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A METHOD FOR CALCULATING COLLISIONS OF LIGHT NUCLEI BASED ON TWO-CENTRE GENERATOR COORDINATE FUNCTIONS[*)]

M.V.Mihailović[+] and M.Poljšak
J. Stefan Institute, University of Ljubljana, Ljubljana, Yugoslavia

1. INTRODUCTION

There were few attempts[1)] to perform a complete calculation of collisions of nuclei in the generator coordinate (GC) basis, but, till now, only elastic scattering of nuclei with zero spin was treated. There were many open problems which made the method unapplicable for more complex calculations. Recently[2)], the Kohn-Kato variational method has been used to formulate a framework for description of multichannel reactions. In this formalism the structure of colliding fragments in the asymptotic region is described by shell model wave functions and the relative motion is described in terms of an amplitude which is a function of distance between shell model potentials of two fragments, instead of a function of relative coordinates of two fragments.

This talk contains the list of problems we have solved recently, so that we can start calculating collisions of light nuclei in the GC basis without going to the resonating group or the R matrix formalism.

We shall limit ourselves to reactions of the type

$$A_i + B_i \rightarrow A_j + B_j \ , \quad i,j = 1, \ \ldots \ N_c \qquad (1.1)$$

where j goes over the set of indices representing elastic and inelastic scattering as well as rearrangement reactions, N_c is the number of open channels. We shall consider the solution of the Schrödinger equation which corresponds to the incoming wave in the j-th channel and which satisfies the boundary conditions

[+]Talk presented by M.V.Mihailović

$$|\underset{\sim}{r}_j|\ \psi_j = 0\ , \quad |\underset{\sim}{r}_j| = 0$$

$$\psi_j = \mathcal{F}_j + \sum_j K_{ji}\, \mathcal{G}_j\ , \quad |\underset{\sim}{r}_j| \to \infty \tag{1.2}$$

if the channel is open ($E_j = E - E_{Aj} - E_{Bj} \geq 0$), and

$$\psi_j \to 0, \quad |\underset{\sim}{r}_j| \to \infty$$

if the channel is closed ($E_j < 0$).

In eq. (1.2) $\underset{\sim}{r}_j$ is the relative coordinate of the centres-of-mass of the two nuclei A_j and B_j,

$$\underset{\sim}{r}_j = \underset{\sim}{x}^{Aj}_{c.m.} - \underset{\sim}{x}^{Bj}_{c.m.}\ ,$$

and E_{Aj} and E_{Bj} are their respective internal energies. The functions $\mathcal{F}_j$ and $\mathcal{G}_j$ are many-body functions which asymptotically have the form

$$\begin{Bmatrix} \mathcal{F}_j \\ \mathcal{G}_j \end{Bmatrix} = \mathcal{A} \begin{Bmatrix} F_j(\underset{\sim}{r}_j) \\ G_j(\underset{\sim}{r}_j) \end{Bmatrix} \phi_{Aj}(\xi_{Aj})\, \phi_{Bj}(\xi_{Bj})\ . \tag{1.3}$$

where $\xi_{Aj} = (\underset{\sim}{x}_1 - \underset{\sim}{x}^{Aj}_{c.m.}, \ \cdots\ \underset{\sim}{x}_{Aj} - \underset{\sim}{x}^{Aj}_{c.m.})$, and $\xi_{Bj} = (\underset{\sim}{x}_{Aj+1} - \underset{\sim}{x}^{Bj}_{c.m.}, \ \cdots\ \underset{\sim}{x}_{A+B} - \underset{\sim}{x}^{Bj}_{c.m.})$, are the internal coordinates of the nuclei A_j and B_j, respectively. The functions ϕ_{Aj} and ϕ_{Bj} represent the intrinsic states of the nuclei A_j and B_j, and are completely antisymmetric in all their variables. The operator $\mathcal{A}$ is an operator which antisymmetrizes the two clusters A_j and B_j. At very large values of the channel coordinate $\underset{\sim}{r}_j$ F_j and G_j are the regular and irregular Coulomb functions. The quantities K_{ij} are the elements of the K-matrix between the asymptotic channel states.

2. TWO-CENTRE GENERATOR COORDINATE BASIS FOR THE DESCRIPTION OF COLLISIONS

2.1. Generator coordinate functions

Except at high energy the collisions between complex nuclei are peripheral processes in the sense that the nucleons of colliding fragments remain largely in their initial systems. An appropriate basis for describing such processes are two-centre shell-model wave functions. A basis particularly convenient for calculation is obtained[2] if one starts with single particle wave functions in two separated harmonic oscillator wells and then constructs many body Slater determinants of the rank A + B. These determinants form a generator coordinate basis and the generator coordinate $\underset{\sim}{S}$ represents the separation between the two wells:

$$\phi_{(AB)i}(\underset{\sim}{x}_1 \cdots \underset{\sim}{x}_{A+B}, \underset{\sim}{S}) = \mathcal{A}\left[\phi_{Ai}(\underset{\sim}{x}_1, \ldots \underset{\sim}{x}_{Ai}, \underset{\sim}{S}_1)\ \phi_{Bi}(\underset{\sim}{x}_{Ai+1} \cdots \underset{\sim}{x}_{A+B}, \underset{\sim}{S}_2)\right], \quad \underset{\sim}{S} = \underset{\sim}{S}_1 - \underset{\sim}{S}_2 . \tag{2.1}$$

In general ϕ_{Ai} and ϕ_{Bi} could be sums of distinct shell-model configurations ϕ_{Aik} and ϕ_{Bik} centred at $\underset{\sim}{S}_1$ and $\underset{\sim}{S}_2$, respectively,

$$\phi_{Ai} = \sum_k a_k\, \phi_{Aik}(\underset{\sim}{x}_1 \cdots \underset{\sim}{x}_{Ai}, \underset{\sim}{S}_1), \quad \phi_{Bi} = \sum_k b_k\, \phi_{Bik}(\underset{\sim}{x}_{Ai+1} \cdots \underset{\sim}{x}_{A+B}, \underset{\sim}{S}_2) .$$

The generator coordinate basis (2.1) has a useful property that the spurious centre-of-mass motion is automatically eliminated for a large class of functions (2.1), namely those describing the system of approximately equal fragments and those channels which contain fragment wave functions ϕ_{Ai} and ϕ_{Bi} which can be described by configurations with no holes in the closed shell. With this restriction the function (2.1) can be written[2] in the form

$$\phi_{(AB)i}(\underset{\sim}{x}_1 \cdots \underset{\sim}{x}_{A+B}, \underset{\sim}{S}) = N(|\underset{\sim}{S}|)\phi_{CM}(\underset{\sim}{R}_{CM})\,\mathcal{A}\left[\exp\left(-\tfrac{1}{2}\beta_i(\underset{\sim}{r}_i - \underset{\sim}{S})^2\right) \phi_{Ai}(\xi_{Ai})\ \phi_{Bi}(\xi_{Bi})\right] \tag{2.1'}$$

In the following we shall restrict ourselves to this class of functions.

2.2. The explicit form of the trial functions

A GC wave function

$$\psi_i(\underset{\sim}{x}_1,\ldots\underset{\sim}{x}_{A+B}) = \int d^3\underset{\sim}{S}\; f_i(\underset{\sim}{S})\; \phi_{(AB)i}\;(\underset{\sim}{x}_1,\ldots\underset{\sim}{x}_{A+B},\underset{\sim}{S}) \qquad (2.4)$$

has to satisfy the boundary conditions (1.2) for $|\underset{\sim}{r}_i| \to \infty$. By introducing (2.1') into (2.4) and by comparing it to eq. (1.3) one gets the following equation for the GC amplitude $f_i^c(\underset{\sim}{S})$

$$\int d^3\underset{\sim}{S}\; \exp(-\tfrac{1}{2}\beta'(\underset{\sim}{r}_i - \underset{\sim}{S})^2)\; \begin{pmatrix} f^c_{i,\mathrm{reg}}(\underset{\sim}{S}) \\ f^c_{i,\mathrm{irr}}(\underset{\sim}{S}) \end{pmatrix} = \begin{pmatrix} F_i(\underset{\sim}{r}_i) \\ G_i^{\mathrm{reg}}(\underset{\sim}{r}_i) \end{pmatrix} \qquad (2.5)$$

$$|\underset{\sim}{r}_i| \to \infty$$

A convenient trial function with correct asymptotic behavior is

$$\begin{aligned}\psi^t_j &= \sum_p C_p\, \phi_{AB}(\underset{\sim}{x}_1,\ldots\underset{\sim}{x}_{A+B},\underset{\sim}{S}_p) + \int d^3\underset{\sim}{S}\; f^c_{j,\mathrm{reg}}(\underset{\sim}{S})\; \phi_{(AB)j}(\underset{\sim}{x}_1\ldots\underset{\sim}{x}_{A+B},\underset{\sim}{S}) \\ &+ \sum_i K^t_{ji}\; d^3\underset{\sim}{S}\; f^c_{i,\mathrm{irr}}(\underset{\sim}{S})\; \phi_{AB)i}(\underset{\sim}{x}_1,\ldots\underset{\sim}{x}_{A+B},\underset{\sim}{S}) \\ &= \sum_p C_p\, \phi_p + \mathfrak{F}_j + \sum_i K^t_{ji}\mathfrak{G}_i\end{aligned} \qquad (2.6)$$

The $|\underset{\sim}{S}_p|$ are chosen in the interval (0, $S_o \approx$ the sum of radii of fragments), so the sum $\sum_p C_p\phi_p$ is supposed to describe the compound system.

There were two open problems in connection with the trial function (2.6): (i) finding a satisfactory solution of the boundary condition problem (2.5) and (ii) projection of angular momentum eigenstates from a two-centre GC function.

2.3. Boundary condition problem

There were several attempts[3), 1.b)] to solve the integral equation (2.5), but all existing formulae are valid for rather large value of S only. This restricts their applicability because the sum in eq. (2.6) has to go then over large values of S_p .

As the wave function has to be regular at the origin, we regularize first the irregular Coulomb function (indicated in (2.5)), by a prescription[4)] based on the Lipmmann-Schwinger integral equation.

We proceed then in the following way:

(1) Using the semiclassical method we obtain the following expression for the GC amplitude

$$f_L(kS) = f_L(kS) + O(1/(kS)^3), \quad kS \to \infty$$

$$\tilde{f}_L(kS) = 4\pi^{1/2} \exp\left[k^2(1-2\eta/kS)/4\beta\right]\left[g_L(kS) - k^4\eta^2 g_L'(kS)/8\beta^2 k^2 S^2\right],$$

where g_L stays for both F_L and G_L^{reg} in eq. (2.5). This expression we used for $S > S_o$, S_o being chosen in such a way, that in the integral equation rewritten in the form

$$\int_o^{S_o} K(kr,kS)\, f_L(kS)\, d(kS) = g_L(kS) - \int_{S_o}^{\infty} K(kr,kS)\, \tilde{f}_L(kS)\, d(kS) + \delta g_L$$

the quantity δg_L satisfies $\max_{o \le r \le \infty} |\delta g_L| < \varepsilon$ for a small prescribed

(2) To get the solution for $S \le S_o$ we expand g in terms of Fourier-Bessel series and f in terms of a Dini series. The integral equation transforms into a system of ill-conditioned linear equations

$$\sum_{i=1}^{n} K_{ji}\, a_i = b_j + \delta b_j , \quad j = 1,2, \ldots m .$$

The method of statistical regularization[5] is used then to obtain the coefficients a_i. We assume that the unknown function $f_L(kS)$ is bounded in the mean as $\sum_{i=1}^{n} a_i^2 \leq \omega$ and we choose a Gaussian form for the a priory density distribution of probability for the solution a_i

$$P(\underset{\sim}{a}) = \text{const.} \exp\left(-\frac{n}{2\omega} \sum_{i=1}^{n} a_i^2\right)$$

If the assumption of boundness of $f_L^{(kS)}$ is correct, this procedure enables us to calculate any linear functional of the function $f_L(kS)$ as accurately as needed. For a test the GC amplitude for $^4He + ^6Li$ scattering is checked for energies between 0.1 MeV and 100 MeV using only few (ten) terms in Dini expansion. We obtained for all $0 \leq r < \infty$

$$\max \left| \sum_{0}^{\infty} K(kS,kS)\ f_L(kS)\ d(kS) - \varepsilon_L(kr) \right| < 10^{-3} \quad .$$

2.4. Projection of angular momentum eigenstates from the two-centre GC function

The trial function (2.6) has to be an eigen function of the angular momentum

$$\psi_{JM}(\underset{\sim}{X}) = \sum_{k K} \int d\underset{\sim}{S}\ f^{JM}_{K}(\underset{\sim}{S})\ \phi^{JM}_{K}(\underset{\sim}{X},\underset{\sim}{S}) \quad ,$$

$$\phi^{JM}_{K}(\underset{\sim}{X},\underset{\sim}{S}) = \frac{2J+1}{8\pi^2} \int d\Omega\, \mathcal{D}^{J}_{MK}(\Omega)^{*}\, R(\Omega)\, \phi_k(\underset{\sim}{X},\underset{\sim}{S}) \quad , \quad \underset{\sim}{X} = (\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots \underset{\sim}{x}_{A+B})$$

So the basic matrix elements in calculation of collisions and the structure is of the form

$$\begin{Bmatrix} H^{JM}_{k'K',kK}(\underset{\sim}{S}',\underset{\sim}{S}) \\ N^{JM}_{k'K',kK}(\underset{\sim}{S}',\underset{\sim}{S}) \end{Bmatrix} = \left\langle \phi_{k'}(\underset{\sim}{X},\underset{\sim}{S}') \middle| (P^{J}_{MK})^{+} \begin{Bmatrix} H \\ I \end{Bmatrix} P^{J}_{MK} \middle| \phi_k(\underset{\sim}{X},\underset{\sim}{S}) \right\rangle \quad (2.7)$$

We based our calculation on the following relation

$$R(\Omega)\,\phi\,(\underset{\sim}{x},\underset{\sim}{S}) = \sum_{k'} c_{k',k}(\Omega)\,\phi_{k'}(\underset{\sim}{x},\underset{\sim}{\tilde{S}}),\quad \underset{\sim}{\tilde{S}} = R(\Omega^{-1})\underset{\sim}{S} \qquad (2.8)$$

which expresses the effect of the rotation of coordinates $\underset{\sim}{x} = (\underset{\sim}{x}_1,\ldots\underset{\sim}{x}_{A+B})$ in terms of rotation of the GC coordinate $\underset{\sim}{S}$. The coefficients c are expressed in terms of the $\mathcal{D}$ functions. The index k' runs only over different configurations of valance nucleons in major shells of fragments.

By using the relation (2.8), the matrix elements (2.7) between projected wave functions can be expressed in terms of the unprojected functions, $\langle \phi_{k'}(\underset{\sim}{x},\underset{\sim}{S'}) \left\{ \begin{matrix} H \\ I \end{matrix} \right\} \phi_k(\underset{\sim}{x},\underset{\sim}{S}) \rangle$, as

$$\sum_{k''k'''}\sum_{\lambda\mu\mu''}\sum_{\lambda'\mu'\mu'''} Y_{\lambda'\mu'''}(\hat{\underset{\sim}{S}})\,\varphi^{J\lambda'}_{MK'k'''k'\mu'''\mu'} \begin{Bmatrix} H_{k''\lambda'\mu',k'''\lambda\mu}(S',S) \\ N_{k''\lambda'\mu',k'''\lambda\mu}(S',S) \end{Bmatrix} \varphi^{J\lambda}_{MKk''k\mu''\mu}\, Y_{\lambda\mu}(\hat{\underset{\sim}{S}})$$

with

$$\varphi^{J}_{MKk''k\mu''\mu} = \int d\Omega\, \mathcal{D}^{J}_{MK}(\Omega)^{*}\, c_{k''k}(\Omega)\, \mathcal{D}^{J}_{\mu''\mu}(\Omega).$$

All coefficients c and φ can be obtained in analytic form.

We use this projection method to calculate the eigen states of the "compound" system. This will enable us to distinguish contributions of particular states. Also approximate summations over complete sets which occur in reaction theory are reduced to a small number of terms.

M.Poljšak will show how we used this projection method to calculate molecule-like states of light nuclei.

3. KOHN-KATO VARIATIONAL METHOD FOR THE K MATRIX

3.1. The expression for the K matrix

The ceefficients C_p and K^t_{ji} in the trial function (2.6) are determined by using Kohn's variational principle

$$\langle \delta\psi_j | H - E | \psi_i^t \rangle = 0 \ .$$

This equation is equivalent to a system of $N_c(N_c + N_p)$ linear equations for $N_c.N_p$ unknown coefficients C_p and N_c^2, unknown matrix elements K_{ij}^t. This stationary solution ψ_i^t is used then to calculate Kato's approximate expression for the K matrix[6,2)]

$$K_{ji} \approx K_{ij}^t - \frac{1}{w}\langle \psi_j^t | H - E | \psi_i^t \rangle,$$ (w is a constant depending on the normalization)

By using the notation of eq. (2.6) and by introducing the following operator

$$\Delta = H - E - (H - E) \sum_{p'} \sum_{p} |\phi_{p'}\rangle\langle\phi_{p'}| H - E|\phi_p\rangle^{-1}\langle\phi_p|(H - E) \qquad (3.1)$$

one gets

$$K_{ji} = -\left[(\Delta_{\mathcal{F}\mathcal{F}})_{ij} - ((\Delta_{q\mathcal{F}}^T)(\Delta_{qq})^{-1}(\Delta_{q\mathcal{F}}))_{ij}\right]/w \qquad (3.2)$$

where

$$(\Delta_{\mathcal{F}\mathcal{F}})_{ij} = \langle \mathcal{F}_i | \Delta | \mathcal{F}_j \rangle \ , \text{ etc.}$$

There are two reasons for using a variational method for the K matrix: all variational coefficients C_p and K_{ij}^t are obtained from a system of linear equations and one can perform the numerical calculation with real quantities only.

3.2. Pseudochannels

In collisions of nuclei usually a large number of reaction channels is open. In measurements and theoretical calculations one limits oneself to few open channels. The effect of the neglected channels is usually compensated by introducing a phenomenological complex optical potential.

We were studing a different method for compensating for neglected open channels which consists in introducing one (or few) additional "pseudo" channel(s) defined by an average energy and a suitable description of channel fragments without modifying the Hamiltonian.

The indices in the expression (3.2) run over the "pseudo-channel" and the channels explicitely taken into account.

Some experience in choosing parameters of the "pseudo" channel is obtained from the calculations on soluble models[7]. There are indications that the results are less dependent on the energy of the "pseudo" channel, than on the parameters describing the fragments in the "pseudo" channels. This is convenient, because the time consuming calculation of the overlap integrals for different energies would be reduced.

4. THE CALCULATION OF TRANSITION AMPLITUDES $(\Delta_{ff})_{ij}$, $(\Delta_{fg})_{ij}$ AND $(\Delta_{gg})_{ij}$

A typical matrix element of the operator , eq. (3.1), in the expression for the K matrix (3.2) is of the form

$$(\Delta_{ff})_{ij} = \int d^3\underset{\sim}{S}' \int d^3\underset{\sim}{S}\; f^c_{i,reg}(\underset{\sim}{S}')\, \Lambda_{ij}(\underset{\sim}{S}',\underset{\sim}{S})\, f^c_{j,reg}(\underset{\sim}{S}) \,, \tag{4.1}$$

where

$$\Lambda_{i,j}(\underset{\sim}{S}',\underset{\sim}{S}) = \langle \phi_{(AB)i}(\underset{\sim}{x}_1,\ldots\underset{\sim}{x}_{A+B},\underset{\sim}{S}') | \Delta | \phi_{(AB)_j}(x_1,\ldots x_{A+B},S) \tag{4.2}$$

The crucial test for the usefulness of the theory is the effort and the computational time needed for calculation of the form factors (4.2) and the amplitudes (4.1). In this section I shall try to illustrate the difficulties and I shall explain two techniques we are using in order to simplify calculations.

4.1. Calculation of the form factor

By substituting the function (2.1) into (4.2) one gets for the form factor

$$\Lambda_{\pm}(\underset{\sim}{S}',\underset{\sim}{S}) = \sum_{k_1 k_1' k_2 k_2'} a_{k_1'} b_{k_2'} \langle \phi_{Ak_1'Bk_2'}(\underset{\sim}{x},\underset{\sim}{S}') | H - E | \phi_{Ak_1Bk_2}(\underset{\sim}{x},\underset{\sim}{S}) \rangle a_{k_1} a_{k_2}$$

$$- \sum_{pp'} \sum_{n} \sum_{k,k'} \frac{C_{nk'p}\, C_{nkp}}{E_n - E} \sum_{kk'} a_{k_1'} b_{k_2'} \langle \phi_{Ak_1'Bk_2'}(\underset{\sim}{x},\underset{\sim}{S}') | H - E |$$

$$\phi_{(AB)k'}(\underset{\sim}{x},\underset{\sim}{S}_{p'}) \rangle \langle \phi_{(AB)k'}(\underset{\sim}{x},\underset{\sim}{S}_{p'}) | H - E | \phi_{Ak_1Bk_2}(\underset{\sim}{x},\underset{\sim}{S}) \qquad (4.3)$$

where we have diagonalized the Hamiltonian in the basis of square integrable functions $\phi_{(AB)k}(x,S_p)$, i.e.

$$H|n\rangle = E_n|n\rangle \,, \quad |n\rangle = \sum_{kp} C_{nkp}\, \phi_{(AB)k}(\underset{\sim}{x},\underset{\sim}{S}_p) \qquad (4.3')$$

So the evaluation of $\Lambda_{\pm}(\underset{\sim}{S}',\underset{\sim}{S})$ involves only the calculation of matrix elements of (H - E) between Slater determinants $\phi_{(AB)k}(\underset{\sim}{x},\underset{\sim}{S})$. This looks like a straightforward job, but there is quite a large number of such matrix elements and each matrix elements has many terms. For illustration in the reaction $^4He + {}^3H \rightarrow (^4He + {}^3H) + (^6Li + n)$ there are 31 matrix expressions $\langle \phi_{(AB)k'}(\underset{\sim}{x},\underset{\sim}{S}') | H - E | \phi_{(AB)k}(\underset{\sim}{x},\underset{\sim}{S}) \rangle$ from which all the others can be obtained by simple permutations of the components of $\underset{\sim}{S}$ and $\underset{\sim}{S}'$. A typical element contains about 500 terms. A by hand calculation is practically impossible.

We learned to calculate analytic expressions for $\langle \phi_{(AB)k'}(\underset{\sim}{x},\underset{\sim}{S}') | H - E | \phi_{(AB)k}(\underset{\sim}{x},\underset{\sim}{S}) \rangle$ on the computer using the programs for symbolic algebra SCHOONSCHIP (on CDC computers) and REDUCE2 (on IBM computers). Both of these programs were developed for calculations in high energy physics, but we learned how to use them (especially SCHOONSCHIP) efficiently in our

many body calculations. As it looks now the calculation of these expressions will not be the major part of the total calculation. For illustration an expression for the part which corresponds to the potential energy of a Gaussian potential is shown on the side. The general structure of these elements is a sum of products of polinomials in S'_x S'_y S'_z S_x,S_y,S_z and exponential functions.

$$\sum_{\substack{N \\ l',m',n',l,m,n}} C^{k'k}_{N,l',m',n',l,m,n}\, S_x'^{l'}\, S_y'^{m'}\, S_z'^{n'}\, S_x^{l}\, S_y^{m}\, S_z^{n}$$

$$\exp(-\alpha^{k'k}_N S'^2 - \beta^{k'k}_N S^2 + \gamma^{k'k}_N S'S) \qquad (4.4)$$

In the numerical calculation which follows one stores and uses the coefficients $C^{k'k}_{N,l',m',n',l,m,n}$, $\alpha^{k'k}_n$, $\beta^{k'k}_n$, $\gamma^{k'k}_n$ and exponentials l',m',n',l,m,n.

4.2. Calculation of transition amplitudes

By inserting expressions of the form (4.4) into eq. (4.1) one gets for the transition amplitude the expression of the form

$$\Delta_{f_j f_i} = \sum_{m,\nu_j} [L',m',p_j\nu_j|j_f m_f]\, R_{\nu m}(\hat{k}_j) \cdot \sum_{m,\nu_i} [L,m,p_i\nu_i|j_i m_i]\, R(\hat{k}_i) \cdot$$

$$\cdot \Big\{ HE_{e',L',m',p_j\nu_j;\, e,L,m,p_i\nu_i} - \sum_{n_e} HP_{e',L',m',p_j\nu_j;\, n_e}\, HP_{n_e;\, e,L,m,p_i\nu_i} / (E_{n_e} - E) \Big\}$$

where

$$HE_{e',L',m',p_j\nu_j;\, e,L,m,p_i\nu_i} = \sum_{k'k} a^{k'p_j\nu_j}_{k'}\, a^{kp_i\nu_i}_{k} \sum_{N,l',m',n',l,m,n} C^{k'k}_{N,l',m',n',l,m,n} \sum_{\lambda} DR(\lambda,l',m',n',L',m',l,m,n,L,m)$$

$$\cdot \int_0^\infty ds'\, s'^{l'+m'+n'+2}\, e^{-\alpha_n s'^2} f_{j,L'}(s') \int_0^\infty ds\, s^{l+m+n+2}\, e^{-\beta_n s^2}\, i_\lambda(-\gamma_n s's)\, f_{i,L}(s)$$

and

$$HP_{n_e,s,L,\Pi',b_i,\nu_i} = \sum_{k'k} a^{d_i b_i \nu_i}_{k} \cdot \sum_{\substack{N \\ l',m',n',l,m,n}} C^{k'k}_{\mu,l',m',n',l,m,n} \sum_{\lambda} DR(\lambda,l',m',n',L',\Pi',l,m,n,L,\Pi) \cdot$$

$$\cdot \sum_{p} S'^{l'm'n'+lmn+2}_{p} \cdot e^{-d_n S'^2_p} f^{J\Pi\gamma}_{n_e,k',L',\Pi'}(S'_p) \int_0^a dS\, S^{l+m+n+2} \cdot e^{-\beta_\lambda S^2} i_\lambda(-\gamma_{\delta'} S'S) \cdot f^{c.}_{i,L}(S)$$

Functions DR . together with vector coupling coefficients take care of the angular momentum coupling; most of components of DR are common for all calculations and they could be efficiently prepared in advance. Calculation of two-dimensional integrals represents a problem: there are too many of them to be prepared in advance. We found, however, one can express them as a finite sum of products of one-dimensional integrals by expending the spherical Bessel function of the imaginary argument $i_\lambda(\gamma S'S)$ either in Taylor series or a series of products of associate Laguarre polynomials. Both series converge fast, for example the formula based on Taylor series provides an accuracy better than 10^{-8} with less than 10 terms. These fast converging factorizations of two-dimensional integrals reduce enormously the amount of numerical work in calculating transition amplitudes.

5. CONCLUSION

In this talk a report is given on the status of a microscopic theory for the analysis of reactions between light nuclei within the framework of the GCM using the Kohn-Kato variational principle. The variational trial function contains a sum of square integrable functions of the two-centre GCM

type and asymptotic channel functions. Having solved the problem of projection of eigenstates of angular momentum from two-centre GC functions which we use to describe the compound system and having found a better solution for the channel functions, we expect that this formalism could handle the internal region and the region which corresponds to the touching of fragments more appropriately than other microscopic methods. This formalism is also consistent in the sense that all quantities entering the expression for the transition operator are calculated using the same effective Hamiltonian. The only input parameters are those which describe the effective two-body interaction which for the sake of consistency, have to be chosen so as to predict the structure of the fragments in the channel as well as the states of the combined system. (The details of the structure of nuclei appear in the form factor $\Lambda(\underset{\sim}{s}',\underset{\sim}{s})$, eq. 4.3, through the configuration mixing coefficients a_k, b_k (eq. (2.1))as well as through the coefficients C_{nqp} describing the combined system and the corresponding energies E_n, eq. (4.3').) Finally, the proposed formalism has an advantage from the computational standpoint: we work everywhere, in the reaction and in the channel region, with the same basis so that we have to calculate one type of matrix elements only. This might give us the chance to handle some reactions which are more complicated than those treated microscopically till now.

There are several open problems, the most of them beeing common to all other microscopic methods. The most difficult is the problem of choosing the effective two body force which describes both the structure of colliding fragments and the reaction cross section. Many potentials provide often proper binding energy of the fragments, but the scattering cross sections are different. This is illustrated in Fig. 1. The situation is even worse when the same effective force cannot describe the structure of both fragments. Microscopic calculations are lengthly so that approaching the problem by trying different forces would not be very useful.

The second open problem is related to the description of fragments in a truncated shell model space. (The first problem is related to this one). In a space spanned by a small number of functions often one adjusts the oscillator parameter in order to get the lowest ground state energy. For unequal nuclei this leads to different oscillator lengths of colliding fragments. In the proposed formalism we used an average value of these two oscillator length and in addition we allow no configurations with holes in the closed shells. In this way problems of spurious centre-of-mass motion are avoided, it is easier to calculate matrix elements and to introduce the scattering boundary conditions. The formalism can be extended to avoid the restriction of frosen cores. Instead of eq. (2.5) for the generator coordinate amplitude f one gets a system of integral equations. This extension is important for describing channels where a fragment is excited to a state of opposite parity.

Till now this formalism has been applied[9] to elastic scattering $^4He + ^4He$ and to the calculation of molecule - like states[6] of ^7Li using a wave function which is a superposition of cluster configurations of $(^4He + ^3H)$ and $(^6Li + n)$. This states we need as intermediate states in the calculation of the reaction $(^4He + ^3H) \rightarrow (^4He + ^3H) + (^6Li + n)$, which is in progress. In this reaction and in the reaction $^6Li + ^4He$ (elastic and inelastic scattering) which is also in progress, we are including all configurations of ^6Li in the p-shell. In all these calculations we are using the nuclear two-body potential and the Coulomb interaction represented by a sum of Gaussian two-body potentials.

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Dr. R.Beck and Dr. M.A.Nagarajan are working together with us on the reactions $^3H + H$ and $^6Li + He$. Many analyses contained in this talk arose out of numerous discussions with them.

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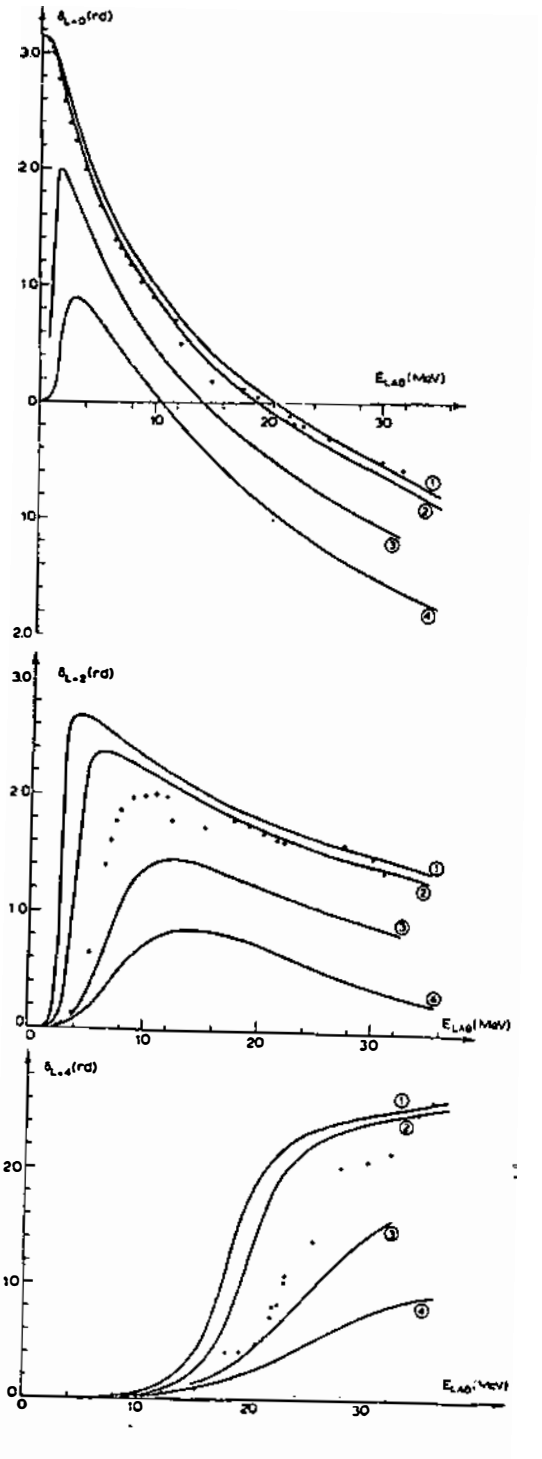

Fig. 1.

The phase shifts for the elastic scattering $^4He + {}^4He$. The curves 1, 2 and 3 are obtained with the Volkov potential V2, the Volkov potential V1 and the Brink-Boeker potential B1, respectively.

DISCUSSION

M. Kamimura: Your methods for deriving the exchange kernel and for solving the rearrangement collision are quite interesting to me, since I am also attacking the problem based on 3-Cluster RGM. In such a rearrangement collision it would be interesting to examine the role of exchange effect due to Coulomb interaction as well as due to nuclear interaction. But usually the calculation of Coulomb exchange kernel is much more difficult than that of nuclear exchange kernel. Then I would like to know how this problem is treated in your work.

M.V. Mihailović: For smaller systems (as $\alpha+\alpha$) we expressed the Coulomb force as a superposition of Gaussian potentials

$$V^C(r_{ij}) = e^2/(2\, r_{ij}) = e^2/\sqrt{\pi}) \int_0^\infty dt \exp(-t^2 r_{ij}^2)$$

After calculating the matrix element for a Gaussian potential we then integrate over the dummy variable t.

In recent calculations we are approximating the integral in the above expression with a sum of six Gaussian functions. Coefficients and ranges of Gaussian functions are chosen to represent as good as possible the Coulomb potential in the region $r_{ij} \sim$ (sum of radii of fragments).

R.J. Philpott: You mentioned that you were using the Kohn--Hulthen variational method. I just wanted to say, as pointed out by Schmid and co-workers, that the Kohn-Hulthen method does not converge very well. Improved convergence can be obtained from the same matrix elements using the techniques described by Schmid and Schwager (see ref. 42 of my talk).

M.V. Mihailović: We are aware of that problem.

A. Tohsaki-Suzuki: May you teach me a few details on "Schoonschip"? Is this code used for the nuclear collision problem only?

M.V. Mihailović: "Schoonschip" is a program for symbolic evaluation of algebraic expressions. The program is also capable

of performing several elaborate substitutions. It is developed by people at CERN for calculation in high energy physics. For calculations of nuclear collisions efficient manupilations with matrices are necessary.