the role of 1 and 2 is exchanged, so the set  $C$  of independent variables are

$$(\theta' = \theta_2, \phi' = \phi_2, \Theta, \chi): C$$

The relations between  $A$ ,  $B$  and  $C$  are visualized in Fig. 1.

The relations between  $A$  and  $B$  and that between respective canonical variables are given by

$$\begin{aligned} \theta &= \theta_1, & \phi &= \phi_1 \\ \cos \Theta &= \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_2 - \phi_1), & (7) \\ \cot \psi &= \cos \theta_1 \cot(\phi_2 - \phi_1) - \cot \theta_2 \sin \theta_1 \operatorname{cosec}(\phi_2 - \phi_1), \end{aligned}$$

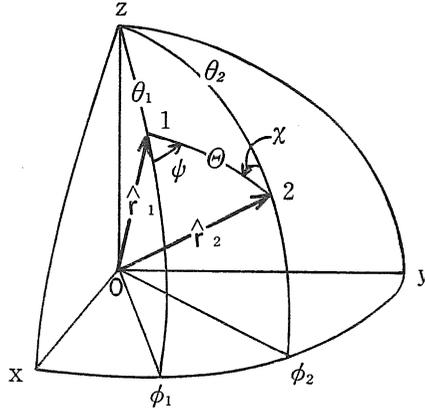


Fig. 1. Perspective drawing of Euler angles on a unit Sphere

and

$$\begin{aligned}\frac{\partial}{\partial \theta_1} &= -\cos \psi \frac{\partial}{\partial \Theta} + \cot \Theta \sin \psi \frac{\partial}{\partial \psi} + \frac{\partial}{\partial \theta}, \\ \frac{1}{\sin \theta_1} \frac{\partial}{\partial \phi_1} &= -\sin \psi \frac{\partial}{\partial \Theta} - (\cot \theta + \cot \Theta \cos \psi) \frac{\partial}{\partial \psi} + \frac{1}{\sin \theta} \frac{\partial}{\partial \phi}, \\ \frac{\partial}{\partial \theta_2} &= \cos \chi \frac{\partial}{\partial \Theta} - \frac{\sin \chi}{\sin \Theta} \frac{\partial}{\partial \psi}, \\ \frac{1}{\sin \theta_2} \frac{\partial}{\partial \phi_2} &= \sin \chi \frac{\partial}{\partial \Theta} + \frac{\cos \chi}{\sin \Theta} \frac{\partial}{\partial \psi}.\end{aligned}\quad (8)$$

Eq's (7) and (8) are derived [1] by using the formulas in spherical trigonometry and the chain rule of the partial differentiation. For the sake of convenience we list those formulas in Appendix a. As a first application of Eq. (8) we shall express  $\mathbf{L}$ , which is defined by (6) in terms of  $A$ , by the set  $B$ . The results [2] are well known

$$\begin{aligned}L_{\pm} &\equiv L_1 \pm iL_2 = e^{\pm i\phi} \left( \pm \frac{\partial}{\partial \theta} - \frac{i}{\sin \theta} \left( \frac{\partial}{\partial \psi} - \cos \theta \frac{\partial}{\partial \phi} \right) \right), \\ L_3 &\equiv M = -i \frac{\partial}{\partial \phi} \\ L^2 &= - \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \left( \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial \psi^2} - 2 \cos \theta \frac{\partial^2}{\partial \phi \partial \psi} \right) \right].\end{aligned}\quad (9)$$

The eigenfunctions and the eigenvalues are also well known [7]. Note that  $\mathbf{L}$  does not include  $\Theta$  so  $\Theta$  is invariant under the rotation.

Definitions of  $K$ ,  $K'$  and  $N$ .

We define an operator  $K$  by

$$K \equiv -i \frac{\partial}{\partial \psi} \quad (10)$$

in terms of  $B$ . From its definition,  $K$  is the component of  $\mathbf{L}$  around  $\mathbf{r}_1$  in the body fixed moving coordinate system. Note that  $K$  is commutable with  $L_{\pm}$  and  $L_3$  which are the components of  $\mathbf{L}$  in  $A$ . (In Fig. 1, the rotations around  $O1$  and around  $Oz$  are commutable.) As is stressed in the introduction we must treat two particles 1 and 2 in a symmetrical way. So we define the second operator  $K'$  by

$$K' \equiv -i \frac{\partial}{\partial \chi} \quad (11)$$

in terms of  $C$ . By using formulas in Appendix a we can express  $K'$  in terms of  $B$ ,

$$\begin{aligned} K' &= -i \left( \frac{\partial \theta}{\partial \chi} \Big|_{\theta, \theta', \phi'} \cdot \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial \chi} \Big|_{\theta, \theta', \phi'} \cdot \frac{\partial}{\partial \phi} + \frac{\partial \psi}{\partial \chi} \Big|_{\theta, \theta', \phi'} \cdot \frac{\partial}{\partial \psi} \right) \\ &= -i \sin \Theta \left[ \sin \psi \frac{\partial}{\partial \theta} - \frac{\cos \psi}{\sin \theta} \frac{\partial}{\partial \phi} + (\cot \Theta + \cos \psi \cot \theta) \frac{\partial}{\partial \psi} \right]. \end{aligned} \quad (12)$$

From its definition  $K'$  is the component of  $\mathbf{L}$  around  $\mathbf{r}_2$  in the body fixed moving frame. Finally, we define third operator  $N$  by

$$\sin \Theta \cdot N \equiv -i [K, K']. \quad (13)$$

As is shown in Fig. 1, two unit vectors  $\hat{\mathbf{r}}_1$  and  $\hat{\mathbf{r}}_2$  make angle  $\Theta$  so  $\hat{\mathbf{r}}_1 \times \hat{\mathbf{r}}_2 = \sin \Theta \cdot \mathbf{n}$ , where  $\mathbf{n}$  is a unit normal vector through the origin to the instantaneous plane  $O12$ . Therefore  $N$  is the component of  $\mathbf{L}$  around  $\mathbf{n}$  in the body fixed moving coordinate. Substituting (10) and (12) into (13), we get

$$N = i \left[ \cos \psi \frac{\partial}{\partial \theta} + \frac{\sin \psi}{\sin \theta} \frac{\partial}{\partial \phi} - \sin \psi \cot \theta \frac{\partial}{\partial \psi} \right]. \quad (14)$$

From Eq's. (10), (12) and (14) we get the commutation relations

$$\begin{aligned} \sin \Theta [N, K] &= iK' - i \cos \Theta K, \\ \sin \Theta [N, K'] &= -iK + i \cos \Theta K'. \end{aligned} \quad (15)$$

Eq. (15) are those relations which are expected from the definitions of  $K$ ,  $K'$  and  $N$ . Finally, we can prove that

$$L^2 = N^2 + [K^2 + K'^2 - \cos \Theta (KK' + K'K)] / \sin^2 \Theta, \quad (16)$$

because if we substitute (10), (12) and (14) into the r.h.s. of (16), we get (9).

### §3. Single Particle Operators

In this section we shall express single particle operators, given by (5) and (6), first by the set  $B$  and then by  $K$ ,  $K'$  and  $N$  given in the last section.

$$2\mu_{3i}T_i = \frac{1}{r_i} \frac{\partial^2}{\partial r_i^2} r_i + \frac{L_i^2}{r_i^2}, \quad (i=1, 2) \quad (17)$$

$$L_i^2 = -\frac{\partial^2}{\partial \theta_i^2} - \cot \theta_i \frac{\partial}{\partial \theta_i} - \frac{1}{\sin^2 \theta_i} \frac{\partial^2}{\partial \phi_i^2}. \quad (18)$$

We substitute (8) into (18) and get [1]

$$\begin{aligned} -L_1^2 &= \frac{\partial^2}{\partial \Theta^2} + \cot \Theta \frac{\partial}{\partial \Theta} + \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \\ &+ (\cot^2 \Theta + \cot^2 \theta + 2 \cot \Theta \cos \psi \cot \theta) \frac{\partial^2}{\partial \psi^2} \\ &+ 2 \left( -\cos \psi \frac{\partial}{\partial \theta} + \sin \psi \cot \theta \frac{\partial}{\partial \psi} - \frac{\sin \psi}{\sin \theta} \frac{\partial}{\partial \phi} \right) \frac{\partial}{\partial \Theta} \\ &+ 2 \left( \cot \Theta \left( \sin \psi \frac{\partial}{\partial \theta} - \frac{\cos \psi}{\sin \theta} \frac{\partial}{\partial \phi} \right) - \frac{\cos \theta}{\sin^2 \theta} \frac{\partial}{\partial \phi} \right) \frac{\partial}{\partial \psi}, \end{aligned} \quad (19)$$

and

$$-L_2^2 = \frac{\partial^2}{\partial \Theta^2} + \cot \Theta \frac{\partial}{\partial \Theta} + \frac{1}{\sin^2 \Theta} \frac{\partial^2}{\partial \psi^2}. \quad (20)$$

If we substitute (10), (12) and (14) into (19) and (20) we can simplify (19) as

$$L_1^2 = p_z(1-z^2)p_z + L^2 - 2 \sin \Theta N p_z + \frac{1}{1-z^2} (2zK'K - K^2) \quad (21)$$

and

$$L_2^2 = p_z(1-z^2)p_z + (1-z^2)^{-1}K^2 \quad (22)$$

where we have set

$$z = \cos \Theta,$$

$$p_z \equiv -i \frac{\partial}{\partial z} \Big|_{\phi, \theta, \psi} = \frac{i}{\sin \Theta} \frac{\partial}{\partial \Theta} \Big|_{\phi, \theta, \psi} \quad (23)$$

Marked asymmetry between (21) and (22) is due to the definition of  $p_z$ , Eq. (23). Though  $z$  is symmetric between 1 and 2, but the canonical conjugate of it,  $p_z$ , is defined in the system  $B$ , and hence asymmetric. We denote the corresponding operator in

the system  $C$  as  $p'_z$ :

$$p'_z \equiv -i \frac{\partial}{\partial z} \Big|_{\varphi', \theta', x} = \frac{i}{\sin \Theta} \frac{\partial}{\partial \Theta} \Big|_{\varphi', \theta', x} \quad (24)$$

The r.h.s. of (24) is expressed by the set  $A$ ;

$$\begin{aligned} \frac{\partial}{\partial \Theta} \Big|_{\varphi', \theta', x} &= \frac{\partial \theta_1}{\partial \Theta} \Big|_{\varphi_2, \theta_2, x} \cdot \frac{\partial}{\partial \theta_1} + \frac{\partial \phi_1}{\partial \Theta} \Big|_{\varphi_2, \theta_2, x} \cdot \frac{\partial}{\partial \phi_1} \\ &= -\cos \psi \frac{\partial}{\partial \theta_1} - \frac{\sin \psi}{\sin \theta_1} \frac{\partial}{\partial \phi_1}, \end{aligned}$$

where we used formulas in Appendix a. Substituting (8) into the above, and using (14), we get the relation between  $p'_z$  and  $p_z$ ,

$$p'_z = p_z - N/\sin \Theta. \quad (25)$$

We define a symmetric variable  $p$ , which is canonical conjugate to  $z$ , by

$$p = (p_z + p'_z)/2 = p_z - N/2 \sin \Theta. \quad (26)$$

Substituting (26) into (21) and (22) and using (16) we obtain symmetric forms as follows;

$$I_1^2 = p(1-z^2)p - N \sin \Theta p - \frac{iN}{2} \cot \Theta + \frac{N^2}{4} + \frac{K'^2}{1-z^2}, \quad (27)$$

$$I_2^2 = p(1-z^2)p + N \sin \Theta p + \frac{iN}{2} \cot \Theta + \frac{N^2}{4} + \frac{K^2}{1-z^2}. \quad (28)$$

Finally we must express  $-m_3 T_3 = \mathcal{V}_1 \cdot \mathcal{V}_2$ , defined in terms of  $A$ , first by the set  $B$  and then by  $K, K'$  and  $N$  and  $p$ . The procedure is straightforward but rather tedious. We write the result only,

$$\begin{aligned} \mathcal{V}_1 \cdot \mathcal{V}_2 &= z \frac{\partial^2}{\partial r_2 \partial r_1} + \frac{i \sin \Theta}{r_1} \left( \sin \Theta p - \frac{N}{2} \right) \frac{\partial}{\partial r_2} \\ &\quad + \frac{i \sin \Theta}{r_2} \left( \sin \Theta p + \frac{N}{2} \right) \frac{\partial}{\partial r_1} + \left[ zp(1-z^2)p \right. \\ &\quad \left. + i(1-z^2)p - \frac{zN^2}{4} + \frac{K'K + KK'}{2(1-z^2)} \right]. \end{aligned} \quad (29)$$

We remark that all of  $I_1^2, I_2^2$  and  $\mathcal{V}_1 \cdot \mathcal{V}_2$  are hermitian and under the exchange operation  $\varepsilon_{12}$ , Eqs. (27), (28) and (29) are covariant provided

$$\begin{aligned} \varepsilon_{12} N &= -N, \\ \varepsilon_{12} K &= K', \end{aligned} \quad (30)$$

$$\varepsilon_{12}K' = K,$$

$z, p$  are invariant.

#### §4. Operators $K_1, K_2$ and $N$

In the body fixed moving frame, the defining axes of  $K$  and  $K'$  make angle  $\Theta$ .

Hence, we define two operators  $K_1$  and  $K_2$  by

$$\begin{aligned} K &= \alpha K_1 + \beta K_2, \\ K' &= \beta K_1 + \alpha K_2, \end{aligned} \quad (31)$$

$$\text{with } \left. \begin{array}{l} \alpha \\ \beta \end{array} \right\} = \cos\left(\frac{\pi}{4} \mp \frac{\Theta}{2}\right) = \frac{1}{\sqrt{2}}\left(\cos\frac{\Theta}{2} \pm \sin\frac{\Theta}{2}\right).$$

Owing to Eqs. (13), (15) and (31),  $K_1, K_2$  and  $N$  satisfy the usual commutation relations of angular momentum,

$$\begin{aligned} [K_1, K_2] &= iN, \\ [K_2, N] &= iK_1, \\ [N, K_1] &= iK_2. \end{aligned} \quad (32)$$

Eq. (16) reduces to

$$\mathbf{L}^2 = K_1^2 + K_2^2 + N^2 \quad (33)$$

As is remarked in Sec. 2,  $L_3 = M = -i\frac{\partial}{\partial\phi}$  is commutable with all of  $K_1, K_2, N$  and  $\mathbf{L}^2$ .  $\mathbf{L}^2, M$  and  $N$  form a complete set of commuting observables. We denote the normalized eigen ket  $|l, m, n\rangle$  having respective eigenvalues  $l(l+1), m, n$ :

$$\begin{aligned} \mathbf{L}^2|l, m, n\rangle &= l(l+1)|l, m, n\rangle, \\ M|l, m, n\rangle &= m|l, m, n\rangle, \\ N|l, m, n\rangle &= n|l, m, n\rangle. \end{aligned} \quad (34)$$

If the parity operator is denoted as  $\mathcal{P}$ , Bhatia and Temkin [4] showed that

$$\mathcal{P}|l, m, n\rangle = (-1)^n|l, m, n\rangle, \quad (35)$$

and

$$\varepsilon_{12}|l, m, n\rangle = (-1)^l|l, m, -n\rangle. \quad (36)$$

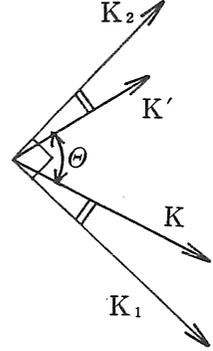


Fig. 2.

By virtue of (32) we can form *the raising and lowering operators in  $n$*

$$K_{\pm} = K_1 \pm iK_2, \quad (37)$$

$$K_{\pm}|l, m, n\rangle = \sqrt{(l \mp n)(l \pm n + 1)}|l, m, n \pm 1\rangle. \quad (38)$$

Repeating (38), we have

$$K_{\pm}^2|l, m, n\rangle = \lambda_l(\mp n)|l, m, n \pm 2\rangle \quad (39)$$

with

$$\lambda_l(n) = \sqrt{(l-n+1)(l-n+2)(l+n)(l+n-1)}. \quad (40)$$

Note that

$$\lambda_l(-n+2) = \lambda_l(n). \quad (41)$$

We also have

$$K_-K_+|l, m, n\rangle = (l-n)(l+n+1)|l, m, n\rangle \quad (42)$$

and

$$K_+K_-|l, m, n\rangle = (l-n)(l+n-1)|l, m, n\rangle.$$

Our final task in this section is to express  $K^2$ ,  $K'^2$  and  $KK' + K'K$ , which appear in single particle operators, in terms of  $K_+$  and  $K_-$ . The calculations are easy,

$$\begin{aligned} K^2 &= -\frac{i}{4}(e^{i\theta}K_+^2 - \bar{e}^{i\theta}K_-^2) + \frac{\mathbf{L}^2 - N^2}{2}, \\ K'^2 &= -\frac{i}{4}(\bar{e}^{i\theta}K_+^2 - e^{i\theta}K_-^2) + \frac{\mathbf{L}^2 - N^2}{2}, \end{aligned} \quad (43)$$

and

$$KK' + K'K = (K_+^2 - K_-^2)/2i. \quad (44)$$

## §5. Radial Equations

In this section we derive the radial equations. As an illustration of our procedure, we take a simple case of two-electron with fixed nucleus, because the general case is trivially performed by making use of (5), (29) and (44) in an exactly similar manner. The Schrödinger equation is

$$(E - H)\Psi_{Elm} = 0, \quad (45)$$

with

$$H = \left[ -\frac{1}{r_1} \frac{\partial^2}{\partial r_1^2} r_1 - \frac{1}{r_2} \frac{\partial^2}{\partial r_2^2} r_2 + \frac{l_1^2}{r_1^2} + \frac{l_2^2}{r_2^2} \right] / 2m + V(r_1, r_2, z). \quad (46)$$

We expand  $\Psi_{Elm}$  by using the complete set  $|l, m, n\rangle$ ;

$$\Psi_{Elm} = \sum_n g_n^l(r_1, r_2, z) |l, m, n\rangle. \quad (47)$$

Because of the parity property of (35), the sum about  $n$  goes over every second value of  $n$ , [4]. Substituting (43) into (27) and (28), using (39), (45) and (46), equating every factor of  $|l, m, n\rangle$  to zero, we get at once the following radial equation

$$(a - nb) g_n(r_1, r_2, z) + (c - d) \lambda(n+2) g_{n+2}(r_1, r_2, z) - (c + d) \lambda(-n+2) g_{n-2}(r_1, r_2, z) = 0, \quad (48)$$

where we make the abbreviations

$$a = -\frac{1}{r_1} \frac{\partial^2}{\partial r_1^2} r_1 - \frac{1}{r_2} \frac{\partial^2}{\partial r_2^2} r_2 + \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \left\{ p(1-z^2)p + \frac{n^2}{4} + \frac{l(l+1) - n^2}{2(1-z^2)} \right\} + 2m(V-E), \quad (49)$$

$$b = \left( \frac{1}{r_1^2} - \frac{1}{r_2^2} \right) \left( \sqrt{1-z^2} p + \frac{i}{2} \frac{z}{\sqrt{1-z^2}} \right), \quad (50)$$

$$c = \frac{iz}{4(1-z^2)} \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right), \quad (51)$$

$$d = \frac{1}{4\sqrt{1-z^2}} \left( \frac{1}{r_1^2} - \frac{1}{r_2^2} \right). \quad (52)$$

In Eq. (48) we suppressed common suffix  $l$  in  $g_n^l(r_1, r_2, z)$  and  $\lambda_l(n)$ . Note that  $a$  and  $c$  are even and  $b$  and  $d$  are odd under  $\varepsilon_{12}$ . The equation for  $g_n(r_2, r_1, z)$  is obtained from (48) with reversed sign for  $b$  and  $d$ . We define  $g_n^\pm$ , which are even or odd under  $\varepsilon_{12}$ , by

$$g_n^\pm = (g_n(r_1, r_2, z) \pm g_n(r_2, r_1, z)) / 2. \quad (53)$$

$g_n^\pm$  satisfies

$$a g_n^\pm - n b g_n^\mp + \lambda(n+2) (b g_{n+2}^\pm - c g_{n+2}^\mp) - \lambda(-n+2) (b g_{n-2}^\pm + c g_{n-2}^\mp) = 0.$$

In order to make eigen kets of  $\varepsilon_{12}$  for the rotational variables, we must follow the similar procedure as above;

$$|\pm, l, m, n\rangle \equiv |l, m, n\rangle \pm (-1)^l |l, m, -n\rangle, \quad (55)$$

$$\varepsilon_{12} |\pm, l, m, n\rangle = \pm |\pm, l, m, n\rangle. \quad (56)$$

Corresponding to (55), we must also make the linear combinations of  $g_n^\pm$  and  $g_{\pm n}^\pm$ , but we skip this procedure, because in Ref. [4] the details are described.

### §6. Discussion

In this section we shall examine the third term of Eq. (5) with an explicit form (29), which is neglected in the last section, as a consistency check of our procedure. For this purpose it would be enough to consider the simple case of equal masses,  $m_1 = m_2 = m_3 = m$  and  $2\mu_{31} = 2\mu_{23} = m$ , and  $L=0$ . In this case terms including  $K, K', N$  and  $L^2$  can be neglected. From (5) and (29) we have

$$\begin{aligned}
 -mT = & \frac{1}{r_1} \frac{\partial^2}{\partial r_1^2} \cdot r_1 + \frac{1}{r_2} \frac{\partial^2}{\partial r_2^2} \cdot r_2 + \left( \frac{1}{r_1^2} + \frac{1}{r_2^2} \right) \frac{\partial}{\partial z} (1-z^2) \frac{\partial}{\partial z} \\
 & + z \frac{\partial^2}{\partial r_2 \partial r_1} + (1-z^2) \left( \frac{1}{r_1} \frac{\partial}{\partial r_2} + \frac{1}{r_2} \frac{\partial}{\partial r_1} \right) \frac{\partial}{\partial z} \\
 & - \frac{1}{r_1 r_2} \left( z(1-z^2) \frac{\partial^2}{\partial z^2} - (1+z^2) \frac{\partial}{\partial z} \right).
 \end{aligned} \tag{57}$$

To examine the symmetry between three particles, we must use

$$r_3 = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 z}, \tag{58}$$

instead of  $z$ . Relevant formulas for this transformation are listed in Appendix b. In terms of  $r_1, r_2$  and  $r_3$  (57) can be written in a symmetrical and simple form [9];

$$\begin{aligned}
 -mT = & \frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} + \frac{\partial^2}{\partial r_3^2} + \cos \Theta_3 \frac{\partial^2}{\partial r_1 \partial r_2} + \cos \Theta_1 \frac{\partial^2}{\partial r_2 \partial r_3} \\
 & + \cos \Theta_2 \frac{\partial^2}{\partial r_3 \partial r_1} + \frac{2}{r_1} \frac{\partial}{\partial r_1} + \frac{2}{r_2} \frac{\partial}{\partial r_2} + \frac{2}{r_3} \frac{\partial}{\partial r_3},
 \end{aligned} \tag{59}$$

where

$$\cos \Theta_k = \frac{r_i^2 + r_j^2 - r_k^2}{2r_i r_j}, \tag{60}$$

( $i, j, k$ ): cyclic permutation of (1, 2, 3),

and  $r_1, r_2$  and  $r_3$  must satisfy the triangle inequalities. With an appropriate central potential the Schrödinger equation with (59) is worth while to study. For a more realistic application of (59) to nuclear problem, we must generalize our procedure to include tensor force and  $Ls$  coupling [6], [9].

### Acknowledgement

The author thanks to Dr. Shinichi Watanabe for informing the paper [4] and turning his attention to this problem.

### Appendix a

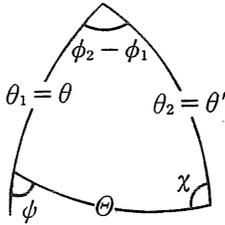


Fig. 3.

In this appendix we list the formulas in spherical trigonometry which are relevant to the text.

$$\frac{\sin \chi}{\sin \theta} = \frac{\sin \psi}{\sin \theta'} = \frac{\sin (\phi_2 - \phi_1)}{\sin \Theta}, \quad (\text{a.1})$$

$$\cos \theta_1 = \cos \theta' \cos \Theta + \sin \theta' \sin \Theta \cos \chi, \quad (\text{a.2})$$

$$\cos (\phi_2 - \phi_1) = \cos \chi \cos \psi + \sin \chi \sin \psi \cos \Theta, \quad (\text{a.3})$$

$$\cot \Theta \sin \theta_2 = \cos \theta_2 \cos \chi + \cot (\phi_2 - \phi_1) \sin \chi, \quad (\text{a.4})$$

$$\sin \Theta \cos \chi = \cos \theta_1 \sin \theta_2 - \sin \theta_1 \cos \theta_2 \cos (\phi_2 - \phi_1), \quad (\text{a.5})$$

$$\sin (\phi_2 - \phi_1) \cos \theta_2 = \cos \psi \sin \chi + \sin \psi \cos \chi \cos \Theta. \quad (\text{a.6})$$

Owing to the symmetries between  $\theta_1, \theta_2$  and  $\Theta$ , and between  $\phi_2 - \phi_1, \pi - \psi$  and  $\chi$ , there are three varieties for (a.2) and (a.3) and six varieties for (a.4), (a.5) and (a.6).

### Appendix b

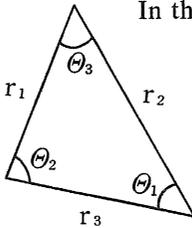


Fig. 4.

In this appendix we list the transformation formulas defined by (58).

$$\frac{\partial}{\partial z} = -\frac{r_1 r_2}{r_3} \frac{\partial}{\partial r_3}, \quad (\text{b.1})$$

$$\frac{\partial}{\partial r_1} = \frac{\partial}{\partial r_1} + \cos \Theta_2 \frac{\partial}{\partial r_3}, \quad (\text{b.2})$$

$$\frac{\partial^2}{\partial z^2} = -\frac{r_1^2 r_2^2}{r_3^2} \left( \frac{\partial^2}{\partial r_3^2} + \frac{\partial}{r_3 \partial r_3} \right), \quad (\text{b.3})$$

$$\frac{\partial^2}{\partial r_1^2} = \frac{\partial^2}{\partial r_1^2} + 2 \cos \Theta_2 \frac{\partial^2}{\partial r_3 \partial r_1} + \cos^2 \Theta_2 \frac{\partial^2}{\partial r_3^2} + \frac{4S^2}{r_1^2 r_3^3} \frac{\partial}{\partial r_3}, \quad (\text{b.4})$$

$$\begin{aligned} \frac{\partial^2}{\partial r_2 \partial r_1} &= \frac{\partial^2}{\partial r_2 \partial r_1} + \cos \Theta_2 \frac{\partial^2}{\partial r_2 \partial r_3} + \cos \Theta_1 \frac{\partial^2}{\partial r_1 \partial r_3} + \cos \Theta_1 \cos \Theta_2 \frac{\partial^2}{\partial r_3^2} \\ &\quad - \frac{4S^2}{r_1 r_2 r_3^3} \frac{\partial}{\partial r_3}, \end{aligned} \quad (\text{b.5})$$

$$\frac{\partial^2}{\partial r_1 \partial z} = -\frac{r_1 r_2}{r_3} \frac{\partial^2}{\partial r_1 \partial r_3} - \frac{r_2^2 \cos \Theta_1}{r_3^2} \frac{\partial}{\partial r_3} - \frac{r_1 r_2}{r_3} \cos \Theta_2 \frac{\partial^2}{\partial r_3^2}. \quad (\text{b.6})$$

In these formulas, the independent variables in l.h.s. are  $r_1$ ,  $r_2$  and  $z$ , and those in r.h.s. are  $r_1$ ,  $r_2$  and  $r_3$ .  $\Theta_j$  is given by (60) and  $S$  is the area of the triangle in Fig. 4,

$$16S^2 = (r_1 + r_2 + r_3)(r_1 + r_2 - r_3)(r_2 + r_3 - r_1)(r_3 + r_1 - r_2).$$

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