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Generator Coordinate Description of Molecule-Like States of p-Shell Nuclei

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States of the compound nucleus formed in a nuclear reaction play an important role in the microscopic R-matrix theory of reactions[1] as well as in the variational approach to collisions[2]. If the colliding nuclei are tightly bound it is likely that the compound nucleus has a two-cluster molecular structure, the clusters of which are the colliding nuclei. If only the projectile or the target is tightly bound, in the compound nucleus some nucleons might be transfered between the clusters and such a state can suitably be described as a superposition of two or more molecule-like states.

The purpose of this paper is to study the molecule-like states of p-shell nuclei in the basis of two-centre generator coordinate wave functions. Firstly we describe the basis wave functions, secondly we outline a new method for the projection of a basis wave function onto the space of angular momentum eigenstates, thirdly we describe the calculation of matrix elements of the Hamiltonian and the identity operator and finally we present the results of the calculation of molecule-like states of ^{7}Li, treating its structure as a superposition of the following two-cluster molecular structures: ^{3}H + ^{4}He and ^{6}Li + n.

[+]Talk presented by M.Poljšak

1. Two centre generator coordinate wave functions

In order to construct a basis of wave functions appropriate for the description of states of a compound nucleus we start with two-centre generator coordinate functions of the form

$$\Phi_{\chi}(\underset{\sim}{x},\underset{\sim}{S}) = \mathcal{A}\left\{\Phi_{A\chi_1}(\underset{\sim}{x}_1,\ldots,\underset{\sim}{x}_A,\underset{\sim}{S}_A)\,\Phi_{B\chi_2}(\underset{\sim}{x}_{A+1},\ldots,\underset{\sim}{x}_{A+B};\underset{\sim}{S}_B)\right\}$$

$$\underset{\sim}{S} = \underset{\sim}{S}_A - \underset{\sim}{S}_B \qquad \chi = (\chi_1,\chi_2) \qquad \underset{\sim}{x} = (\underset{\sim}{x}_1,\underset{\sim}{x}_2,\ldots,\underset{\sim}{x}_{A+B}) \qquad (1)$$

The functions $\Phi_{A\chi_1}$ and $\Phi_{B\chi_2}$ are Slater determinants constructed out of single particle functions which are eigenfunctions of harmonic oscillator potentials centred at $\underset{\sim}{S}_A$ and $\underset{\sim}{S}_B$, respectively. The indices χ_1 and χ_2 denote particular shell model configurations. In order to avoid the problem of spurious centre - of - mass motion we shall restrict ourselves to configurations with no holes in the closed shells and to the cases where the oscillator parameters of both wells are equal. The antisymmetrizer $\mathcal{A}$ takes care of the exchange of nucleons between the two fragments.

2. Projection of angular momentum eigenstates from the two-centre generator coordinate functions

The generator coordinate basis wave functions are obtained by applying to functions (1) the projection operator

$$P^J_{MK} = \frac{2J+1}{8\pi^2}\int d\Omega\, \mathcal{D}^{J\,*}_{MK}(\Omega)\, R(\Omega)$$

Here $R(\Omega)$ is the rotation operator that rotates the coordinates of all the nucleons $\underset{\sim}{x}$ through the Euler angles Ω and $\mathcal{D}^J_{MK}(\Omega)$ are elements of its matrix representation.

Our method of projection is based on the following relation which expresses the effect of the rotation of coordinates $\underset{\sim}{x}$ in terms of the rotation of the generator coordinate $\underset{\sim}{S}$

$$R(\Omega)\ \phi_{\chi}(\underset{\sim}{x},\underset{\sim}{S}) = \sum_{\chi' \epsilon \mathcal{X}} c_{\chi'\chi}(\Omega)\ \phi_{\chi'}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}), \quad \underset{\sim}{\tilde{S}} = R(\Omega^{-1})\underset{\sim}{S} \tag{2}$$

where the coefficients $c_{\chi'\chi}(\Omega)$ are expressible in terms of the $\mathfrak{D}$ functions and $\mathcal{X}$ is the set of all different configurations of valence nucleons in the major shell only.

We shall establish the relation (2) for the nucleus ^{7}Li treating it as a composite of two clusters ^{6}Li and n. This cluster structure contains all relevant information concerning the method of angular momentum projection.

Let the single particle potential of the nucleons in the cluster ^{6}Li be a harmonic oscillator potential centred at $\underset{\sim}{S}_A$ and let the remaining neutron move in a harmonic oscillator potential centred at $\underset{\sim}{S}_B$.

We shall use the Cartesian representation for single nucleon wave functions: $\phi_{0,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_i)$, $i \in \{A,B\}$, for the ground state and $\phi_{n,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_A)$, $n \in \{1,2,3\}$, which has an additional node along the Cartesian axis x_n, for the first excited state. When the nucleons of both clusters occupy the lowest possible states, a GC function of such a system has the form

$$\phi_{n_p\sigma_p n_n \sigma_n \chi_A}(\underset{\sim}{x},\underset{\sim}{S}) = \mathcal{A}\Big\{\phi_{0,-\frac{1}{2},-\frac{1}{2}}(\underset{\sim}{x}_1,\underset{\sim}{S}_A)\ \phi_{0,-\frac{1}{2},+\frac{1}{2}}(\underset{\sim}{x}_2,\underset{\sim}{S}_A)$$

$$\phi_{0,+\frac{1}{2},-\frac{1}{2}}(\underset{\sim}{x}_3,\underset{\sim}{S}_A)\ \phi_{0,+\frac{1}{2},+\frac{1}{2}}(\underset{\sim}{x}_4,\underset{\sim}{S}_A)\ \phi_{n_F,\sigma_F,-\frac{1}{2}}(\underset{\sim}{x}_5,\underset{\sim}{S}_A)\ \phi_{n_n,\sigma_n,+\frac{1}{2}}(\underset{\sim}{x}_6,\underset{\sim}{S}_A)$$

$$\phi_{0,\chi_{-1},+\frac{1}{2}}(\underset{\sim}{x}_7,\underset{\sim}{S}_B)\Big\} \tag{3}$$

The effect of the rotation operator on the single particle functions is as follows:

i) $$R(\Omega)\ \phi_{0,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_i) = \sum_{m_s'} \mathfrak{D}^{\frac{1}{2}}_{m_s'm_s}(\Omega)\ \phi_{0,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_i) \tag{4}$$

because the space part of a ls function is an exponential function depending on $|\underset{\sim}{x} - \underset{\sim}{S}_i|$ only and the spin part transforms in the following way

$$R(\Omega)\chi^{\frac{1}{2}}_{m_s} = \sum \mathcal{D}^{\frac{1}{2}}_{m_s' m_s}(\Omega)\chi^{\frac{1}{2}}_{m_s'}$$

ii) The lp single-particle wave function $\phi_{n,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_A)$ is a product of $\phi_{0,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_A)$ and the first degree polinomial $(x_n - S_{An})$.

The effect of the rotation of the Cartisian coordinate x_n is given by

$$R(\Omega)x_n = \sum_{n'} a_{n'n}(\Omega)\, x_{n'}$$

where the coefficients $a_{n'n}$ can be expressed by the $\mathcal{D}$ functions, for example

$$a_{11}(\Omega) = \tfrac{1}{2}\left[\mathcal{D}^1_{-1-1}(\Omega) - \mathcal{D}^1_{-11}(\Omega) - \mathcal{D}^1_{1-1}(\Omega) + \mathcal{D}^1_{11}(\Omega)\right].$$

Then we have

$$\begin{aligned}
R(\Omega)\,\phi_{n,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_A) &= R(\Omega)\left[(x_n - S_{An})\,\phi_{0,m_s,m_t}(\underset{\sim}{x},\underset{\sim}{S}_A)\right] \\
&= \Big(\sum_{n'} a_{n'n}(\Omega)x_{n'} - S_{An}\Big)\sum_{m_s'} \mathcal{D}^{\frac{1}{2}}_{m_s' m_s}(\Omega)\,\phi_{0,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_A) \\
&= \Big(\sum_{n'} a_{n'n}(\Omega)(x_{n'} - \tilde{S}_{An'})\Big)\sum_{m_s'} \mathcal{D}^{\frac{1}{2}}_{m_s' m_s}(\Omega)\,\phi_{0,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_A) \\
&\quad + \Big(\sum_{n'} a_{n'n}(\Omega)\,\tilde{S}_{An'} - S_{An}\Big)\sum_{m_s'} \mathcal{D}^{\frac{1}{2}}_{m_s' m_s}(\Omega)\,\phi_{0,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_A) \\
&= \sum_{n'} a_{n'n}(\Omega)\sum_{m_s'} \mathcal{D}^{\frac{1}{2}}_{m_s' m_s}(\Omega)\,\phi_{n,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_A) \\
&\quad + \Big(\sum_{n'} a_{n'n}(\Omega)\,\tilde{S}_{An'} - S_{An}\Big)\sum_{m_s'} \mathcal{D}^{\frac{1}{2}}_{m_s' m_s}(\Omega)\,\phi_{0,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_A)
\end{aligned} \tag{5}$$

If we apply the rotation operator to the GO function (3) we have to replace the single particle wave functions by the rotated [illegible] in the resulting function each of the four [illegible]

single particle states is occupied, the terms of the rotated lp single particle state (eq. 5) which contain $\phi_{0,m_s',m_t}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}_A)$ do not contribute to the rotated many-particle GC function and we have

$$R(\Omega)\,\phi_{n_p\sigma_p n_n\sigma_n\varkappa_n}(\underset{\sim}{x},\underset{\sim}{S}) = \sum_{n_p'\sigma_p' n_n'\sigma_n'\varkappa_n'} a_{n_p'n_p}(\Omega)\;\mathcal{D}^{\frac{1}{2}}_{\sigma_p'\sigma_p}(\Omega)$$

$$\times\, a_{n_n'n_n}(\Omega)\,\mathcal{D}^{\frac{1}{2}}_{\sigma_n'\sigma_n}(\Omega)\,\mathcal{D}^{\frac{1}{2}}_{\varkappa_n'\varkappa_n}(\Omega)\,\phi_{n_p'\sigma_p' n_n'\sigma_n'\varkappa_n'}(\underset{\sim}{x},\underset{\sim}{\tilde{S}})$$

which is a particular example of eq. (2).

By using relation (2) we can now establish the following statement: the vector space spanned by the set $\{P^J_{MK}\phi_\varkappa(\underset{\sim}{x},\underset{\sim}{S}_o)\,|\,-J\leqslant K\leqslant J\ \&\ \varkappa\in\mathcal{H}\}$ where $\underset{\sim}{S}_o$ is a fixed vector, does not depend on the direction of $\underset{\sim}{S}_o$. Proof: Let us choose a configuration $\varkappa\in\mathcal{H}$ and a vector $\underset{\sim}{S}$, which has the some length as $\underset{\sim}{S}_o$. Let Ω be the Euler angles such that $\underset{\sim}{S}_o = R(\Omega)\underset{\sim}{S}$. The function $P^J_{MK}\phi_\varkappa(\underset{\sim}{x},\underset{\sim}{S})$ can be expressed in the form

$$P^J_{MK}\phi(\underset{\sim}{x},\underset{\sim}{S}) = P^J_{MK}R(\Omega)\,R^{-1}(\Omega)\,\phi_\varkappa(\underset{\sim}{x},\underset{\sim}{S})$$

$$= P^J_{MK}R(\Omega)\sum_{\varkappa'} c_{\varkappa'\varkappa}(\Omega^{-1})\,\phi_{\varkappa'}(\underset{\sim}{x},\underset{\sim}{S}_o)$$

$$= \frac{2J+1}{8\pi^2}\sum_{\varkappa'} c_{\varkappa'\varkappa}(\Omega^{-1})\int d\omega\;\mathcal{D}^{J*}_{MK}(\omega)\,R(\omega)\,R(\Omega)\,\phi_{\varkappa'}(\underset{\sim}{x},\underset{\sim}{S}_o)$$

$$= \frac{2J+1}{8\pi^2}\sum_{\varkappa'} c_{\varkappa'\varkappa}(\Omega^{-1})\int d\omega\;\mathcal{D}^{J*}_{MK}(\omega)\,R(\Omega\omega)\,\phi_{\varkappa'}(\underset{\sim}{x},\underset{\sim}{S}_o)$$

If we denote the combined rotation $\Omega.\omega$ by σ, then

$$\mathcal{D}^{J*}_{MK}(\omega) = \sum_m \mathcal{D}^{J*}_{Mm}(\sigma)\;\mathcal{D}^{J}_{Km}(\Omega)$$

and therefore

$$P^J_{MK}\phi_\varkappa(\underset{\sim}{x},\underset{\sim}{S}) = \frac{2J+1}{8\pi^2}\sum_{\varkappa} c_{\varkappa'\varkappa}(\Omega^{-1})\int d\sigma\sum_m \mathcal{D}^{J*}_{Mm}(\sigma)\;\mathcal{D}^{J}_{Km}(\Omega)$$

$$\times\, R(\sigma)\,\phi_{\varkappa'}(\underset{\sim}{x},\underset{\sim}{S}_o)$$

$$\sum_{\chi'} \sum_{m} c_{\chi'\chi}(\Omega^{-1}) \quad \mathcal{D}^{J}_{Km}(\Omega)\, P^{J}_{Mm}\, \Phi_{\chi'}(\underset{\sim}{x},\underset{\sim}{S}_{o})$$

Any element of the set of projected wave functions corresponding to $\underset{\sim}{S}$ can thus be expressed as a linear combination of functions corresponding to $\underset{\sim}{S}_{o}$, which completes the proof.

3. Matrix elements of the Hamiltonian and the identity operator

The matrix elements of the Hamiltonian H and the identity operator I between two projected GC wave functions can be calculated in terms of overlaps of the unprojected functions (1) in the following way:

$$\langle \Phi_{\chi}(\underset{\sim}{S}) | (P^{J}_{MK})^{\dagger} \begin{Bmatrix} H \\ I \end{Bmatrix} P^{J}_{MK'} | \Phi_{\chi'}(\underset{\sim}{S}') \rangle = \langle \Phi_{\chi}(\underset{\sim}{S}) | \begin{Bmatrix} H \\ I \end{Bmatrix} P^{J}_{KK'} | \Phi_{\chi'}(\underset{\sim}{S}') \rangle$$

$$= \frac{2J+1}{8\pi^{2}} \sum_{\chi''} \int d\Omega \quad \mathcal{D}^{J*}_{KK'}(\Omega)\, c_{\chi''\chi}(\Omega)\, \langle \Phi_{\chi}(\underset{\sim}{S}) | \begin{Bmatrix} H \\ I \end{Bmatrix} | \Phi_{\chi''}(\underset{\sim}{\tilde{S}}') \rangle$$

By expanding the matrix elements of H and I between unprojected GC wave functions in terms of spherical harmonic functions:

$$\langle \Phi_{\chi}(\underset{\sim}{S}) | \begin{Bmatrix} H \\ I \end{Bmatrix} | \Phi_{\chi''}(\underset{\sim}{\tilde{S}}') \rangle = \sum_{\lambda\mu} \sum_{\lambda''\mu''} \begin{Bmatrix} H_{\chi\lambda\mu,\chi''\lambda''\mu''}(S,S') \\ N_{\chi\lambda\mu,\chi''\lambda''\mu''}(S,S') \end{Bmatrix} Y^{*}_{\lambda\mu}(\hat{\underset{\sim}{S}})\, Y_{\lambda''\mu''}(\hat{\underset{\sim}{\tilde{S}}})$$

$$= \sum_{\lambda\mu} \sum_{\lambda''\mu''} \begin{Bmatrix} H_{\chi\lambda\mu,\chi''\lambda''\mu''}(S,S') \\ N_{\chi\lambda\mu,\chi''\lambda''\mu''}(S,S') \end{Bmatrix} \quad Y^{*}_{\lambda\mu}(\hat{\underset{\sim}{S}})\, \mathcal{D}^{\lambda''}_{\mu'\mu''}(\Omega)\, Y_{\lambda'\mu'}(\hat{\underset{\sim}{S}}')$$

and choosing $\underset{\sim}{S}$ and $\underset{\sim}{S}'$, according to the statement proven in the previous section, in the z direction, we get

$$\langle \Phi_{\chi}(\underset{\sim}{S}) | \begin{Bmatrix} H \\ I \end{Bmatrix} | \Phi_{\chi''}(\underset{\sim}{\tilde{S}}') \rangle = \sum_{\lambda''\mu''} \sum_{\lambda} \begin{Bmatrix} H_{\chi\lambda 0,\chi''\lambda''\mu''}(S,S') \\ N_{\chi\lambda 0,\chi''\lambda''\mu''}(S,S') \end{Bmatrix} \frac{[(2\lambda+1)(2\lambda''+1)]^{\frac{1}{2}}}{4\pi} \mathcal{D}^{\lambda''}_{0\mu''}(\Omega)$$

Defining then

$$\varphi^{J\lambda}_{KK'\chi''\chi'\mu'\mu} = \int d\Omega\, \mathcal{D}^{J}_{KK'}(\Omega)\, c_{\chi''\chi'}(\Omega)\, \mathcal{D}^{\lambda}_{\mu'\mu}(\Omega) , \qquad (6)$$

nally we obtain

$$\langle \Phi_{\varkappa}(S) | (P^{J}_{MK})^{\dagger} \begin{Bmatrix} H \\ I \end{Bmatrix} P^{J}_{MK'} | \Phi_{\varkappa'}(S') \rangle =$$

$$\frac{2J+1}{8\pi^2} \sum_{\varkappa''} \sum_{\lambda} \sum_{\lambda''\mu''} \frac{[(2\lambda+1)(2\lambda''+1)]^{\frac{1}{2}}}{4\pi} \begin{Bmatrix} H_{\varkappa\lambda 0,\, \varkappa''\lambda''\mu''}(S,S') \\ N_{\varkappa\lambda 0,\, \varkappa''\lambda''\mu''}(S,S') \end{Bmatrix} \mathcal{C}^{J\lambda''}_{KK'\varkappa''\varkappa' 0\mu'} \quad (7)$$

Since the coefficients $c_{\varkappa'\varkappa}(\Omega)$ are given in terms of functions $\mathfrak{D}$ we can express the coefficients $\mathcal{C}$ from eq. (7) by the vector coupling coefficients. The projection process is then an algebraic one rather than a numerical integration.

4. Molecule-like states of ^{7}Li

In order to find the two-centre molecule-like states of nuclei one has to solve the wave equation of Schrödinger within the space spanned by the set of functions $\{P^{J}_{MK}\Phi_{\varkappa}(\underline{x},S) | -J \leq K \leq J \;\&\; \varkappa\epsilon\mathcal{H} \;\&\; S\epsilon[0,\infty)\}$. This differential eq. is equivalent to the Hill-Wheeler integral equation of the form

$$\sum_{\varkappa' K'} \int dS' \langle O_{\varkappa}(S) | (P^{J}_{MK})^{\dagger} (H - EI) P^{J}_{MK'} | \Phi_{\varkappa'}(S') \rangle f_{\varkappa' K'}(S') = 0 \quad (8)$$

the kernels of which are given by eq. (7).

For illustration eq. (8) has been solved for the nucleus ^{7}Li first treating it as a composite of two clusters ^{4}He and ^{3}H. Both clusters were described in terms of Slater determinants constructed out of 1s single particle functions. As the nuclear two-body interaction the Volkov effective two-body potential[3] was used. The two-body Coulomb interaction was represented by a sum of Gaussian functions. This representation is reliable for interparticle distances from 0.2 fm to 20 fm. Outside this interval the exact Coulomb interaction is stronger.

The energy levels of ^{7}Li calculated with the angular momentum and parity projected generator coordinate basis wave functions are shown by the dashed lines in fig. 1. The results without Coulomb interactions are shown by the lower two full lines. The diagram suggests that the system has only two

degenerate states stable with respect to desintegration into ^{4}He and ^{2}H. For these two states eq. (5) has been solved by replacing the integral over S by the sum of few terms. The result for the energy of the ground state is $E(J = \frac{1^-}{2}, \frac{3^-}{2}) = (-35.54 \pm 0.02)$ MeV. Let us note that the ground state energy calculated by the GCM is 1.0 MeV below that obtained by the projected Hartree-Fock method[4], where the same effective interaction was used.

Next we treated the nucleus ^{7}Li as a composite of the cluster ^{6}Li and n, where the cluster ^{6}Li was allowed to be only in the ground state configuration. The energy of ^{7}Li in a state with $J^\pi = \frac{1^-}{2}$ calculated with projected GC basis functions is shown by the upper full line in fig. 1.

Finally we described the ground state of ^{7}Li by a superposition of wave functions for clustering in ^{3}H + ^{4}He and ^{6}Li + n. The ground state energy of ^{7}Li was then 0.1 MeV below that corresponding to clusters ^{3}H and ^{4}He only.

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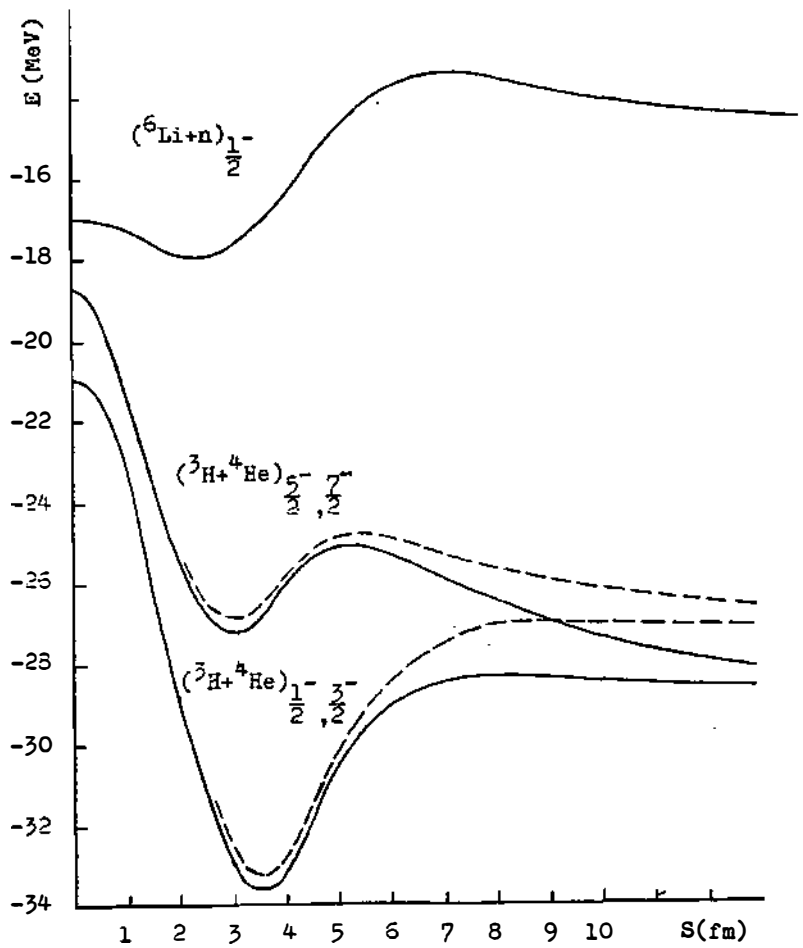

Fig. 1. Energy levels of the nucleus ^7Li as functions of the distance between the centres of single particle potentials of the constituent clusters. When the Coulomb interaction is neglected the calculation gives the lower two full lines for the cluster structure $^3H+^4He$ and the upper full line for ^6Li+n, where ^6Li is allowed to be in the ground state configuration only. The Coulomb interaction shifts the lower two full lines into the dashed lines.

DISCUSSION

M. Kamimura: I would like to know whether or not you made the calculation in which the two kinds of configurations $^{3}He + ^{4}He$ and $^{6}Li + n$ are diagonalized at each separation distance? If so it must be very interesting because one can see where the strength of rearrangement effect is large, namely where the energy-surface difference is large between the calculation with $^{3}He + ^{4}He$ only and that with $^{3}He + ^{4}He$ plus $^{6}Li + n$. Such a calculation must be very helpful for the study of rearrangement collision.

M. Poljšak: We have taken into account both configurations $^{3}He + ^{4}He$ and $^{6}Li + n$ only for the states of ^{7}Li with $J^{\pi} = 1/2^{-}$. The energy of the lowest such state was 0.1 MeV below the energy of the same state when only the configuration $^{3}H + ^{4}He$ was allowed. For states with $J^{\pi} = 5/2^{-}$, $7/2^{-}$ only the configuration $^{3}H + ^{4}He$ was considered. The inclusion of the configuration $^{6}Li + n$ is in progress.

B.G.Giraud: When rotating the generator function containing clusters with spins, it is not necessary to sum over the spin labels if you use a helicity formalism, namely if the quantization axis is the generator coordinate vector $\underset{\sim}{S}$ itself.

M. Poljšak: The use of the helicity formalism simplifies the projection onto the space of eigenfunctions of angular momentum operators, but the projection on parity eigenstates is more complicated.