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by

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ON THE SCATTERING OF HEAVY IONS AT LOW ENERGY IN THE FRAME WORK OF MOLECULAR ORBITALS *

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ABSTRACT

In this paper we give a generalization of the model of nuclear reactions proposed by W. Von Oertzen in the framework of molecular orbitals. The different equations leading to the cross section are derived and discussed. It turns out that the helicity scheme is the most appropriate one.

Some emphasis is given to reactions including elastic scattering and elastic transfer for which this approach is well suited.

We discuss both the unadiabatic and Coriolis coupling terms which appear in the equations, and we show how these terms are partly calcelled if one takes into account one part of the recoil effect.

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1. INTRODUCTION

Many new experimental data on heavy ion scattering have been obtained recently and among those, we are specially interested in elastic and inelastic scattering, transfer of one nucleon or hole, of nuclei which may be described with an inert core surrounded with valence nucleons.

What we call a core in these reactions may be understood qualitatively in the following way:

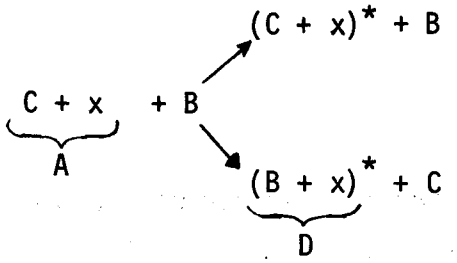
If we describe each nucleus by its central average potential, the scattering process may be analysed in terms of a two-center-nuclear shell model in which the distance between the two centers is approximately the separation between the two colliding nuclei. Due mainly to the coulomb repulsion and to absorption the reaction is generally peripheral [1]; this means that only the nucleons sitting near the surface of each nuclei will be involved in the process and that the relative distance of approach R of the two nuclei is bounded by a minimum value R_{min}. For this closest distance of approach the potential wells are as shown on fig. 1.

For the lower shells, the probability of tunneling of the nucleons from one nucleus to the other one is very small. They are therefore assumed to be not perturbed in the collision process. These shells, which are closed shells, form the cores. The other shells, generally the upper shells, in which the nucleons or holes can move from one nucleus to the other one are called the valence shells. The composition of the cores depend on the energy of the scattering.

In this model, we shall assume that the antisymmetrization between one nucleon belonging to one core and the other ones belonging to the other core

may be neglected, except if the cores are identical. In that case a new symmetry which corresponds to the exchange of the cores occurs.

In this paper, we shall restrict ourselves to the analysis of the reactions in which one of the interacting nuclei is described in terms of a core plus a valence nucleon (or cluster) x, the other one being a bare core. Such reactions may be written as



(1-a) (elastic or inelastic scattering)

(1-b) (transfer of the particule x)

where the star indicates that an excited state may be reached.

In general, both channels are present. They are very often calculated by different methods: optical potential analysis, diffractionnal methods, Glauber theory, etc. ... for the elastic channel, mainly DWBA for inelastic and transfer channels. However, these channels may be strongly coupled and it is important to consider them on the same footing. Furthermore, if the cores B and C are identical, the two channels defined in expressions (1-a) and (1-b) become indiscernable and interfer. This feature has been shown in several experiments, such as $C^{12} + C^{13}$ [2, 3], $Si^{28} + Si^{29}$ [4] and $F^{19} + O^{18}$ [5] in which the oscillations observed in the angular distribution are not of the diffractive type. It is interesting therefore, to all these respects to have a model which includes these physical situations.

A first approach may be to consider the complete antisymmetrization between all the nucleons. This has been done for light nuclei by the groups of K.

Wildermuth [6], H. Hackenbroich [7]. Works are in progress for heavier nuclei in which only a part of the antisymmetrization is taken into account as discussed above [8].

A second approach may be borrowed to molecular physics for low energy reactions [9]. In this case, one part of the antisymmetrization is simulated phenomenologically while the exchange of the transferred particle x between the two cores is taken into account more correctly. This mechanism has been discussed recently both from an experimental and a theoretical aspect by W. Von Oertzen et al [3, 10], J. Y. Park et al [11] and two of us [12].

The qualitative idea is the following. When the two nuclei A and B approach each other slowly, the field of the core B distorts the wave function of the motion of x around the core C to which it is bounded. This distortion is such that the particle x may be trapped in the field of B. In that situation x moves around both cores B and C faster than the cores themselves in their mutual approach. This adiabatic description of the process is very similar to what occurs in molecular physics so that an analysis in terms of nuclear molecular orbitals seems very well suited. In the asymptotic states both the elastic (or inelastic) and the transfer channel may be reached according as whether the particle x moves around the core C or the core B in the final state, as it is shown schematically on fig. 2.

According to this mechanism, the particle x can perform several revolutions around the two cores before it "chooses" to stay either with C or with B; this is a multistep process, in the meaning that x is exchanged several times between B and C. Contrarywise if the relative velocity of the two cores is large with respect to the orbital velocity of x, then the wave function of the nuclei involved will just be distorted weakly leading to a one step transfer process well described by the DWBA.

This argument does not mean, indeed, that the DWBA may not be well appropriated for low energy scattering, since the validity of the DWBA is roughly related to the ratio of the exchange to the core-core potentials. If this ratio allows a treatment of the exchange potential to first order only, one expects that both methods will lead to equivalent results, as it has been shown in simple situations by G. Baur and C. K. Gelbke [13]. In fact, the reactions discussed in ref. 2, 4 have been also successfully analysed with the DWBA [13, 14].

It is therefore interesting to extend the model which has been put forward by W. Von Oertzen [3] to situations in which the nuclei may be excited to compare it with the DWBA and to look for possible "nuclear molecules".

Due to axial symmetry around the axes joining the two cores, it will be very usefull to introduce an intrinsic frame of reference bounded to B and C. As it happens in the unified model [15] of deformed nuclei, the total spin projection on this axis of symmetry is a good quantum number (except for the Coriolis effect). Since this axis becomes parallel to the relative momentum of the two cores in the asymptotic final state it will be very convenient to work in the helicity scheme.

This model will look like an extension to scattering problems of the unified model of Bohr and Mottelson for bound states, the intrinsic wave function describing strongly deformed nuclei with a two center potential. Indeed the so called vibration coupling terms will be here very important and will lead to unadiabatic effects. Furthermore, microscopic descriptions of this situation may be undertaken as it has been done for instance by W. Von Oertzen and N. Norenberg [10]. We shall not discuss this microscopic approach at all.

In the next section we shall recall our notations and sketch the general ideas of the model. In section 3, we shall discuss the relative motion of the two cores and section 4 will be devoted to the analysis of the coupling terms, mainly the kinetic energy coupling and the Coriolis coupling. In this last section; we shall recall some properties of the molecular orbitals and derive simple approximations to illustrate our discussion.

2. DESCRIPTION OF THE MODEL

2.1 - GENERAL CONSIDERATIONS

To simplify the presentation of our model, we shall neglect the antisymmetrization between the nucleons of the core and those of the cluster x and furthermore, to reduce the algebra, we shall assume that only one parentage is important.

Let $|\psi>$ be the wave function describing the scattering state corresponding to the reaction $A + B \nearrow^{A + B}_{C + D} \searrow$, where $A = C + x$ and $D = B + x$. We look for a solution of the Schrodinger equation

$$H|\psi> = (\Sigma_i \frac{-\Delta_i}{2m_i} + \Sigma_{i<j} V_{ij})|\psi> = E|\psi> \qquad (2.1)$$

which may be written as

$$|\psi> = \sum_{S_f M_f} \chi^{S_f M_f}_{AB}(\underset{\sim}{R}_{AB})|J_A\ J_B;\ S_f\ M_f> + \chi^{S_f M_f}_{DC}(\underset{\sim}{R}_{DC})|J_D\ J_C;\ S_f\ M_f> \qquad (2.2)$$

with the boundary conditions

$$|\psi> \xrightarrow[R_{AB} \to \infty]{} e^{i\underset{\sim}{K}_i \cdot \underset{\sim}{R}_{AB}}|J_A\ J_B;\ S_i\ M_i> + \sum_{S_f\ M_f\ J'_A} \frac{e^{iK_f\ R_{AB}}}{R_{AB}} x \qquad (2.3)$$

$$f^{S_f\ S_i\ J_A}_{M_f\ M_i\ J'_A}\ |J'_A\ J_B;\ S_f\ M_f>$$

or

$$|\psi> \xrightarrow[R_{CD}\to\infty]{} \sum_{S_f\ M_f\ J'_D} \frac{e^{ik'_f R_{DC}}}{R_{DC}}\ g^{S_f\ S_i\ J_D}_{M_f\ M_i\ J'_D}\ |J'_D\ J_C;\ S_f\ M_f> \qquad (2.4)$$

Since we have neglected exchange effects, we can label the nucleons of each core and write

$$H = H_C + H_B + H_x - \frac{\Delta_{rCx}}{2m_{Cx}} - \frac{\Delta_{RAB}}{2m_{AB}} + \Sigma_{i\epsilon C\ j\epsilon B} V_{ij} + \Sigma_{i\epsilon C\ j\epsilon x} V_{ij} + \Sigma_{i\epsilon B\ j\epsilon x} V_{ij} + \Sigma_{i\epsilon B\ j\epsilon x} V_{ij} \qquad (2.5)$$

where $H_{B(C,x)}$ describes the internal motion in each core. For instance, we have

$$H_B = -\Sigma_{i\epsilon B} \frac{\Delta_i}{2m_i} + \Sigma_{i<j,\ i\epsilon B\ j\epsilon B} V_{ij} \qquad (2.6)$$

i.e.

$$H_B\ |\underline{\psi}_B^{j_B,\ m_B}(\underline{\rho}_B)> = \underline{\varepsilon}_B^{j_B}\ |\underline{\psi}_B^{j_B,\ m_B}(\underline{\rho}_B)> \qquad (2.7)$$

where $\underline{\varepsilon}_B^{j_B}$ is the binding energy and $|\underline{\psi}_B^{j_B,\ m_B}(\underline{\rho}_B)>$ the internal wave-function of the core B, and so on for H_C and H_x. Multiplying eq. (2.1) by the complex conjugate of the spacial part $\underline{\psi}_B$, $\underline{\psi}_C$, $\underline{\psi}_x$ of the wave function of the cores B, C, x and integrating over all internal spacial coordinates we are led to

$$0 = -\frac{\Delta r_{Cx}}{2m_{Cx}} - \frac{\Delta_{RAB}}{2m_{AB}} + \tilde{V}_{CB}(R_{CB}) + \tilde{V}_{Cx}(r_{Cx}) + \tilde{V}_{Bx}(r_{Bx}) + \varepsilon_C + \varepsilon_B + \varepsilon_x - E)|\phi> \qquad (2.8)$$

where

$$|\phi> = \int \pi_i\ d\rho_{iB}\ \pi_j\ d\rho_{jC}\ \pi_k\ d\rho_{kx}\ \psi(\rho_{iB})\ \psi(\rho_{iC})\ \psi_x(\rho_{ix})|\psi> \qquad (2.9)$$

and

$$\tilde{V}_{\alpha\beta} = \langle \psi_C \, \psi_B \, \psi_x \, | \sum_{\substack{i\in\alpha \\ j\in\beta}} V_{ij} \, (\underset{\sim}{R}_{\alpha\beta} + (\underset{\sim}{\rho}_i - \underset{\sim}{\rho}_j) | \psi_C \, \psi_B \, \psi_x \rangle \tag{2.10}$$

We note that $\tilde{V}_{\alpha\beta}$ is a local potential. Would have we included exchange effects, all the potentials in eq. (2.8) would have become non local. However, as said above, these exchange effects are small because of the peripheral character of our process. Nevertheless they may be simulated if one thinks that the potentials $\tilde{V}$ introduced in eq. (2.8) are equivalent to the non local ones and are therefore energy dependent. Furthermore, there is no coupling equations b because we neglected core excitations. In our model, it turns out that the functions $\phi_{\ell,j}(\underset{\sim}{r}_{Cx})$ describing the relative motion of the cores C and the cluster x are solutions of the reduced equation

$$-\frac{\Delta_{rCx}}{2m_{Cx}} + \tilde{V}_{Cx}\,(\underset{\sim}{r}_{Cx}) \;\; \phi_{\ell C,jx}\,(\underset{\sim}{r}_{Cx}) = (\varepsilon_A - \varepsilon_C - \varepsilon_x)_{jx} \;\; \phi_{\ell C,jx}(\underset{\sim}{r}_{Cx}) \tag{2.11}$$

In writing eq. (2.8), we have made an arbitrary choice of independent variables; this choice is not unique and we can as well choose the sets $(\underset{\sim}{r}_{Bx}, \underset{\sim}{R}_{CD})$ or $(\underset{\sim}{r}, \underset{\sim}{R})$ which are shown on fig. 3. The transformation of eq. (2.8) obtained with these new variables is straightforward since

$$-\frac{\Delta_{rCx}}{2m_{Cx}} - \frac{\Delta_{RAB}}{2m_{AB}} = -\frac{\Delta r_{Bx}}{2m_{Bx}} - \frac{\Delta R_{CD}}{2m_{CD}} = -\frac{\Delta r}{2m} - \frac{\Delta R}{2M} \tag{2.12a}$$

where

$$m_{\alpha\beta} = \frac{m_\alpha \; m_\beta}{m_\alpha + m_\beta}\,, \quad m = \frac{m_x(m_B + m_C)}{m_B + m_C + m_x}\,, \quad M = \frac{m_B \; m_C}{m_B + m_C}$$

The different relations between these variables are easily derived. We have

$$\underset{\sim}{r} + \frac{m_{BC}}{m_B}\underset{\sim}{R} = \underset{\sim}{r}_{Bx}$$

$$\underset{\sim}{r} - \frac{m_{BC}}{m_C}\underset{\sim}{R} = \underset{\sim}{r}_{Cx}$$

$$\frac{m_{Cx}}{m_C}\underset{\sim}{r} + \frac{m_{BC}}{m_{AB}}\underset{\sim}{R} = \underset{\sim}{R}_{AB} \qquad (2.12\text{-b})$$

$$\frac{m_{Cx}}{m_B}\underset{\sim}{r} - \frac{m_{BC}}{m_{CD}}\underset{\sim}{R} = \underset{\sim}{R}_{CD}$$

Since the potentials in eq. (2.8) have the cylindrical symmetry around the axis joining the two cores B and C, it is interesting to introduce explicitely the variables $\underset{\sim}{R}$ and $\underset{\sim}{r}$ in the equation and to solve the problem with these variables.

To summarize, assuming that nuclei are described by one parentage only, that there are no core excitation, that the exchange of nucleons belonging to two different cores may be neglected or simulated, our problem reduces in solving eq. (2.8), written with the variables $\underset{\sim}{r}$ and $\underset{\sim}{R}$, with the following boundary conditions

$$|\Phi\rangle \xrightarrow[R\to\infty]{} \sum_{\alpha'\beta}\left\{\Phi^{S_f}_{\alpha'}{}^{M_f}(\underset{\sim}{r}_{Cx})\exp\frac{i\,K_f\,m_{Cx}\,\underset{\sim}{r}\cdot\underset{\sim}{R}}{m_C\,R}\left[\exp\frac{i\,m_{BC}\,\underset{\sim}{K}\cdot\underset{\sim}{R}}{m_{AB}}\right.\right.\delta_{if}$$

$$\left.\left. + \frac{1}{R}\exp\left(\frac{i\,K_f\,m_{BC}\,R}{m_{AB}}\right) f_{S_iS_f} + \Phi^{S_fM_f}_{\beta}(\underset{\sim}{r}_{Bx}) \times \frac{1}{R}\exp\left(iK_f\frac{m_{Bx}}{m_C\,R}\underset{\sim}{r}\,\underset{\sim}{R} + \frac{m_{BC}}{m_{CD}}\right)\right] g_{S_iS_f}\right\} \qquad (2.13)$$

where

$$\Phi^{SM}_{\alpha'}(\underset{\sim}{r}_{Cx}) = \sum_{j_x\,\ell}\left\{\left\{\left\{\left\{\phi^{\alpha}_{\ell}(r_{Cx})\,|\beta\mu\rangle\right\}^{m_x}_{j_x}\;|J_C\;m_C\rangle\right\}^{m_A}_{J_A}\;|J_B\;m_B\rangle\right\}^{M}_{S} \qquad (2.14)$$

or

$$\Phi^{SM}_{\alpha' J_A J_B}(\underset{\sim}{r}_{Cx}) = \sum_{\substack{J_{BC}\ J_x \\ M_{BC}\ m_x}} \begin{pmatrix} J_{BC} & J_x \\ M_{BC} & m_x \end{pmatrix} \begin{vmatrix} S \\ M \end{pmatrix} \Phi^{J_{BC},\ J_x}_{\alpha'\ J_A,\ J_B} \tag{2.15}$$

where

$$\Phi^{J_{BC},\ J_C}_{\alpha' J_B\ J_C\ J_A\ J_B} = \sum_{\ell} (-)^{J_x + J_{BC} + J_B + J_A} \hat{J}_{BC}\, \hat{J}_A \left\{ \begin{matrix} J_C & J_B & J_{BC} \\ J_{AB} & J_x & J_A \end{matrix} \right\} \Phi^{\alpha'}_{\ell}(r_{Cx}) |s\mu> \Big\}^{m_x}_{J_x} \tag{2.16}$$

$$\cdot\ |J_C\ J_B;\ J_{BC}\ M_{BC}>$$

The index α stands for all the quantum numbers necessary to caracterize the state. The phase which appears in expression (2.13) corresponds to one part of the recoil effect.

2.2 - INTRINSIC-WAVE-FUNCTION

Since we restricted ourselves to the situation in which the relative motion of the cores B and C is very slow compared with the orbital motion of x, we look for the solutions of eq. (2.8) which can be projected on the wave functions corresponding to fixed values of R. These functions may be written

$$|\Phi> = \sum_n \chi_n(\underset{\sim}{R})\ |\Phi_n(\underset{\sim}{r}, \underset{\sim}{R})> \tag{2.17}$$

where $|\Phi_n(\underset{\sim}{r}, \underset{\sim}{R})>$ are solutions of eq. (2.8) corresponding to fixed values of $\underset{\sim}{R}$.

As it is done in molecular physics, in order to make explicitely apparent the different symmetries which may occur, we introduce a moving frame of reference as sketched on fig. 4.

The Euler angles defining this moving frame are $(\alpha,\beta,0)$ where α and β are the angles defining the position of $\underset{\sim}{R} = \underset{\sim}{R}_C - \underset{\sim}{R}_B$ in the laboratory fixed frame of reference, see fig. 4a. In the moving frame, see fig. 4b, $\underset{\sim}{r}$ is defined by

the spherical coordinates (r, Θ, ϕ). Since the three vectors $\underset{\sim}{r}$, $\underset{\sim}{r}_{Bx}$ and $\underset{\sim}{r}_{Cx}$ are in the same "vertical" plane, they are defined with the same ϕ angle.

In this moving frame these functions $|\Phi_n(\underset{\sim}{r}, R)>$ are solutions of

$$\mathcal{H}_e|\Phi_n^{\Lambda}(r, R)> = E_n^{\Lambda}(R)|\Phi_n^{\Lambda}(\underset{\sim}{r}, R)> \tag{2.18}$$

$$\Sigma_\zeta|\Phi_n^{\Lambda}(\underset{\sim}{r}, R)> = \Lambda|\Phi_n^{\Lambda}(\underset{\sim}{r}, R)> \tag{2.19}$$

where

$$\mathcal{H}_e = -\frac{\Delta_r}{2m} + \tilde{V}_{Cx} + \tilde{V}_{Bx} \tag{2.20}$$

Σ_ζ is the projection of $\underset{\sim}{\Sigma}$ on the ζ axis of the moving frame, and $\underset{\sim}{\Sigma} = \underset{\sim}{j}_B + \underset{\sim}{j}_C + \underset{\sim}{\ell} + \underset{\sim}{s}_x$, $\underset{\sim}{\ell}$ being the angular momentum associated to the variable $\underset{\sim}{r}$. The energy $E_n^{\Lambda}(R)$ is the molecular exchange potential. In this moving frame, it is only a function of R. Eq. (2.19) holds because it is easy to check that

$$\left[\mathcal{H}_e, \Sigma_\zeta\right] = 0 \tag{2.21}$$

If furthermore the cores B and C are identical, the molecule has a center of symmetry. In that case, the parity which changes $\underset{\sim}{r} \to -\underset{\sim}{r}$ commutes with $\mathcal{H}_e$. We can label the wave functions with an index p such that

$$\pi|\Phi_{n,p}^{\Lambda}(\underset{\sim}{r}, R)> = |\Phi_{n,p}^{\Lambda}(-\underset{\sim}{r}, R)> = (-1)^p\ |\Phi_{n,p}^{\Lambda}(\underset{\sim}{r}, R)> \tag{2.22}$$

These wave functions are the intrinsic wave functions. They must satisfy the following boundary conditions:

$$|\Phi_{n\bar{s}}^{\Lambda}(\underset{\sim}{r}, R)> \xrightarrow[r \to \infty,\ R \text{ fixed}]{} 0 \tag{2.23}$$

$$|\Phi_{n\bar{s}}^{\Lambda}(\underset{\sim}{r}, R)> \xrightarrow[R \to \infty,\ r_{Cx} \text{ fixed}]{} |\Phi_{s,\alpha}^{\Lambda}(\underset{\sim}{r}_{Cx})> \tag{2.24}$$

$$|\Phi_{n\bar{s}}^{\Lambda}(\underset{\sim}{r}, R)> \xrightarrow[R \to \infty\ r_{Bx} \text{ fixed}]{} |\Phi_{s,\alpha}^{\Lambda}(\underset{\sim}{r}_{Bx})> \tag{2.25}$$

where $|\Phi^{\Lambda}_{S,\alpha}(\underset{\sim}{r})>$ is the function (2.14) expressed in the moving frame. The index S labels the total spin of these asymptotic nuclear states, i.e. for instance

$$S^2|\Phi^{\Lambda}_{S,\alpha}(\underset{\sim}{r}_{Cx})> = S(S+1)|\Phi^{\Lambda}_{S,\alpha}(\underset{\sim}{r}_{Cx})> \tag{2.26}$$

where $\underset{\sim}{S} = \underset{\sim}{J}_B + \underset{\sim}{J}_C + \underset{\sim}{s}_x + \underset{\sim}{\ell}_{Cx}$, where $\underset{\sim}{\ell}_{Cx} = \underset{\sim}{r}_{Cx} \wedge \underset{\sim}{P}_{Cx}$. The index Λ is not changed in the asymptotic state because it is easy to check that

$$\Sigma_\zeta = S_\zeta \tag{2.27}$$

For each value of R, these intrinsic wave functions are orthonormalized according to

$$\int \underset{\sim}{dr} < \Phi^{\Lambda}_{n}(\underset{\sim}{r}, R) \; |\Phi^{\Lambda}_{n'}(\underset{\sim}{r}, R)> = \delta_{\Lambda\Lambda'}\, \delta_{nn'} \tag{2.28}$$

We notice that these intrinsic wave functions are not eigenstates of Σ^2 but that only their asymptotic expressions are eigenstates of S^2. This is the reason for which we introduced the label $\bar{S}$.

In order to simplify the writing, the index n will stand throughout the paper (except when necessary as in eq. (3.28) for instance) for $(n, \bar{s})$. These intrinsic states depend explicitly only on the modulus of $\underset{\sim}{R}$. They indeed depend implicitly on the angles defining $\underset{\sim}{R}$ because the frame in which they are represented depends on these angles, as it is discussed in section 3.1 and the appendix.

We want to mention a difficulty due to specific choice of intrinsic wave which we have made in eq. (2.18). When $R \to \infty$ with r_{Cx}(or r_{Bx}) fixed and from expressions (2.12), eq. (2.18) reduces to (R is fixed):

$$\left(-\frac{\Delta r_{Cx}}{2m} + \tilde{V}_{Cx} \right) \; |\Phi^{\Lambda}_{n}(\underset{\sim}{r}, \infty)> = E^{\Lambda}_{n}(\infty) \; |\Phi^{\Lambda}_{n}(\underset{\sim}{r}, \infty)> \tag{2.29}$$

However, the equation which leads to the asymptotic expressions $|\Phi^{\Lambda}_{S,\alpha}(\underset{\sim}{r}_{Cx})>$

is eq. (2.11) which is different from eq. (2.29). This would mean that

i) $E_n^{\Lambda}(\infty)$ is different from $(\varepsilon_A - \varepsilon_C - \varepsilon_x)$

ii) $|\Phi_n^{\Lambda}(\underset{\sim}{r}, \infty)>$ does not fulfill the condition (2.24, 25).

Nevertheless it is shown in section 4.4 that in the LCNO approximation one can use a new basis in which this problem does not occur.

Eq. (2.18) describes nothing but a strongly deformed nucleus whose average potential is a two center potential, with a continuous deformation parameter R. Such a problem has been solved many times in nuclear physics, either using an exact solution for harmonic potentials [16], or a more sophisticated Hartree-Fock procedure [17] or even using the JWKB approximation [18].

In this paper, we shall not look for exact solutions of eq. (2.18), but for rather simple approximate forms which will allow us to discuss in a simpler form the different coupling terms.

In order to fulfill the boundary conditions, we shall look for a solution which is a linear combination of nuclear orbitals (LCNO) as it has been first proposed by G. Breit [19]. Such a solution will be accurate in our problem, because we expect that the cores of the colliding nuclei will stay apart from each other, as we discussed it in the introduction, and G. Reidmeister [17] has shown that the LCNO is a good approximation of the exact solution in the asymptotic region. We set:

$$|\Phi_n^{\Lambda}(\underset{\sim}{r}, R)> = \sum_{S\geq\Lambda} \left(\sum_{\alpha} C_{\alpha n}^{S\Lambda}(R) \, |\Phi_{\alpha}^{S\Lambda}(\underset{\sim}{r}_{Cx})> + \sum_{\beta} C_{\beta n}^{S\Lambda}(R) |\Phi_{\beta}^{S\Lambda}(\underset{\sim}{r}_{Bx})> \right) \qquad (2.30a)$$

where R is a fixed quantity and $C_{\alpha,n}^{S\Lambda}(R)$ and $C_{\beta,n}^{S\Lambda}(R)$ are parameters; α and β are indices which specify the states of the nuclei $A_{(C + x)}$ or $D_{(B + x)}$ and n specifies other quantum number necessary to define the intrinsic wave function.

The functions $|\Phi_\alpha^{S\Lambda}(\underset{\sim}{r}_{Cx})>$ and $|\Phi_\beta^{S\Lambda}(\underset{\sim}{r}_{Bx})>$ are given by expression (2.14) or expression (2.15).

If the two cores are identical, the wave function $|\Phi_n^{\Lambda}(\underset{\sim}{r}, R)>$ must furthermore fulfill the condition (2.22). Since in that case $\underset{\sim}{r}_{Cx} = \underset{\sim}{r} - \frac{\underset{\sim}{R}}{2}$, $\underset{\sim}{r}_{Bx} = \underset{\sim}{r} + \frac{\underset{\sim}{R}}{2}$, it turns out that changing $\underset{\sim}{r} \to -\underset{\sim}{r}$ induces the transformation $\underset{\sim}{r}_{Cx} \leftrightarrow -\underset{\sim}{r}_{Bx}$. It is easy to show therefore that the combination

$$|\Phi_n^{\Lambda p}(\underset{\sim}{r}, R)> = \sum_{S\geq\Lambda} \sum_{\alpha} C_{\alpha n}^{S\Lambda}(R) \frac{(|\Phi_\alpha^{S,\Lambda}(\underset{\sim}{r}_{Cx})> + (-)^{p-\pi}|\Phi_\alpha^{S}(\underset{\sim}{r}_{Bx})>)}{\sqrt{2}} \qquad (2.30b)$$

satisfies the required condition if π is the parity of the nuclear state, i.e.

$$|\Phi_\alpha^{S\Lambda}(-\underset{\sim}{r}_{Cx})> = (-1)^{\pi} |\Phi_\alpha^{S\Lambda}(\underset{\sim}{r}_{Cx})>$$

Inserting expression (2.30) into eq. (2.18) and using the Ritz variational principle we obtain very easily [20] the solutions which we are looking for. W. Von Oertzen and al. [3, 10] have given some general properties of these wave functions in simple situations and we refer to their papers. In section 4 we shall give some examples of this procedure and shall recall some properties of these intrinsic wave functions.

2.3 - THE RELATIVE MOTION WAVE FUNCTION

Once we have solved eq. (2.18) with the proper boundary conditions, we look for solutions of eq. (2.8) expanded on the intrinsic wave functions

$$|\psi(\underset{\sim}{R}, \underset{\sim}{r})> = \sum_{\Lambda n} \chi_n^{\Lambda}(\underset{\sim}{R}) |\Phi_n^{\Lambda}(R, \underset{\sim}{r})> , \qquad (2.31)$$

$\chi_n^{\Lambda}(\underset{\sim}{R})$ describing the relative motion of the two cores in the fixed frame of reference. The index n includes all necessary quantum numbers to specify the

state. particularly J_{BC}, the spin state of the two cores B and C as it is seen in expression (2.16).

Inserting expression (2.31) into eq. (2.8) and performing the scalar product on the variable $\underset{\sim}{r}$ one obtains, after taking into account the transformation (2.12)

$$\left[-\frac{\Delta_R}{2M} - (E - \varepsilon_B - \varepsilon_C - \varepsilon_x) \right] \chi_n^{\Lambda}(\underset{\sim}{R}) - \sum_{n'} < \Phi_n^{\Lambda} \mid \frac{\Delta_R}{2M} \Phi^{\Lambda}{}_{n'} > \chi_{n'}^{\Lambda}(\underset{\sim}{R}) -$$

$$- \frac{1}{M} \sum_{n'} <\Phi_n^{\Lambda}|\nabla_R \Phi_{n'}^{\Lambda}> \underset{\sim}{\nabla}_R \chi_{n'}^{\Lambda}(\underset{\sim}{R}) + \sum_{n',\Lambda'} < \Phi_n^{\Lambda} \mid \tilde{V}_{BC} \mid \Phi_{n'}^{\Lambda'} > + \qquad (2.32)$$

$$+ E_n^{\Lambda}(R)\ \chi_n^{\Lambda}(\underset{\sim}{R}) = 0$$

This equation and its solutions will be discussed in section 3, while the different coupling terms will be analysed in section 4.

The physical origin of these different coupling terms are unadiabatic terms:

* the so-called Coriolis coupling (due to the fact that the transfer is analysed in a moving frame)
* the kinetic energy coupling (which depends on the ratio $\frac{m_x}{m_C + m_B}$ as well as on the relative energy as it will be discussed in section 4).

- the potential coupling terms corresponding to excitations due to the relative motion. The term $\bar{E}_n^{\Lambda}(R)$ is the molecular potential which is produced by the revolution of the particle x around both the cores B and C. It must be noted that the terms depending on Λ will lead to coupling on the angular momentum of the relative motion as it will be discussed in the next section.

In order to solve eq. (2.32), we must specify the boundary conditions which we require for $\chi_n^{\Lambda}(\underset{\sim}{R})$. The physical boundary conditions are given with the variables $\underset{\sim}{R}_{AB}$ or $\underset{\sim}{R}_{DC}$, but not $\underset{\sim}{R}$ (see equations (2.3) and (2.4)). From expressions (2.12), one sees that if $m_x \ll m_B$ and $m_x \ll m_C$, we would have

$$\underset{\sim}{R} \simeq \underset{\sim}{R}_{AB} \simeq -\underset{\sim}{R}_{CD}$$

so that the boundary conditions on $\chi_n^{\Lambda}(\underset{\sim}{R})$ would be those given by expressions (2.3) and (2.4). This would occur if we neglected the recoil effect. If this recoil is taken into account, we can still use expressions (2.3) and (2.4) in which we replace $\underset{\sim}{R}_{AB}$ (or $\underset{\sim}{R}_{CD}$) by $\underset{\sim}{R}(-\underset{\sim}{R})$ provided that we multiply the intrinsic wave function by a phase factor as sketched in expression (2.13). In this case eq. (2.32) is modified in a manner discussed in the next section.

2.4 - DISCUSSION

The previous model is built to describe elastic and transfer reactions by taking into account the possible deformation of the colliding nuclei both in the outgoing and ingoing channels, due to their relative field. This continuous adiabatic deformation is contained in the continuous transformation of the nuclear wave function $\Phi_n(\underset{\sim}{r}_{Cx})$ into the intrinsic wave function $|\Phi_n(R, \underset{\sim}{r})>$ as a function of R. This slow deformation allows a rotation of the transferred particle x around the two cores, constituting an intermediate molecular state corresponding to several exchanges of the particle x between the two cores. This is what we call a multi-step process.

This model is borrowed to molecular physics where such situations arise frequently. There are however differences due to the difference of the forces involved in both cases and to the ratios of the masses of the cores and the

orbiting particle which are very different. The consequences are

- non adiabatic terms more important
- interactions due to the spin of the cores more important
- recoil effect must be included.

The recoil effect is appeared in both the intrinsic wave function and the relative wave function, but as it will be seen later, there is a kind of compensation between these two contributions.

The domain of validity of this model is discussed in section 4. It turns out to lie around the Coulomb barrier. It is related both to the incident energy and to the energy of excitation of the first level of the colliding nuclei. The larger the masses of the cores are, the smaller the recoil effect will be, but the Coulomb barrier being higher, the relative energy must be increased, increasing the non adiabatic terms. There is therefore an optimum which has to be estimated.

3. RELATIVE MOTION AND SCATTERING AMPLITUDE

As stated in section 2, we look for a solution of eq. (2.8) given in terms of the expression (2.31).

Inserting this ansatz into eq. (2.8) and taking into account eq. (2.18), we obtain, after taking into account the transformation (2.12):

$$\sum_{n\Lambda} \left[-\frac{\Delta_R}{2M} + \tilde{V}_{BC}(\underset{\sim}{R}) + E^{\Lambda}(R) \right] \chi_n^{\Lambda}(\underset{\sim}{R}) \mid \Phi_n^{\Lambda}(\underset{\sim}{r}, R) > =$$

$$= (E - \varepsilon_C - \varepsilon_B - \varepsilon_X) \sum_{n\Lambda} \chi^{\Lambda}(\underset{\sim}{R}) \mid \Phi_n^{\Lambda}(\underset{\sim}{r}, R) > \qquad (3.1)$$

3.1 - ANALYSIS OF THE LAPLACIAN OPERATOR

Since $|\Phi_n^\Lambda(\underset{\sim}{r}, R)>$ is expressed in the moving frame, the action of Δ_R on this wave function must be studied carefully. We know that

$$\Delta_R = \frac{1}{R}\frac{\partial^2}{\partial R^2} R - \frac{\tilde{L}^2}{R^2} \tag{3.2}$$

where $\tilde{L}^2$ contains partial derivatives with respect to the angles of $\underset{\sim}{R}$, but for fixed values of $\underset{\sim}{r}$ in the fixed frame. This operator does act therefore on $|\Phi_n^\Lambda(\underset{\sim}{r}, R)>$. Using the arguments of L. Landau and E. Lifchitz [21], it is shown in the appendix that

$$\tilde{L}^2\ \chi_n^\Lambda(\underset{\sim}{R})\,|\Phi_n^\Lambda(\underset{\sim}{r}, R)> = (\underset{\sim}{\mathcal{L}} - \underset{\sim}{\ell})^2\ \chi_n^\Lambda(\underset{\sim}{R})\,|\ \Phi_n^\Lambda(\underset{\sim}{r}, R)> \tag{3.3}$$

where $\underset{\sim}{\mathcal{L}}$ is the angular momentum of the rigid body formed with the cores B and C and the transferred particle x if they were fixed in the moving frame; $\underset{\sim}{\ell}$ is the angular momentum of the transferred particle in the moving frame; an equivalent expression appears indeed also in the collective model of deformed nuclei.

The relation (3.3) is not the most appropriate one. In fact $|\Phi_n^\Lambda(\underset{\sim}{r}, R)>$ is not an eigenstate of ℓ_Z, it is an eigenstate of Σ_Z as it has been discussed in section 2 (cf. eq. (2.19)).

If we introduce $\underset{\sim}{J} = \underset{\sim}{\mathcal{L}} + \underset{\sim}{J}_B + \underset{\sim}{J}_C + \underset{\sim}{s}_x$, i.e. the total angular momentum of the rigid body in the moving frame, eq. (3.3) may be re-written:

$$\tilde{L}^2\ \chi_n^\Lambda(\underset{\sim}{R})\,|\Phi_n^\Lambda(\underset{\sim}{r}, R)> = (\underset{\sim}{J}^2 + \underset{\sim}{\Sigma}^2 - 2\ \underset{\sim}{\Sigma}\cdot\underset{\sim}{J})\ \chi_n^\Lambda(\underset{\sim}{R})\ |\Phi_n^\Lambda(\underset{\sim}{r}, R)> \tag{3.4}$$

From this transformation, one sees that it is convenient to look for a solution of eq. (3.1) which may be written as

$$\chi_n^\Lambda(\underset{\sim}{R}) = \sum_{JM} (2J+1)\ \frac{f_{nJ}^\Lambda(R)}{R}\ D_M^{J*}(\alpha,\beta, 0) \tag{3.5}$$

where $D^{J*}_{M\Lambda}(\alpha,\beta,0)$ is the well known rotation matrix.

Inserting expression (3.5) into eq. (3.1) and taking into account eq.(3.4) one obtains the coupled equations:

$$\left[-\frac{\partial^2}{\partial R^2} + \frac{J(J+1) - 2\Lambda^2}{R^2} + 2M\, E^{\Lambda}_{n}(R) - k^2 \right] f^{\Lambda}_{nJ}(R) =$$

$$\sum_{n'} \left\{ 2 < n\,\Lambda \left| \frac{\partial}{\partial R} \right| n'\Lambda > \frac{\partial}{\partial R} + <n\Lambda \left| \frac{\partial^2}{\partial R^2} \right| n'\Lambda > - \frac{<n\Lambda|\Sigma^2|n'\Lambda>}{R^2} \right\} f^{\Lambda}_{n'J}(R)$$

$$- \frac{2M}{8\pi^2}(2J+1) \sum_{\Lambda' n'} < n\Lambda \,|D^{J}_{M}\, \tilde{V}_{BC}\, D^{J*}_{M\Lambda}| n'\Lambda' > f^{\Lambda'}_{n'J}(R)$$

$$+ \frac{1}{R^2} \sum_{n'} \left\{ \sqrt{(J+\Lambda+1)(J-\Lambda)} < n\Lambda \mid \Sigma_- | n'\Lambda+1 > f^{\Lambda+1}_{n'J}(R) \right. \qquad (3.6)$$

$$\left. + \sqrt{(J-\Lambda+1)(J+\Lambda)} < n\Lambda|\Sigma_+|n'\Lambda-1 > f^{\Lambda-1}_{n'J}(R) \right\}$$

where $\Sigma_{\pm} = \Sigma_x \pm i\,\Sigma_y$, $|n\Lambda>$ stands for $|\Phi^{\Lambda}_{n}(\underset{\sim}{r}, R)>$ and, $k^2 = 2M(E-\varepsilon_C-\varepsilon_B-\varepsilon_X)$. As it is discussed in the appendix, the term $2\underset{\sim}{\Sigma}\cdot\underset{\sim}{J}\, D^{J*}_{M\Lambda}(\alpha,\beta,0)|n\Lambda>$ yields $2\Lambda^2\ D^{J*}_{M\Lambda}(\alpha,\beta,0)|n\Lambda>$ and not zero because the operators $\frac{\partial}{\partial\phi}$ and $\frac{\partial^2}{\partial\phi^2}$ which are part of $\mathscr{L}^2$ and $\mathscr{L}_\zeta$ act not only on $D^{J*}_{M\Lambda}(\alpha,\beta,0)$ but also on the wave function $|\Phi^{\Lambda}_{n}(\underset{\sim}{r}, R)>$ yielding the terms in Λ. In fact, it is shown in section 4 (see eq. (4.23) and (4.43)) that in a representation which diagonalises a symmetrized hamiltonian in the LCNO representation, several coupling terms cancel. In eq. (3.6), the different coupling terms appear explicitly: The first type is diagonal in Λ and couples only different orbitals with the same value of Λ. This type includes the kinetic energy coupling terms and the diagonal part of the Coriolis term $< n\Lambda|\ \underset{\sim}{\Sigma}^2|n'\Lambda>$.

The second type is not diagonal in Λ. It includes mainly the non diagonal part of the Coriolis coupling, $< n\Lambda|\Sigma_{\mp}|n'\Lambda\pm1 >$ and if $\tilde{V}_{BC}(R)$ is not central a coupling due to the optical potential of the two colliding cores.

Below, we shall see how these coupling terms induce transitions on the orbital momentum of the relative motion of the colliding cores. In section 4 we shall discuss these terms in more detail, and show that there are some cancellations among them (see eq. (4.23)).

In this representation, we see that except for the couplings in n, there is no more than three coupled equations in Λ. Even, due to symmetries between Λ and $-\Lambda$, this number may be reduced in some cases. In the regular representation, one may have more coupled equations.

3.2 - ASYMPTOTIC CONDITIONS AND HELICITY AMPLITUDES

In the fixed frame one imposes the asymptotic condition (2.13). As it has been discussed in section 2, the molecular orbitals have the nuclear wave functions as a limit. Considering first collision without rearrangement and neglecting the recoil, the condition (2.13) may be written as

$$|\psi > \longrightarrow \sum_{S'} \left(e^{i\underset{\sim}{k}\cdot\underset{\sim}{R}} \delta_{SS'} + f_{SS'} \frac{e^{ikR}}{R} \right) |\Phi^{M}_{S'}(\underset{\sim}{r}_{Cx}) > \qquad (3.7)$$

where $|\Phi^{M}_{S'}(\underset{\sim}{r}_{Cx}) >$ is referred to the laboratory fixed frame of reference. If one expresses $|\Phi^{M}_{S'}(\underset{\sim}{r}_{Cx}) >$ in the moving frame, it can be easily derived from the properties of the rotations, that

$$e^{i\underset{\sim}{k}\cdot\underset{\sim}{R}}|\Phi^{M}_{S}(\underset{\sim}{r}_{Cx}) > = \sum_{J\Lambda} (2J+1)\, \varepsilon^{\Lambda M}_{SJ}(kR) D^{J*}_{M\Lambda}(\alpha,\beta,0)|\, \Phi^{\Lambda}_{S}(\underset{\sim}{r}_{Cx}) > \qquad (3.8)$$

where

$$\varepsilon_{SJ}^{\Lambda M}(kR) = \sum_{\ell}(2\ell+1)i^{\ell}\, j_{\ell}(kR) \begin{pmatrix} \ell & S & J \\ 0 & -M & M \end{pmatrix} \begin{pmatrix} \ell & S & J \\ 0 & -\Lambda & \Lambda \end{pmatrix} (-1)^{\Lambda-M} \tag{3.9}$$

One notes that

$$\varepsilon_{SJ}^{\Lambda M}(kR) = \varepsilon_{SJ}^{-\Lambda-M}(kR)$$

From the previous discussion on the Laplacian operator, one sees that these functions $\varepsilon_{SJ}^{\Lambda M}$ are given by the set of coupled equations

$$\left(-\frac{1}{R}\frac{\partial^2}{\partial R^2}R + \frac{J(J+1) + S(S+1) - 2\Lambda^2}{R^2} - k^2\right) \varepsilon_{SJ}^{\Lambda M}(kR) =$$

$$= \frac{1}{R^2}\left\{\sqrt{(J-\Lambda)(J+\Lambda+1)(S-\Lambda)(S+\Lambda+1)}\ \varepsilon_{SJ}^{\Lambda-1,M}(kR)\right\} .$$

$$+ \sqrt{(J+\Lambda)(J-\Lambda+1)(S+\Lambda)(S-\Lambda+1)}\ \varepsilon_{SJ}^{\Lambda+1,M}(kR)\Big\} . \tag{3.10}$$

In fact, inserting eq. (3.9) into eq. (3.10) one obtains the well known equation for the Bessel function $j_{\ell}(kR)$ by using the recursion formula:

$$\left[2\, m_1 m_2 + j_1(j_1+1) - j_2(j_2+1) - j_3(j_3+1)\right] \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & -m_2 & m_2 \end{pmatrix} =$$

$$= \left[j_3(j_3+1) - m_1(m_1+1)\right]^{\frac{1}{2}}\left[j_2(j_2+1) - m_2(m_2+1)\right]^{\frac{1}{2}} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & -m_2 & m_2+1 \end{pmatrix} + \tag{3.11}$$

$$+ \left[j_3(j_3+1) - m_1(m_1-1)\right]^{\frac{1}{2}}\left[j_2(j_2+1) - m_2(m_2-1)\right]^{\frac{1}{2}} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & -m_2 & m_2-1 \end{pmatrix}$$

We show in section 4.3 that

$$\langle (n\bar{S})\Lambda | \underset{\sim}{\Sigma}^2 | (n'\bar{S}')\Lambda \rangle \xrightarrow[R\to\infty]{} \left[S(S+1) + R^2 \langle n\Lambda | \frac{\partial^2}{\partial R^2} | n'\Lambda \rangle \right] \delta_{nn'} \delta_{\quad} + 2M\,\delta E \tag{3.12a}$$

$$\langle (n\bar{S})\Lambda \, | \Sigma_{\pm} | (n'S')\Lambda \rangle \xrightarrow[R\to\infty]{} \left[(S\pm\Lambda)(S'\mp\Lambda+1) \right]^{\frac{1}{2}} \delta_{nn'} \delta_{SS'} \tag{3.12b}$$

and

$$\langle n\Lambda | \frac{\partial}{\partial R} | n'\Lambda \rangle \xrightarrow[R\to\infty]{} 0 \, .$$

where δE is an energy correction corresponding to the recoil effect and which can be included in $E_n^{\Lambda}(R)$ by a suitable change of intrinsic wave function (see sect. 4.4). Therefore, eq. (3.10) is the limit of eq. (3.6) outside the range of the nuclear potential.

In analogy to the plane waves, the full wave-functions can be expanded as follows in the asymptotic region:

$$\psi_S^M = \sum_{J\Lambda S'} (2J+1)\, F_{JSS'}^{\Lambda M}(k,R)\, D^{J*}_{M\Lambda}(\alpha,\beta,0) \, | \, \Phi_{S'}^{\Lambda}(\underset{\sim}{r}_{Cx}) \rangle \tag{3.13}$$

where

$$F_{JSS'}^{\Lambda M}(kR) = \sum_{\ell\ell'} (-)^{\ell'-\ell+S-S'+\Lambda-M} (2\ell+1)(2\ell'+1) i^{\ell} \begin{pmatrix} \ell S J \\ 0\, M-M \end{pmatrix} \begin{pmatrix} \ell' S' J \\ 0\, \Lambda\, -\Lambda \end{pmatrix} \psi^{J}_{\substack{\ell'\ell \\ S'S}}(kR) \tag{3.14}$$

and $\psi^{J}_{\substack{\ell'\ell \\ S'S}}(kR)$ being the standard scattering wave function in the asymptotic region.

The expansion (3.13) is not exact in the interaction region, because as it has been emphasized in section 2, the molecular wave functions are not eigenfunctions of $\underset{\sim}{\Sigma}^2$. In this case they are labelled by

$$| \Phi_{n\bar{S}}^{\Lambda} \rangle \longrightarrow | \Phi_S^{\Lambda} \rangle$$

In order to establish the connection with phase shifts, we should examine equations (3.13) and (3.8) in the asymptotic region $R \to \infty$. Asymptotically eq. (3.8) becomes

$$e^{i\underset{\sim}{k}\cdot\underset{\sim}{R}}|\Phi_S^M> \longrightarrow \sum_{J\Lambda}(2J+1)\left(\delta_{M\Lambda}\ \frac{e^{ikR}}{2ikR} - \alpha^{\Lambda M}_{JSS'}\ \frac{e^{-ikR}}{2ikR}\right) D^{J*}_{M\Lambda}(\alpha,\beta,0)|\ \Phi_S^\Lambda> \qquad (3.15)$$

where

$$\alpha^{\Lambda M}_{JSS'} = \sum_{\ell}\ (2\ell+1)(-1)^{\Lambda-M}\begin{pmatrix}\ell & S & J\\ 0 & -M & M\end{pmatrix}\begin{pmatrix}\ell & S' & J\\ 0 & -\Lambda & \Lambda\end{pmatrix}\ \delta_{SS'} \qquad (3.16)$$

The asymptotic behaviour of the components of the wave function (3.14) takes on the standard form in terms of the S-matrix, i.e.

$$\psi^J_{\ell'\ell}(kR) \xrightarrow[R\to\infty]{} \frac{1}{2kR}\ i^{\ell'+1}\left[e^{-ikR}\ \delta_{\ell'\ell} - (-1)^{\ell'}\ S^J_{\ell'\ell}\ e^{ikR}\right] \qquad (3.17)$$
$$S'S \qquad\qquad\qquad\qquad\qquad\qquad S'S \qquad\qquad S'S$$

Inserting this expression into eq. (3.13), we get

$$\psi_S^M \xrightarrow[R\to\infty]{} \sum_{J\Lambda S'}(2J+1)\left[-\alpha^{\Lambda m}_{JSS'}\ \frac{e^{-ikR}}{2ikR} + S^{\Lambda M}_{JSS'}\ \frac{e^{ikR}}{2ikR}\right] D^{J*}_{M\Lambda}(\alpha,\beta,0)|\ \Phi^\Lambda_{S'}> \qquad (3.18)$$

where $\alpha^{\Lambda M}_{JSS'}$ is defined by expression (3.16) and

$$S^{\Lambda M}_{JSS'} = \sum_{\ell\ell'}\ i^{\ell+\ell'}\ \sqrt{(2\ell+1)(2\ell'+1)}\ S^J_{\ell'\ell}\ \begin{pmatrix}\ell & S & J\\ 0 & M & -M\end{pmatrix}\ \begin{pmatrix}\ell' & S' & J\\ 0 & \Lambda & -\Lambda\end{pmatrix}(-)^{\ell+S-S'+\Lambda-M}$$
$$S'S$$

Since each LCNO has a determined nuclear orbital $|\Phi^\Lambda_S>$ as limit, one can identify eq. (3.18) with eq. (3.7). Taking into account eq. (3.15), the scattering amplitude is written as follows

$$f_{SM\to S'\Lambda}(\alpha,\beta) = \sum_J\ (2J+1)\ a^{\Lambda M}_{JSS'}\ D^{J*}_{M\Lambda}(\alpha,\beta,0) \qquad (3.20)$$

where

$$a^{\Lambda M}_{JSS'} = \frac{S^{\Lambda M}_{JSS'} - \delta_{M\Lambda}}{2ik} \tag{3.21}$$

is the helicity amplitude. The fact that the radial part of the asymptotic expansion of the LCNO contains the helicity amplitude of scattering has the following kinematic origin. When $R \to \infty$, the axes of the molecule tend to the direction of the scattered particle in the exit channel, which is parallel to the final relative momentum.

As our principal concern is to describe the collision of heavy ions near the Coulomb barrier its interaction effects must be included. In this case the solution of eq. (3.10) is:

$$\varepsilon^{\Lambda M}_{SJ}(kR) = \frac{1}{kR} \sum_{\ell} (2\ell+1) i^{\ell} e^{i\sigma_\ell} F_\ell(\gamma; kR) \begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} \begin{pmatrix} \ell & S & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} (-1)^{\Lambda - M} \tag{3.22}$$

where σ_ℓ is the Coulomb phase shift and F_ℓ the regular Coulomb wave function. Equations (3.13) and (3.14) are still valid if expression (3.17) is replaced by

$$\psi^{J}_{\substack{\ell'\ell \\ S'S}} \xrightarrow[R \to \infty]{} \frac{1}{2kR} i^{\ell'+1} \left[u^{-}_{\ell} \; \delta_{\substack{\ell'\ell \\ S'S}} - u^{+}_{\ell} \; S^{J}_{\substack{\ell'\ell \\ S'S}} \right] \tag{3.23}$$

where $u^{\pm}_{\ell} = (G_\ell \pm i F_\ell) e^{i\sigma_R}$ * and G_ℓ is the irregular Coulomb wave function.

Proceeding as above, one obtains for the nuclear scattering amplitude

$$a^{\Lambda M}_{nJSS'} = \frac{H^{\Lambda M}_{JSS'} - \beta^{\Lambda M}_{JSS}}{2ik} \tag{3.24}$$

where

$$\beta^{\Lambda M}_{JSS} = \sum_{\ell} \sqrt{2\ell+1} \; (-1)^{\Lambda - M} \begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} \begin{pmatrix} \ell & S & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} e^{2i\sigma_\ell} \tag{3.25}$$

and

$$H^{\Lambda M}_{JSS'} = \sum_{\ell\ell'} i^{\ell+\ell'} (-1)^{\ell+S-S'+\Lambda-M} \sqrt{(2\ell+1)(2\ell'+1)} \begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} S^{J}_{\ell'\ell} \, e^{2i\sigma_\ell} \tag{3.26}$$

---

* Note that this phase convention is not the standard one.

The scattering amplitude is then given by

$$f_{SM \to S'\Lambda}(\alpha,\beta) = f_C(\alpha,\beta)\delta_{SS'}\delta_{\Lambda M} + \sum_J (2J+1)\, a^M_{nJSS'}\, D^{J*}_{M\Lambda}(\alpha,\beta,0) \qquad (3.27)$$

3.3 - COUPLED SCHRÖDINGER EQUATIONS

Instead of eq. (3.6), it may be interesting to write an equation which exhibits explicitly the relative angular momentum of the two cores. For plane waves the relative wave function exhibiting the relative angular momentum is $j_\ell(kR)$. Expression (3.14) is therefore the ansatz which allows to transform the well known Schrödinger equation into de helicity representation and coversely.

By analogy, we shall look for a solution of (3.6) which reads

$$f^{\Lambda}_{(n)J}(kR) = \sum_{\ell'\ell} (-1)^{\ell'-\ell+S-S'+\Lambda-M} \sqrt{(2\ell+1)(2\ell'+1)}\; i^{\ell} \begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \underset{(nS')S}{\psi^{J}_{\ell'\ell}}(kR) \qquad (3.28)$$

where S' is the spin of the nuclear state which is the asymptotic limit of the molecular state $|\Phi^{\Lambda}_n>$ (see expression (2.24)). Although this expression looks like expression (3.14), it has a different meaning because $\underset{(nS')S}{\psi^{J}_{\ell'\ell}}(kR)$ does not describe exactly the relative motion of the cores in the fixed frame during the interaction. It is related to the function describing this relative motion by the expression (A-10) shown in the appendix. It turns out that ℓ' is the angular momentum of the relative motion only in the asymptotic region. Nevertheless, as it is shown in the appendix, when $R \to \infty$, the limit of the function

$\psi^J_{\ell,\ell}$ is the function $\psi^J_{\ell'\ell}$ appearing in eq. (3.14) so that both functions have
$(nS')S \qquad\qquad S'S$
the same asymptotic expressions and the previous formulae can be used.

Inserting expression (3.28) into eq. (3.6) and using the recursion formula (3.11), one is led to

$$\left[-\frac{\partial^2}{\partial R^2} + \frac{\ell''(\ell''+1)}{R^2} - k^2 \right] \psi^J_{\ell\ell'' nS}(kR) = \sum_{\ell'} v^J_{M_o n\ell''\ell'} \psi^J_{\ell\ell' nS}(kR) +$$

$$+ \sum_{n'\ell'} (A^J_{nn' \ell''\ell'} + v^J_{N_\mu nn' \ell''\ell'} + C^J_{nn' \ell''\ell'}) \psi^J_{\ell\ell' n'S}(kR) \qquad (3.29)$$

where

$$v^J_{M_o n\ell''\ell'} = \sum_{\Lambda} (-1)^{\ell'-\ell''} (2\ell''+1) \begin{pmatrix} \ell'' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} 2ME^{\Lambda}_{\mu}(R) \qquad (3.30)$$

is the molecular exchange potential expressed in the fixed frame,

$$A^J_{\substack{nn' \\ \ell''\ell'}} = \sum_{\Lambda} (-1)^{\ell'-\ell''} (2\ell''+1) \begin{pmatrix} \ell'' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \left\{ 2 < n\Lambda \left| \frac{\partial}{\partial R} \right| n'\Lambda > \frac{\partial}{\partial R} + \right.$$

$$\left. + < n\Lambda \left| \frac{\partial^2}{\partial R^2} \right| n'\Lambda > - \frac{1}{R^2} < n\Lambda | \underset{\sim}{\Sigma}^2 - S'(S'+1) | n'\Lambda > \right\} \qquad (3.31)$$

is the non adiabatic coupling potential, which can be readily simplified as shown in equations (4.23) and (4.33), if $\underset{\sim}{\Sigma}^2$ is carefully analysed.

$$v^J_{N_\mu \substack{nn' \\ \ell''\ell'}} = -\frac{M}{4\pi^2} \sum_{\Lambda,\Lambda'} (-)^{\ell'-\ell''+\Lambda'-\Lambda} (2\ell''+1) \begin{pmatrix} \ell'' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda' & -\Lambda' \end{pmatrix} x$$

$$x < n\Lambda MJ | \tilde{V}_{BC}(\underset{\sim}{R}) | n'\Lambda' MJ > \qquad (3.32)$$

is the nuclear equivalent potential in the fixed frame,

$$C^J_{\substack{nn' \\ \ell''\ell'}} = -\frac{1}{R^2} \sum_{\Lambda} (-)^{\ell'-\ell} (2\ell''+1) \begin{pmatrix} \ell'' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \Bigg\{ \sqrt{(J+\Lambda+1)(J-\Lambda)} \Big[< n\Lambda|\Sigma_-|n'\Lambda+1 > -$$

$$- \sqrt{(S'+\Lambda+1)(S'-\Lambda)} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda+1 & -\Lambda-1 \end{pmatrix} + \sqrt{(J-\Lambda+1)(J+\Lambda)} \Big[< n\Lambda|\Sigma_+|n'\Lambda-1 > \quad -$$

$$- \sqrt{(S'-\Lambda+1)(S'+\Lambda)} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda-1 & -\Lambda+1 \end{pmatrix} \Bigg\} \qquad (3.33)$$

is the so-called Coriolis coupling term expressed in the fixed frame (we recall that the index n stands for $(n\bar{s}')$. This equation shows some interesting features. First we note that all the terms depending on Λ induce tensorial operators which are not diagonal on ℓ, as one expects.

Secondly in one particular case the coupling in ℓ disappears, namely if one restricts oneself to molecular states in which only the $j = 1/2$ states of the two nuclei contribute (ex : $C^{12} + C^{13}$). In that case, since the potential E^{Λ}_n depends only on the absolute value of Λ, it can be factorized and

$$V^J_{M_o\ n\ \ell''\ell'} = 2\ M\ E^{\Lambda}_n\ \delta_{\ell'\ell''} \qquad (3.34)$$

This shows that the molecular potential $E^{\Lambda}_n(R)$ is a true scalar. This point has been also observed by W. Von Oertzen et al. [22] in a different way. Furthermore, as it will be discussed in section 4, all the non diagonal Coriolis coupling term vanish since, in that particular case

$$< n\Lambda|\Sigma_{\mp}|n'\Lambda\pm1 > = \sqrt{(S'\pm\Lambda\mp1)(S'\mp\Lambda)}$$

Our equation becomes equivalent to the equation of W. Von Oertzen [3], if one assumes, as it is generally the case, that the potential $-\tilde{V}_{BC}(R)$ is a scalar, spherically symmetric.

Instead of solving eq. (3.6), one can solve eq. (3.29) in which the functions $\psi_{\ell',\ell}(kR)$ have the asymptotic expressions given by expression (3.17) or (3.23), the helicity amplitude being obtained by the sum expressed by (3.19).

3.4 - IDENTICAL CORES AND CROSS-SECTION

In that case the function $|\psi>$, see eq. (3.13), must be symmetric or anti-symmetric in the interchange of the two cores (i.e. position and spin) according as these cores are bosons or fermions. Therefore

$$|\psi(\underset{\sim}{r}, \underset{\sim}{R}) > = (-)^{2 J_C} P_{BC}|\psi(\underset{\sim}{r}, \underset{\sim}{R}) >$$

where J_C is the spin of one core. In that case, it has been shown in section 2 that the molecular wave functions are furthermore eigenfunctions of the parity, that is

$$| \Phi_n^{\Lambda P}(\underset{\sim}{r}, R) > = (-)^P | \Phi_n^{\Lambda P}(-\underset{\sim}{r}, R) >$$

The expansion (3.13) is replaced by

$$|\psi_s^M(\underset{\sim}{r}, \underset{\sim}{R}) > = \sum_{J\Lambda S'P} (2J+1)\, F^{\Lambda MP}_{JSS'}(R)\, D^{J*}_{M\Lambda}(\alpha,\beta,0)|\Phi^{\Lambda P}_{S'} > \qquad (3.35)$$

The exchange of the spins of the cores induce a phase factor for each core spin state J_{BC} equal to $(-)^{2J_C+J_{BC}}$. The operation $\underset{\sim}{R} \rightarrow -\underset{\sim}{R}$ is expressed in the fixed frame by the operator $\hat{R}$ such that

$$\hat{R}_1 \; D^{J^*}_{M\Lambda}(\alpha,\beta,0) \;\; = D^{J^*}_{M\Lambda}(\alpha + \pi,\; \pi - \beta,\; 0) \; .$$

On the other hand (cf. eq. (2.30b)

$$|\Phi^{\Lambda P}_S(\underset{\sim}{r},\, R) > \; = \sum_{S'} \; C^{\Lambda P}_{SS'}(R) \left[\frac{|\phi^{\Lambda}_{S'}(\underset{\sim}{1}) > \; + \; (-)^{P-\pi} |\phi^{\Lambda}_{S'}(\underset{\sim}{2}) >}{\sqrt{2}} \right] \tag{3.36}$$

where π is the intrinsic parity of the nuclear orbitals, and $\underset{\sim}{1} = \underset{\sim}{r} - \frac{\underset{\sim}{R}}{2}$ and $\underset{\sim}{2} = \underset{\sim}{r} + \frac{\underset{\sim}{R}}{2}$. Thus $\hat{R}_1 |\phi_S{}^{\Lambda P}(\underset{\sim}{1}) > \; = |\phi_S{}^{\overline{\Lambda} P}(\underset{\sim}{2}) >$. Since the spatial symmetry depends on the spin J_{BC} of the cores, we write expression (3.35) as follows

$$|\psi^M_S(\underset{\sim}{R},\, \underset{\sim}{r}) > \; = \sum_{J_{BC}} \; \psi^M_{S\; J_{BC}}(\underset{\sim}{R},\, \underset{\sim}{r}) \; = \sum_{\substack{J_{BC} \\ J\; P}} \sum_{\Lambda\; S'} \; (2J+1) \; F^{\Lambda MP}_{JSS'}(R) \; D^{J^*}_{M\Lambda}(\alpha,\beta,0) |\; \Phi^{\Lambda P}_{SJ_{BC}} > \tag{3.37}$$

where $|\Phi^{\Lambda P}_{S\; J_{BC}} >$ is given by

$$|\Phi^{\Lambda P}_{S\; J_{BC}} > \; = \sum_{j_x\; m_x} \begin{pmatrix} J_{BC} \; j_x \\ M_{BC} \; m_x \end{pmatrix} \Bigg| \begin{matrix} S \\ \Lambda \end{matrix} \Bigg) \quad \Phi^{J_{BC}\; j_x}_{\alpha'} > \tag{3.38}$$

where $|\Phi^{J_{BC}\; j_x}_{\alpha'} >$ is given by (2.16).

Then the correct symmetrized function is expanded as

$$|\psi^M_S(\underset{\sim}{R},\, \underset{\sim}{r}) > \; = \frac{1}{\sqrt{2}} \left[1 + (-)^{2\; J_C} \; \hat{P}_{CB} \right] \sum_{J\Lambda S'P\; J_{BC}} (2J+1) \; F^{\Lambda MP}_{JSS'}(R) \; D^{J^*}_{M\Lambda}(\alpha,\beta,0) |\Phi^{\Lambda P}_{S'\; J_{BC}} > \tag{3.39}$$

From expansion (3.36) we have, for the asymptotic nucleonic wave functions,

$$|\; \Phi^{\Lambda P}_{S'J_{BC}}(\underset{\sim}{r},\, R) > \xrightarrow[R \to \infty]{} \frac{|\phi^{\Lambda}_{S'\; J_{BC}}(1) > \; + \; (-)^{P-\pi} |\phi^{\Lambda}_{S'\; J_{BC}}(2) >}{\sqrt{2}} \tag{3.40}$$

Therefore, if the Coulomb interaction is not included,

$$F^{\Lambda MP}_{JSS'}(R) \xrightarrow[R \to \infty]{} \frac{1}{2ik} \left[- \alpha^{\Lambda MP}_{JSS'} \delta_{SS'} \frac{e^{-ikR}}{R} + S^{\Lambda MP}_{JSS'} \frac{e^{ikR}}{R} \right] \tag{3.41}$$

where $\alpha^{\Lambda MP}_{JSS'}$ and $S^{\Lambda MP}_{JSS'}$ are given by expressions identical to eq. (3.16) and eq. (3.19), but with restricted values of ℓ given by the following selection rule (cf. appendix)

$$(-1)^{\ell} = (-1)^{J_{BC} + \pi - P} \tag{3.42}$$

On the other hand, eq. (3.9) becomes

$$\varepsilon^{\Lambda MP}_{JS}(kR) \xrightarrow[R\to\infty]{} \left[\frac{e^{ikR}}{R} \gamma^{\Lambda MP}_{JSS'} - \alpha^{\Lambda MP}_{JSS'} \delta_{SS'} \frac{e^{-ikR}}{R} \right] \frac{1}{2ik} \tag{3.43}$$

where

$$\gamma^{\Lambda MP}_{JSS'} = \sum_{\ell} \sqrt{(2\ell+1)}\, (-)^{\Lambda - M} \begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} \begin{pmatrix} \ell & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \delta_{SS'} \tag{3.44}$$

with the restricted values of ℓ given by the selection rule (3.42). We then introduce

$$a^{\Lambda MP}_{JSS'} = \frac{S^{\Lambda MP}_{JSS'} - \gamma^{\Lambda MP}_{JSS'}}{2ik} \tag{3.45}$$

and

$$f^{P}_{SM \to S'\Lambda}(\alpha,\beta) = \sum_{J} (2J+1)\, a^{\Lambda MP}_{JSS'}\, D^{J^*}_{M\Lambda}(\alpha,\beta,0) \ . \tag{3.46}$$

Due to the restriction rule (3.42) $f^{P}_{SS'}$ depends on J_{BC}. Inserting eqs. (3.40), (3.41), (3.43), (3.44), (3.45) in eq. (3.39) and making use of

$$\hat{P}_{CB} \left| \phi^{\Lambda}_{S}\, J_{BC}\, (\underset{\sim}{2}) \right> = \left| \phi^{\bar{\Lambda}}_{S}\, J_{BC}\, (\underset{\sim}{1}) \right> = (-)^{2 J_C + J_{BC}} \left| \phi^{-\Lambda}_{S}\, J_{BC}\, (\underset{\sim}{1}) \right> \tag{3.47}$$

(cf. eq. (3.38), one finally obtains, after the summation over p = 1 and 2.

$$|\psi_S^M(R, r) > \xrightarrow[R \to \infty]{} \sum_{J_{BC}} \left[|\Phi_S^M\, J_{BC}(\underset{\sim}{1}) > e^{i\underset{\sim}{k}\cdot\underset{\sim}{R}} + (-)^{J_{BC}} |\Phi_S^M\, J_{BC}(\underset{\sim}{2}) > e^{-i\underset{\sim}{k}\cdot\underset{\sim}{R}} \right] +$$

$$+ \frac{1}{2} \sum_{J_{BC}} \sum_{\Lambda\, S'} \left\{ \left[(f^1 + f^2)_{SM\to S'\Lambda}(\alpha) \, |\Phi_{S'}^{\Lambda}, J_{BC}(\underset{\sim}{1}) > + (-)^{\pi} (f^1 - f^2)_{SM\to S'\Lambda}(\alpha) |\Phi_{S'}^{\Lambda} J_{BC}(\underset{\sim}{2}) > \right] + \right.$$

$$\left. + (-)^{J_{BC}} \left[(f^1 + f^2)_{SM\to S'-\Lambda}(\pi-\alpha) |\Phi_{S'}^{\Lambda} J_{BC}(\underset{\sim}{2}) > + (-)^{\pi} (f^1 - f^2)_{SM\to S'-\Lambda}(\pi-\alpha) |\Phi_{S'}^{\Lambda} J_{BC}(\underset{\sim}{1}) > \right] \right\} \frac{e^{ikR}}{R} \tag{3.48}$$

To derive the cross-section for the reaction in which the initial nucleus has the spin J_A and the final one the spin J_D, it is advantageous to change the coupling scheme in which we worked up to now, i.e.

$$\underset{\sim}{J}_B + \underset{\sim}{J}_C \to \underset{\sim}{J}_{BC}$$

$$\underset{\sim}{J}_{BC} + \underset{\sim}{j} \to \underset{\sim}{S}$$

into another one in which the spin of the final nuclei appear explicitly namely:

$$\underset{\sim}{j} + \underset{\sim}{J}_C \to \underset{\sim}{J}_D$$

$$\underset{\sim}{J}_D + \underset{\sim}{J}_B \to \underset{\sim}{S}$$

This is done by the unitary transformation

$$\left[\Phi_{S'}^{\Lambda} J_{BC} \right] > = \sum_{J_{BC}} < J_B\, J_C (J_{BC}) j;\, S'\Lambda | J_B J_C j (J_D);\, S'\Lambda > | \Phi_{S'}^{\Lambda} J_B > \tag{3.49}$$

where the transformation matrix elements are given by [23]:

$$<J_B J_C (J_{BC}) j; S'\Lambda | J_B J_C j (J_D); S'\Lambda> = (-)^{J_B + J_C + j + S'} \sqrt{(2J_{BC}+1)(2J_D+1)} \begin{Bmatrix} J_B & J_C & J_{BC} \\ j & S' & J_D \end{Bmatrix} \tag{3.50}$$

the curly bracket being the Wigner's 6-j symbol.

Substituting (3.49) and (3.50) into (3.48) we get

$$f_{\substack{SM \to S'\Lambda \\ J_A \quad J_D'}}^{(1)}(\alpha) = \langle \Phi_{S'J_D'}(1) | \psi^M_{S\, J_A} \rangle =$$

$$= \frac{1}{2}\sqrt{(2J_D'+1)(2J_A+1)}\;(-1)^{S'-S} \sum_{J_{BC}} (2J_{BC}+1) \begin{Bmatrix} J_B & J_C & J_{BC} \\ j & S' & J_D' \end{Bmatrix} \times$$

$$\times \begin{Bmatrix} J_B & J_C & J_{BC} \\ j & S & J_A \end{Bmatrix} \left[(f^1+f^2)_{SM\to S'\Lambda}(\alpha) + (-)^{J_{BC}+\pi} (f^1-f^2)_{SM\to S'-\Lambda}(\pi-\alpha) \right]$$

In the same way, we obtain

$$f_{\substack{SM \to S'\Lambda \\ J_A \quad J_D'}}^{(2)}(\alpha) = \langle \Phi_{S'J_D'}(2) | \psi^M_{S\, J_A} \rangle = f_{\substack{SM \to S'\Lambda \\ J_A \quad J_D'}}^{(1)}(\pi-\alpha) \tag{3.52}$$

and the cross-section, which is given by

$$\frac{d\sigma}{d\Omega} = \frac{1}{(2J_A+1)(2J_B+1)} \sum_{\substack{M\Lambda \\ SS'}} \frac{1}{(2S+1)} \left[\left| f_{\substack{SM \to S'\Lambda \\ J_A \quad J_D'}}^{(1)}(\alpha) \right|^2 + \left| f_{\substack{SM \to S'\Lambda \\ J_A \quad J_D'}}^{(2)}(\pi-\alpha) \right|^2 \right] \tag{3.53}$$

can be written

$$\frac{d\sigma}{d\Omega} = \frac{2J_D'+1}{2J_B+1} \sum_{\substack{SS' \\ M\Lambda}} \frac{1}{(2S+1)} \left| \sum_{J_{BC}} (2J_{BC}+1) \begin{Bmatrix} J_B & J_C & J_{BC} \\ j & S & J_A \end{Bmatrix} \begin{Bmatrix} J_B & J_C & J_{BC} \\ j & S' & J_D' \end{Bmatrix} \mathcal{F}^{J_{BC}}_{SM\to S'\Lambda}(\alpha) \right|^2 \tag{3.54}$$

where

$$\mathcal{F}^{J_{BC}}_{SM \to S'\Lambda}(\alpha) = \frac{1}{\sqrt{2}} (f^1+f^2)_{SM \to S'\Lambda}(\alpha) + (-)^{J_{BC}+\pi} \frac{1}{\sqrt{2}} (f^1-f^2)_{SM \to S'-\Lambda}(\pi-\alpha) \tag{3.55}$$

From this general expression, we can deduce the simple following results in some particular cases

i) for $J_B = J_C = 0$, $j = 1/2$ $\quad J_A = J_D = 1/2$ (say $C^{12} + C^{13} \to C^{12} + C^{13}$)

the only possible values of S, S' and J_{BC} are $S = S' = 1/2$, $J_{BC} = 0$; we get after summation over M and Λ

$$\frac{d\sigma}{d\Omega} = \left| \mathcal{F}^{0}_{1/2 \quad 1/2} \right|^2 \tag{3.56}$$

ii) for $J_B = J_C = 1/2$, $j = 1/2$, $J_A = J_D = 0$ (say $C^{13} + C^{14} \to C^{13} + C^{14}$)

J_{BC} can take on the two values 0 or 1 while S and S' are necessarily restricted to the values $S = S' = 1/2$ by the two 6-j symbols appearing in (3.54). We get after the summation over M and Λ

$$\frac{d\sigma}{d\Omega} = \left| \frac{1}{4} \mathcal{F}^{0}_{1/2\ 1/2} + \frac{3}{4} \mathcal{F}^{1}_{1/2 \quad 1/2} \right|^2 \tag{3.57}$$

iii) for $J_B = J_C = 1/2$, $j = 1/2$, $J_A = J_D = 1$ (say $N^{14} + C^{13} \to C^{13} + N^{14}$)

J_{BC} can take again the two values 0 or 1 while S and S' can take on the values 1/2 and 3/2. We get

$$\frac{d\sigma}{d\Omega} = \frac{3}{2} \sum_{M\Lambda} \left\{ \frac{1}{2} \left| \frac{1}{4} \mathcal{F}^{0}_{1/2\ 1/2\ M\ \Lambda} + \frac{1}{12} \mathcal{F}^{1}_{1/2\ 1/2\ M\ \Lambda} \right|^2 + \frac{1}{36} \left(\left| \mathcal{F}_{3/2\ 3/2\ M\ \Lambda} \right|^2 + \frac{1}{2} \left| \mathcal{F}_{1/2\ 3/2\ M\ \Lambda} \right|^2 - \left| \mathcal{F}_{3/2\ 1/2\ M\ \Lambda} \right|^2 \right) \right\} \tag{3.58}$$

These formulae can be compared with the results of W. Von Oertzen et al [10]. The two formulae (3.56) and (3.57) are strictly the same as formulae (2.23) and (2.37) of their paper. Our formulae (3.58) looks somewhat different from their expression (2.38). However, if one assumes that there is no coupling between the spins of the cores and the spin of the orbiting particle as it is done in reference [10] and as it will be generally the case, then our amplitudes are independent of S and S' as well as of and M in that particular case. We can therefore write

$$\mathcal{F}^{J_{BC}}_{\substack{SS' \\ \Lambda M}} \simeq F^{J_{BC}} \delta_{SS'} \tag{3.59}$$

Performing the summation over Λ and M and adding the amplitude which become equal we obtain:

$$\frac{d\sigma}{d\Omega} = \left| \frac{3}{4} F^1 + \frac{1}{4} F^0 \right|^2 + \frac{1}{8} \left| F^1 - F^0 \right|^2 \tag{3.60}$$

which is the formula (2.38) of reference [10].

In the same line, we can make the comparison with the results obtained in molecular physics by F. J. Smith [24] for instance.

4. THE COUPLING TERMS AND RECOIL CORRECTIONS

4.1 - DIFFERENT TYPES OF COUPLING

There are two classes of coupling terms. The first one includes the potential between the two cores, and in eq. (3.29) the exchange potential which is not diagonal in ℓ'. The second class includes the coupling terms describing the non

adiabaticity of the scattering process. In this section we shall be mainly concerned with these terms. Again two types of terms appear:

- The diagonal ones in Λ,

$$< n\Lambda \left| \frac{\partial}{\partial R} \right| n'\Lambda > \tag{4.1}$$

$$< n\Lambda \left| \frac{\partial^2}{\partial R^2} \right| n'\Lambda > \tag{4.2}$$

and

$$< n\Lambda \, |\Sigma^2| n'\Lambda > \tag{4.3}$$

couple states of identical "nucleonic" angular momentum Λ.

- The non diagonal ones in Λ,

$$< n\Lambda |\Sigma_{\pm}| \, n'\Lambda \mp 1 > \tag{4.4}$$

which mix states with different intrinsic angular momentum projection. We shall discuss successively the so-called unadiabatic terms (4.1) and (4.2) and the Coriolis terms (4.3) and (4.4).

4.2 - UNADIABATIC TERMS

4.2-1 - General Considerations

Before analysing the properties of the coupling matrix elements, (4.1), (4.2) and (4.3), we discuss the energy domain where the adiabatic approximation may be used. This can be described in terms of molecular orbitals, in the

following way. One supposes, in analogy to atomic collision that the period of the cluster motion is defined by the quantity $\tau = \hbar/\Delta E_{ij}$ where ΔE_{ij} is the energy difference between the states i, j of the nucleonic system in some nuclear configuration. We denote the effective time of collision interaction by $T_{rel} = d/V_{rel}$, where d is the effective interaction distance and V_{rel} is the relative velocity in collision. When $\tau << T_{rel}$ one has the so-called adiabatic behaviour. Physically this corresponds to the situation in which the cluster x moves around B and C faster than the cores themselves in their mutual approach. This condition imposes the upper limit to the energy of the incident core

$$E_{rel} < \left(\frac{\Delta E_{ij}}{\pi \hbar}\right)^2 \frac{d^2}{2} \mu \qquad (4.5)$$

where E_{rel} is the relative energy of the two cores and μ is the reduced mass in the channel considered. For elastic scattering $\Delta E_{ij}(R)$ may be estimated by the value at infinite separation, $\Delta E_{ij}(\infty)$ which is given by the energy levels of the ion. Actually in (4.5), ΔE_{ij} corresponds to the difference between the energies of two shells and not of two subshells.

On the other hand, the expression (4.5) indicates all the energy levels which must be taken into account in the coupled equations for a given incident energy E, in the C.M. system.

We quote some numbers to give orders of magnitude

Reactions	Emax MeV	Levels to be included for $E > E_0$	E_0 MeV
$Li^7 + \alpha$	6.8	ground state	0.0
		ground state and first level	0.45
$O^{16} + O^{17}$	32	GS	0.0
		GS and first level	0.85
$Ca^{40} + Ca^{41}$	100	GS	

In all these cases the matrix elements of the terms (4.1) and (4.2) are expected to be small. Let us analyse the properties of these elements in more details. Due to the orthogonality of the "molecular wave functions" $|n\Lambda>$, these matrix elements have interesting properties. It is easy to show from the two conditions.

$$\frac{\partial}{\partial R} < n\Lambda | n'\Lambda > = 0$$

$$\frac{\partial^2}{\partial R^2} < n\Lambda | n'\Lambda > = 0$$

the following conclusions:

* the diagonal elements of the term (4.1) are purely imaginary:

$$\mathrm{Re} < n\Lambda \left| \frac{\partial}{\partial R} \right| n\Lambda > = 0 \qquad (4.6)$$

Since these matrix elements are generally real, they turn out to be nul.

* the real part of the diagonal elements of the term (4.2) are simply given by

$$\mathrm{Re} < n\Lambda \left| \frac{\partial^2}{\partial R^2} \right| n\Lambda > = - < \frac{\partial}{\partial R} n\Lambda \left| \frac{\partial}{\partial R} n\Lambda \right| > \qquad (4.7)$$

Since these matrix elements are real, this relation will give the matrix element itself.

* the non diagonal elements of the term (4.1) have the symmetry property

$$< n\Lambda \left| \frac{\partial}{\partial R} n'\Lambda > = - < \frac{\partial}{\partial R} n\Lambda \right| n'\Lambda > \qquad (4.8)$$

If we want to go further on the discussion, we must analyse some simple situations with simple models. We shall restrict ourselves to the two levels model. This model works in two different situations:

a) two different cores, one level (no excitation)

b) two identical cores, two levels (i.e. excitation of one level)

4.2-2 Two Levels Formulae

The situation a) occurs in the reactions

$$C^{13} + O^{16} \longrightarrow \begin{cases} O^{16} + C^{13} \\ O^{17} + C^{12} \end{cases}$$

since the Q of the reaction is - 0.804 MeV. The two reactions may occur at low energy (this is to be compared with the 0.874 MeV level of O^{17}. Furthermore the coulomb barrier are equal in the two channels.

The situation b) occurs in the reactions

$$O^{16} + O^{17} \longrightarrow O^{16} + O^{17}_{GS}$$
$$\searrow \quad O^{16} + O^{17}\ (0.874)$$

In both these cases, we write

$$|n\Lambda > = C^{\Lambda}_{1n}(R)\,|\ \Phi^{\Lambda}_{1j}(\underset{\sim}{r}_1) > + C^{\Lambda}_{2n}(R)\,|\ \phi^{\Lambda}_{2j'}(\underset{\sim}{r}_2) > \qquad (4.9)$$

where $|\phi^{\Lambda}_{1j}>$ and $|\phi^{\Lambda}_{2j'}>$ describe respectively the motion of the valence particle around the core formed either by one of the nuclei in interaction or by the other one.

For instance, in the first example, for $\Lambda = 1/2$ we write (see section 2)

$$|n\ 1/2 > = C^{\frac{1}{2}}_{1n}(R)\ |\Phi^{\frac{1}{2}}_{C^{1/2},\,1/2}(\underset{\sim}{r}_1) > + C^{\frac{1}{2}}_{2n}(R)\,|\Phi^{\frac{1}{2}}_{O^{16},\,5/2}(\underset{\sim}{r}_2) > \qquad (4.10)$$

where $|\Phi^{\frac{1}{2}}_{C^{12},\,1/2} >$ describes the $P_{1/2}$ orbit of the neutron in C^{13} while $|\Phi^{1/2}_{O^{16},\,5/2} >$ describes the $d_{5/2}$ orbit of this neutron in O^{17}; for the second example, taking into account the symmetry due to the identity of the two cores (see section 2), we write

$$|n\Lambda > = C^{\Lambda P}_{5/2,n}\,|\Phi^{\Lambda}_{5/2,P} > + C^{\Lambda P}_{1/2,n}\,|\Phi^{\Lambda}_{1/2,P} > \qquad (4.11)$$

where

$$|\Phi^{\Lambda}_{j,P} > = \frac{1}{\sqrt{2}}\,|\phi^{\Lambda}_{j}(\underset{\sim}{r}_1) + (-)^{P}\,\phi^{\Lambda}_{j}(\underset{\sim}{r}_2) >$$

Here $\Phi^{\Lambda}_{5/2}$. describes the fundamental state of O^{17} and $\Phi^{\Lambda}_{1/2}$ the first excited state (assumed to be a pure $S_{1/2}$ state).

From expression (4.9), the eq. (2.18) can be solved exactly and we obtain the two eigenfunctions

$$|1,\Lambda > = N\left[\phi^{\Lambda}_{1j} + \frac{E_1 - \Delta_{21} - H_{21}}{H_{22} - E_1 - \Delta_{22}}\,\phi^{\Lambda}_{2j'}\right] \qquad (4.12)$$

$$|2, \Lambda > = N\left[\frac{E_2 - \Delta_{12} - H_{12}}{H_{11} - E_2 - \Delta_{11}} \phi^{\Lambda}_{1j} + \phi^{\Lambda}_{2j'} \right] \qquad (4.13)$$

where N is a normalization factor (depending on R), Δ_{ij} and H_{ij} are the matrix elements defined by

$$\Delta_{ij} = \int \phi_{1i}(\underset{\sim}{r}_1)\phi_{2j}(\underset{\sim}{r}_2)d\underset{\sim}{r}_1 \ , \qquad H_{ij} = \int \phi_{1i}(\underset{\sim}{r}_1)\,\mathcal{H}_e\,\phi_{2j}(\underset{\sim}{r}_2)d\underset{\sim}{r}_1$$

The corresponding eigen energies are

$$E_{\underset{1}{-}} = E_1 + E_0 \qquad (4.14)$$

$$E_{\underset{2}{-}} = E_1 - E_0$$

where

$$E_1 = \frac{\Delta_{22} H_{11} + \Delta_{11} H_{22} - (\Delta_{21} H_{12} + \Delta_{12} H_{21})}{2(\Delta_{11} \Delta_{22} - \Delta_{12} \Delta_{21})} \qquad (4.15)$$

$$E_0 = \frac{\sqrt{\{\Delta_{22}H_{11}+\Delta_{11}H_{22} -(\Delta_{21} H_{12}+\Delta_{12}H_{21})\}^2 - 4(\Delta_{11}\Delta_{22}-\Delta_{12}\Delta_{21})(H_{11} H_{22} - H_{12} H_{21})}}{2(\Delta_{11} \Delta_{22} - \Delta_{12} \Delta_{21})}$$

From the properties of the matrix elements discussed in previous works (cf. W. Von Oertzen [3]) and C. Beccaria [12b]) it turns out that

$\mathrm{Lim}_{R\to\infty} \Delta_{ij} = \delta_{ij}$ (as an exponential)

$\mathrm{Lim}_{R\to\infty} H_{ij} = 0$

$\mathrm{Lim}_{R\to\infty} \dfrac{H_{ii}}{\Delta_{ii}} = \varepsilon_i$, where ε_i is the binding energy of the valence system x in the final state i. Therefore, as it is expected,

$$\left|{}^{1,\ \Lambda}_{(2)} > \longrightarrow \left|\phi^{\Lambda}_{1,j}\right.\right\rangle_{(2)} \qquad \text{(binding energy } \varepsilon_1\text{)}_{(2)}$$

To first order, one may write

$$\left|i\Lambda\right> \simeq N \left[\phi^{\Lambda}_{i,j} + \frac{\left[\varepsilon_i + V(R)\right] \Delta_{ki} - H_{ki}}{\varepsilon_k - \varepsilon_i} \phi^{\Lambda}_{k,j_k} \right] \qquad (4.16)$$

where $i + k = 3$ and $V(R)$ is the coulomb potential. From this expression it is easy to calculate the coupling terms, since we only need to calculate expressions of the type

$$\bar{\Delta}_{ik} = \int \phi^{\Lambda}_i{}^{*} \left(\frac{\partial}{\partial R} \phi^{\Lambda}_k \right) \underset{\sim}{dr}$$

and

$$\bar{F}_{ik} = \int \phi^{\Lambda}_i \left(\frac{\partial^2}{\partial R^2} \phi^{\Lambda}_k \right) \underset{\sim}{dr}$$

We notice that the functions ϕ^{Λ}_k are function of R in a very simple way, namely

$$\phi^{\Lambda}_k(\underset{\sim}{r} \pm \mu R \underset{\sim}{e}_3)$$

in other words,

$$\frac{1}{\mu} \frac{\partial}{\partial R} \phi^{\Lambda}_k = \pm \frac{\partial}{\partial r_z} \phi^{\Lambda}_k (r_x, r_y, r_z) \qquad (4.17)$$

and all the calculations can be performed simply using the recursion formulae of the spherical harmonics and of the spherical Bessel functions. Numerical results will be given in a forthcoming paper.

4.3 - THE CORIOLIS TERMS

We shall describe here the procedure which can be used to calculate

these terms. This method must be used also to calculate the matrix elements of the spin-orbit potential.

We shall use the expansion (4.9) to illustrate this procedure. In expressions (4.3) and (4.4) the operators $\Sigma_{\pm}$ and $\underset{\sim}{\Sigma}$ may be written as

$$\underset{\sim}{\Sigma} = \underset{\sim}{J'} + \underset{\sim}{\ell}$$

where $\underset{\sim}{J'}$ is the sum of all spins involved and $\underset{\sim}{\ell} = -i(\underset{\sim}{r} \Lambda \underset{\sim}{\bar{V}}_r)$ (in the moving frame). However, in expression (4.9), the wave functions are centered at the positions of the cores, i.e. $\phi^{\Lambda}_{\beta S}(r_\beta) = \phi^{\Lambda}_{\beta S}(r + \mu_\beta R\, e_3)$ where μ_β is a mass ratio depending on the index which takes on the value 1 or 2, given in eqs. (2.12b).

We must therefore translate the operator $\hat{\underset{\sim}{\ell}}$. We can write:

$$\hat{\underset{\sim}{\ell}} = -i(\underset{\sim}{r}_\beta - \mu_\beta R\, \underset{\sim}{e}_3)\Lambda\ \underset{\sim}{\bar{V}}_r$$

Noting that $\underset{\sim}{\nabla}_r\ \phi(\underset{\sim}{r}_\beta) = \underset{\sim}{\bar{V}}_{r_\beta}\ \phi(\underset{\sim}{r}_\beta)$, one obtains

$$\hat{\underset{\sim}{\ell}}\ \phi_{\beta S}(\underset{\sim}{r}_\beta) = \tilde{\underset{\sim}{\ell}}_\beta\ \phi_{\beta S}(\underset{\sim}{r}_\beta) + \tilde{\underset{\sim}{\mathcal{L}}}_\beta\ \phi_{\beta S}(\underset{\sim}{r}_\beta) \tag{4.18}$$

where

$$\tilde{\underset{\sim}{\ell}}_\beta = -i(r_\beta \Lambda \underset{\sim}{\bar{V}}_{r_\beta})$$

and

$$\tilde{\underset{\sim}{\mathcal{L}}}_\beta = i\mu_\beta R(\underset{\sim}{e}_3 \Lambda \underset{\sim}{\bar{V}}_{r_\beta}) \tag{4.19}$$

From these results, we can calculate all the matrix elements which we need for the operators Σ^2 and $\Sigma_{\pm}$: For any operator σ acting only on the intrinsic variables, we can write from (4.9)

$$< n\Lambda|\sigma|n'\Lambda > = \sum_{\alpha,\beta = 1,2} C^{\Lambda *}_{\alpha n}\ C^{\Lambda}_{\beta n'} < \phi^{\Lambda}_{\alpha S}(\underset{\sim}{r}_\alpha)|\sigma|\ \phi^{\Lambda}_{\beta S'}(\underset{\sim}{r}_\beta)>$$

The different matrix elements of interest are therefore

$$\langle\phi^{\Lambda}_{\alpha S}(\underset{\sim}{r}_\alpha)|\Sigma^2|\phi_{\beta S'}(\underset{\sim}{r}_\beta)\rangle = S'(S'+1)\Delta^{\Lambda}_{\alpha\beta} + \langle\phi^{\Lambda}_{\alpha S}(\underset{\sim}{r}_\alpha)|\mathcal{L}^2_\beta + \mathcal{L}_\beta\, S_\beta + S_\beta\,\mathcal{L}_\beta|\,\phi^{\Lambda}_{\beta S'}\rangle \quad (4.20a)$$

where $\underset{\sim}{S}_\beta = \underset{\sim}{\ell}_\beta + \underset{\sim}{J}'$ and

$$\langle\phi^{\Lambda}_{\alpha S}(\underset{\sim}{r}_\alpha)|\Sigma_\pm|\phi^{\Lambda\mp1}_{\beta S'}(\underset{\sim}{r}_\beta)\rangle = \sqrt{(S'\mp\Lambda+1)(S'\pm\Lambda)}\;\Delta^{\Lambda}_{\alpha\beta} +$$

$$+ \langle\phi^{\Lambda}_{\alpha S}(\underset{\sim}{r}_\alpha)|\mathcal{L}_{\beta\pm}|\,\phi^{\Lambda\mp1}_{\beta S'}(\underset{\sim}{r}_\beta)\rangle \quad (4.20b)$$

the second term of these expressions may be easily calculated using the Wigner-Eckart theorem and the gradiant formula. The result is

$$\langle\phi^{\Lambda}_{\beta' S}|\mathcal{L}^2_\beta|\phi^{\Lambda}_{\beta S'}\rangle = -R^2\,\mu^2_\beta\,\langle\phi^{\Lambda}_{\beta' S}|\,\Delta_{r_\beta} - \frac{1}{\mu^2_\beta}\,\frac{\partial^2}{\partial R^2}\,|\,\phi^{\Lambda}_{\beta S'}\rangle \quad (4.21)$$

$$\langle\phi^{\Lambda}_{\beta' S\ell j}|\mathcal{L}_\beta\cdot J'|\phi^{\Lambda}_{\beta S'\ell' j}\rangle = \sum_{\ell''}\langle\phi^{\Lambda}_{\beta' S\ell j}|\phi^{\Lambda}_{\beta S'\ell' j}\rangle(-1)^{S'-2\Lambda+j+\ell'}\times$$

$$\times\begin{Bmatrix}\ell'' & j & S'\\ j & \ell' & 1\end{Bmatrix}\sqrt{j(j+1)(2j+1)}\,\langle\ell''\|\mathcal{L}\|\ell'\rangle \quad (4.22a)$$

$$\langle\phi^{\Lambda}_{\beta' S\ell j}|\mathcal{L}_\mu|\phi^{\Lambda}_{\beta S'\ell' j}\rangle = \sum_{\ell'' S''}\langle\phi^{\Lambda}_{\beta' S\ell j}|\phi^{\Lambda}_{\beta S''\ell'' j}\rangle(-1)^{S''+S'+\ell''+j-\Lambda+1+\mu}\times$$

$$\times\begin{Bmatrix}\ell'' & \ell' & 1\\ S' & S'' & j\end{Bmatrix}\begin{pmatrix}S'' & 1 & S'\\ -\Lambda & \mu & \Lambda'\end{pmatrix}\sqrt{(2S''+1)(2S'+1)}\,\langle\ell''\|\mathcal{L}\|\ell'\rangle \quad (4.22b)$$

where

$$\langle\ell''\|\mathcal{L}\|\ell'\rangle = \mu_\beta\, R\,\langle\ell''\|\nabla\|\ell'\rangle$$

From (4.21) and (4.20) it is easy to show that

$$\frac{1}{R^2}\langle n\Lambda|\underset{\sim}{\Sigma}|n'\Lambda'\rangle = \frac{1}{R^2}\langle n\Lambda|\sum_\gamma (S_\gamma^2+\mathcal{L}_\gamma S_\gamma + S_\gamma \mathcal{L}_\gamma)\tilde{\delta}_\gamma - \hat{D}|n'\Lambda'\rangle$$

$$+ \langle n\Lambda \left| \frac{\partial^2}{\partial R^2} \right| n'\Lambda'\rangle - \langle n\Lambda|\sum_\gamma \mu_\gamma^2 \Delta_{r_\gamma} \tilde{\delta}_\gamma|n''\Lambda'\rangle \qquad (4.23)$$

where $\tilde{\delta}_\gamma$ means $\tilde{\delta}_\gamma|\phi^\Lambda_{\beta S'}\rangle = \delta_{\gamma\beta}\ |\phi^\Lambda_{\beta S'}$ and

$$\hat{D}|n\Lambda\rangle = \sum_\beta \frac{\partial^2}{\partial R^2} C^\Lambda_{\beta n}(R) + 2\frac{\partial}{\partial R} C^\Lambda_{\beta n}(R) \frac{\partial}{\partial R} \mid \phi^\Lambda_{\beta S}\rangle.$$

From these formulae, one can easily calculate the asymptotic values of the expression (4.20, 22) when $R \to \infty$: All the terms involving the gradiant formula vanish as well as all the non diagonal elements. This shows the results given by eqs. (3.12a).

The last term of eq. (4.23) looks like a correction to the term $2M\, E^\Lambda_n(R)$, it is a compensation to the recoil effect. Let us analyse these recoil corrections in the next subsection.

4.4 - RECOIL CORRECTIONS

As in DWBA calculations, the recoil corrections consist in taking into account the fact that the vectors $\underset{\sim}{R}$, $\underset{\sim}{R}_{AB}$ and $\underset{\sim}{R}_{CD}$ are not parallel (see fig.3).

We have shown in section 2, that this correction has two consequences. The first one is to take into account the difference between eqs. (2.29) and (2.11). In fact, one can rewrite (2.29) as

$$\left\{ -\frac{\Delta r_{Cx}}{2\, m_{Cx}} + \tilde{V}_{Cx} + \Delta_{r_{Cx}} \left(\frac{1}{2m_{Cx}} - \frac{1}{2m} \right) \right\} \phi = E_n(\infty)\phi \ ; \qquad (4.24)$$

the correction which we call H_{Cx} may be written as

$$H_{Cx} = \left(\frac{1}{2m_{Cx}} - \frac{1}{2m}\right) \Delta_{r_{Cx}} = \frac{1}{2} \frac{m_B}{m_C(m_B + m_C)} \Delta_{r_{Cx}} \tag{4.25}$$

We set

$$H_{corr} = \sum_{\gamma} H_{\gamma} \hat{\delta}_{\gamma} \tag{4.26}$$

In the no-recoil DWBA calculation, this correction is neglected, since it is of the order of $\frac{mx}{mc}$. First calculations have shown that if this correction may be of 10% for very unfavorable elastic scattering [12b], it is much more important for inelastic scattering where the reference is not the binding energy of x to the core c, but the excitations energies. Therefore, we shall show how to take these terms into account. It is very easy to check that

$$< n\Lambda|H_{corr}|n'\Lambda> = < n\Lambda \left|\sum_{\gamma} \frac{\mu_{\gamma}^2}{2M} \Delta_{r_{\gamma}} \hat{\delta}_{\gamma}\right| n'\Lambda > \tag{4.27}$$

which is the last term appearing in eq. (4.23). This gives the clue of the method to be used with the LCNO approximation. Instead of looking for eigenfunctions of $\mathcal{H}_e$ as it has been done up to now, we shall look for eigenfunctions of

$$\mathcal{H} = \mathcal{H}_e + H_{corr} \tag{4.28}$$

where $\mathcal{H}_e$ and H_{corr} are given respectively by eqs. (2.20) and (4.26). Let us call them $|\tilde{n\Lambda}>$, such that

$$\mathcal{H}|\tilde{n\Lambda} > = \tilde{E}_n^{\Lambda}|\tilde{n\Lambda} > \tag{4.29}$$

Since $\mathcal{H}$ has the same symmetry as $\mathcal{H}_e$, the quantum number Λ is not changed at all. The advantage of such a representation is that when $R \to \infty$ with fixed values of $\underset{\sim}{r}_{Cx}$ (or $\underset{\sim}{r}_{Bx}$) eq. (4.29) reduces to

$$\left(-\frac{\Delta_{r_{Cx}}}{2m_{Cx}} + V_{Cx} \right) | \tilde{\Phi}^{\tilde{\Lambda}}_n(\underset{\sim}{r}, \infty) > = \tilde{E}^{\tilde{\Lambda}}_n(\infty) | \tilde{\Phi}^{\tilde{\Lambda}}_n(\underset{\sim}{r}, \infty) > \tag{4.30}$$

which is exactly eq. (2.11) so that $\tilde{E}^{\tilde{\Lambda}}_n(\infty)$ is nothing but $(\varepsilon_A - \varepsilon_C - \varepsilon_x)$ as it should be. This overcomes the difficulty quoted through eq. (2.29). Then we rewrite eq. (2.8) as

$$\left(-\frac{\Delta R}{2M} + \tilde{V}_{CB}(\underset{\sim}{R}) + \mathcal{H}_e - H_{corr} \right) | \Phi > = (\varepsilon_C + \varepsilon_B + \varepsilon_x - E) | \Phi > \tag{4.31}$$

A straightforward calculation shows that the term $\sum_{n',\Lambda} < \tilde{n\Lambda} | 2M H_{corr} | \tilde{n\Lambda} > f^{\Lambda}_{n',J}(R)$ is added in the right-end side of eq. (3.6) and this term is just cancelled by the last term of (4.23), so that in the new representation with the LCNO approximation for real radial wave functions, eq. (3.6) reads

$$\left[-\frac{\partial^2}{\partial R^2} + \frac{J(J+1) - 2\Lambda^2}{R^2} + 2M \tilde{E}^{\tilde{\Lambda}}_n(R) - k^2 \right] f^{\Lambda}_{nJ}(R) =$$

$$\sum_{n'} \left\{ -\frac{1}{R^2} < \tilde{n\Lambda} | \sum_{\gamma} (S^2_{\gamma} + \mathcal{L}_{\gamma} S_{\gamma} + S_{\gamma} \mathcal{L}_{\gamma}) \hat{\delta}_{\gamma} - \hat{D} | \tilde{n'\Lambda} > \right\} f^{\Lambda}_{n',J}(R) +$$

$$+ \sum_{n' \neq n} 2 < \tilde{n\Lambda} \left| \frac{\partial}{\partial R} | \tilde{n'\Lambda} > \frac{\partial}{\partial R} f^{\Lambda}_{n',J}(R) - \frac{2M}{8\pi^2} (2J+1) \sum_{\Lambda' n'} < \tilde{n\Lambda} | D^J_{M\Lambda} \tilde{V}_{BC} D^{J*}_{M} | \tilde{n'\Lambda'} > f^{\Lambda}_{n',J}(R) + \right.$$

$$+ \frac{1}{R^2} \sum_{n'} \left\{ \sqrt{(J+\Lambda+1)(J-\Lambda)} < \tilde{n\Lambda} | \Sigma_- | \tilde{n'\Lambda+1} > f^{\Lambda+1}_{n',J}(R) + \right.$$

$$\left. \left. + \sqrt{(J-\Lambda+1)(J+\Lambda)} < \tilde{n\Lambda} | \Sigma_+ | \tilde{n'\Lambda-1} > f^{\Lambda-1}_{n',J}(R) \right\} \right] \tag{4.32}$$

in which several of the coupling terms have been cancelled. In the same way,

eq. (3.31) is simply reduced to

$$\tilde{A}^{J}_{\substack{nn' \\ \ell''\ell'}} = \sum_{\Lambda} (-1)^{\ell'-\ell''}(2\ell''+1) \begin{pmatrix} \ell'' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \Big\{ 2 < \tilde{n\Lambda} \Big| \frac{\partial}{\partial R} \Big| \tilde{n'\Lambda} > \frac{\partial}{\partial R} -$$

$$- \frac{1}{R^2} <\tilde{n\Lambda} \mid \sum_{\gamma} (S^2_{\gamma} - S'(S'+1) + \mathcal{L}_{\beta} S_{\beta} + S_{\beta}\mathcal{L}_{\beta})\hat{\delta}_{\gamma} - \hat{D} \mid \tilde{n'\Lambda} > \Big\}. \qquad (4.33)$$

The second effect of the recoil appears in the asymptotic expression of as shown in eq. (2.13).

We must therefore introduce these phase factors into the molecular wave function, i.e., we look for solutions of eq. (2.8) which reads

$$|\psi > = \sum_{n\Lambda} \chi^{\Lambda}_{n}(\underset{\sim}{R})\, e^{i\, \underset{\sim}{k}_n \cdot \underset{\sim}{r}} | \tilde{\Phi}^{\Lambda}_{n}(\underset{\sim}{r}, R) >$$

with $\underset{\sim}{k}_n = k_{fn} \frac{m_{nx}}{m_n} \frac{\underset{\sim}{R}}{|\underset{\sim}{R}|}$ where the index n labels B or C according as the state n has for limit a nuclear state in which x is bound to B or C. Since $e^{i\, \underset{\sim}{k}_n \cdot \underset{\sim}{r}}$ is invariant in rotations, this factor will only change the equation leading to the molecular wave functions. Asymptotically, the energy $E^{\Lambda}_{n}(R)$ will be shifted as it should be. The relative motion eq. (3.6) or (3.29) will not be changed in shape but this correction introduces matrix elements which depend on the transfered momentum.

V. CONCLUSIONS

In this paper, we have shown that a theory of nuclear reactions can be written in the framework of the molecular orbitals description of intermediate states. This approach leads to an extension of the unified model of deformed nuclei of Bohr and Mottelson to the continuum states and therefore leads naturally to a description of the scattering process in the helicity scheme.

If the equations can be written formally in any case, including all spin couplings, the solution of these equations can be given only in simple situation which fortunately appears in many actual experiments. Namely when the two states approximation as well as the adiabatic approximation can be used; W. Von Oertzen et al. have given many such examples.

This formalism is particularly well suited for the analysis of the so-called elastic and elastic-transfer reactions. These are also analysed using the DWBA formalism [13, 14] and the resonating group method [8] for light nuclei, leading to interesting comparisons, and to the search for the existence of "nuclear molecular" states. This method can be used also if the nuclei are described in the weak-coupling model since core-excitations may be included simply in this formalism. We have shown that several coupling terms can be cancelled if one defines intrinsic states which are eigenstates of a symmetrized intrinsic hamiltonian.

We have also shown how the unadiabatic corrections which are not cancelled, including the Coriolis corrections could be calculated. They give rise to transitions in the angular momentum of the relative motion of the two cores. Finally we have indicated the procedure to take into account the recoil corrections which complicate the analysis.

These two types of corrections as welll as the strong spin orbit orbit coupling which occurs in this nuclear problem make the difference with the analysis of ions-electrons collisions, although the search for Coriolis coupling and recoil corrections are also in progress.

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APPENDIX 1

Using the transformation rules of ref. 21 one gets easily the following relation

$$\underset{\sim}{L} = \underset{\sim}{L}' + \underset{\sim}{\lambda} - \underset{\sim}{\ell}$$

where $\underset{\sim}{L}$ is the angular momentum operator $\underset{\sim}{R} \wedge \underset{\sim}{P}_R$ corresponding to $\underset{\sim}{r}$ fixed in the fixed frame, while $\underset{\sim}{L}'$ is the same operator but for x fixed in the moving frame so that:

$$\underset{\sim}{L}' |\Phi_n^{\Lambda}(\underset{\sim}{r}, R)> = 0 \ .$$

Furthermore $\underset{\sim}{\ell}$ is the angular momentum operator of the particle x, i.e. $\underset{\sim}{\ell} = \underset{\sim}{r} \wedge \underset{\sim}{p}_r$ and $\underset{\sim}{\lambda} = \ell_\zeta(\underset{\sim}{\zeta} + \cot \beta \ \underset{\sim}{\xi})$ in the moving frame where $\ell_\zeta = -i \frac{\partial}{\partial \phi}$ and the different vectors are given in fig. 4 of the text. A straightforward calculation shows that the sum $\underset{\sim}{L}' + \underset{\sim}{\lambda} = \underset{\sim}{\mathcal{L}}$ is nothing but the angular momentum of the rigid body formed with the cores B and C and the particle x fixed in the moving frame. Therefore $\underset{\sim}{L} = \underset{\sim}{\mathcal{L}} - \underset{\sim}{\ell}$. One must not forget that the operator $\frac{\partial}{\partial \phi}$ which appears in $\underset{\sim}{\mathcal{L}}$ (through $\underset{\sim}{\lambda}$) acts also on the intrinsic wave functions $|\Phi_n^{\Lambda}(\underset{\sim}{r})>$.

APPENDIX 2

In deriving the eq. (3.6), we have written the molecular wave function in the system fixed to the cores. Then, in order to carry out the differentiation with respect to the cores variables the form of the derivatives were changed as was discussed in section 3. Another alternative may can be to write the molecular wave function in the space fixed coordinate system so that the derivatives operators maintain their form. We aim to discuss this in this appendix.

We still write the total wave function as discussed in section 3.

$$|\psi(\underset{\sim}{R}, \underset{\sim}{r}) > = \sum_{n\Lambda} \chi_n^{\Lambda}(\underset{\sim}{R}) \; |\Phi_n^{\Lambda}(\underset{\sim}{r}, R) > \tag{A.1}$$

with

$$\chi_n^{\Lambda}(R) = \sum_{JM} (2J+1) \; \frac{f_{MJ}^{\Lambda M}(R)}{R} \; D_{M\Lambda}^{J^*}(\alpha,\beta,0) \tag{A.2}$$

Developing the molecular wave function in the nuclear-orbitals basis, as

$$|\Phi_n^{\Lambda}(\underset{\sim}{r}, R) > = \sum_{S,\alpha \; = \; 1, \; 2} C_{S\alpha}^{n\Lambda}(R) |\Phi_n^{S\Lambda}(\underset{\sim}{r}_{\alpha}) > , \tag{A.3}$$

or in the fixed frame

$$|\Phi_n^{\Lambda}(\underset{\sim}{r}, R) > = \sum_{S,\alpha \; = \; 1, \; 2} C_{S,\alpha}^{n}(R) \sum_{M_S} D_{M_S\Lambda}^{S}(\alpha,\beta,0) |\Phi_{M_S}^{S}(\underset{\sim}{r}_{\alpha}) > \tag{A.4}$$

We now combine formulae (A.4), (A.3) and (A.2) to obtain the total wave function

$$|\psi(\underset{\sim}{R}, \underset{\sim}{r}) > = \sum_{n\Lambda} \sum_{\substack{JM \\ SM_S}} (2J+1) \; \frac{f_{nJ}^{M\Lambda}(R)}{R} \; D_{M\Lambda}^{J^*}(\alpha,\beta,0) \; D_{M_S\Lambda}^{S}(\alpha,\beta,0) | \; \Phi_{M_S}^{S} > \tag{A.5}$$

Noticing that

$$D^{J*}_{M\Lambda}(\Omega) D^{S}_{M_S\Lambda}(\Omega) = (-1)^{\Lambda-M} \sum_{LM_L} \sqrt{2L+1} \begin{pmatrix} J & S & L \\ -M & M_S & m \end{pmatrix} D^{L*}_{mo}(\Omega) \begin{pmatrix} J & S & L \\ -\Lambda & \Lambda & 0 \end{pmatrix}$$

the eq. (A.5) can be rewritten as

$$|\psi(\underset{\sim}{R}, \underset{\sim}{r}) > = (4\pi)^{1/2} \sum_{\substack{JMSM_S \\ \Lambda n\, L\, m}} (-)^{M_S-\Lambda} \sqrt{2L+1}\,(2J+1) \frac{f^{\Lambda M}_{nJ}(R)}{R} \begin{pmatrix} J & S & L \\ -M & M_S & m \end{pmatrix} x$$

$$x\, Y^{-m}_{L}(\hat{R}) \begin{pmatrix} J & S & L \\ -\Lambda & \Lambda & 0 \end{pmatrix} C^{n\Lambda}_{S}(R)\ |\Phi^{S}_{M_S} >$$

In the case of identical cores this function must be symmetrical or antisymmetrical in the interchange of the two cores. Then we must have

$$|\psi(\underset{\sim}{R}, \underset{\sim}{r}) > = (-1)^{2J_C} P_{BC} |\psi(\underset{\sim}{R}, \underset{\sim}{r}) > , \qquad (A.7)$$

as from (A.6), we have

$$P_{BC} |\psi(\underset{\sim}{R}, \underset{\sim}{r}) > = (-)^{L+2J_C+J_{BC}+P-\pi} |\psi(\underset{\sim}{R}, r) > , \qquad (A.8)$$

Consequently $L + J_{BC} + P - \pi$ must be even, which is the selection rule (3.42). Inserting (3.28) into expression (A.6), one obtains:

$$|\psi(\underset{\sim}{R},\underset{\sim}{r})> = \frac{(4\pi)^{1/2}}{R} \sum_{\substack{JMM_S S'' \\ nLm\alpha=1,2}} \left[(2L+1)(2\ell+1)\right]^{1/2} (2J+1)\,(-)^{S-S'+M_S-M-\ell}\, i^{\ell} \begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} x$$

$$\begin{pmatrix} L & S'' & J \\ m & M_S & -M \end{pmatrix} Y^{-m}_{L}(\hat{R})\, \psi^{J}_{\substack{L\ell\alpha \\ (nS')SS''}}(KR)|\ \Phi^{S''}_{M_S}(\underset{\sim}{r}_\alpha) > \qquad (A.9)$$

where the function $\psi^{J}_{L\ell\alpha\ (nS')SS''}(KR)$ describing the relative motion of the two cores in the fixed frame is given by

$$\psi^{J}_{L\ell\alpha\ (nS')SS''}(KR) = \sum_{\ell'} (-1)^{\ell'} \psi^{J}_{\ell'\ell\ (nS')S}(KR)\, G^{Jn}_{L\ell'\alpha\ S''S}(R)\, \sqrt{2\ell'+1} \tag{A.10}$$

where

$$G^{Jn}_{L\ell'\alpha\ S''S}(R) = \sum_{\Lambda} \begin{pmatrix} \ell' & S' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} \begin{pmatrix} L & S'' & J \\ 0 & \Lambda & -\Lambda \end{pmatrix} C^{n\Lambda}_{S''\alpha}(R) \ . \tag{A.11}$$

When $R \to \infty$, it has been shown in the text (see 2.24) that

$$C^{n\,\Lambda}_{S''\alpha}(R) \xrightarrow[R \to \infty]{} \delta_{S'S''}\ \delta_{\alpha\, 1(2)}$$

Therefore

$$G^{Jn}_{L\ell'\alpha\ S''S}(\infty) = \frac{\delta_{L\ell'}\ \delta_{S'S''}}{2\ell' + 1}$$

and

$$\psi^{J}_{L\ell\alpha\ (nS')SS''}(KR) \longrightarrow \frac{(-1)^{L}}{\sqrt{2L+1}}\ \psi^{J}_{L\ell\ S'S}(KR)\ \delta_{S'S''} \ , \tag{A.12}$$

where the function $\psi^{J}_{L,\ell\ S'S}$ is the function introduced in (3.14) as it can be checked immediately, since

$$|\psi(\underset{\sim}{R}, \underset{\sim}{r})> \longrightarrow \frac{(4\pi)^{1/2}}{R} \sum_{\substack{J\ M\ M_S \\ L\ m\ \ell}} i^{\ell} \sqrt{2\ell+1}\ (2J+1)(-)^{S-S'+M_S-M+L-\ell}\ x$$

$$\begin{pmatrix} \ell & S & J \\ 0 & M & -M \end{pmatrix} \begin{pmatrix} L & S' & J \\ m & M_S & -M \end{pmatrix} Y^{-m}_{L}(\hat{R})\ \psi^{J}_{L\ell\ S'S}(KR)\ |\Phi^{M}_{S'}(\underset{\sim}{r})> \tag{A.13}$$

which is exactly the expression given by R. G. Newton [20] in its eq. (15.12) for $\hat{k} = 0$. This shows that the asymptotic expression (3.17) given for $\psi^{J}_{\ell',\ell}(kR)$ $(nS')S$ are correct.

FIGURE CAPTIONS

Figure 1: Representation of the two center potential resulting from the superposition of the potentials defining the two interacting nuclei, when they are at their closest distance of approach (situation (b) of figure 2). The inner shells (hatched area) define the two innert cores.

a) one particle on the last shell is exchanged;
Ex.: $O^{16} + O^{17} \rightarrow O^{16} + O^{17}$

b) one hole on the last shell is exchanged;
Ex.: $O^{16} + N^{15} \rightarrow O^{16} + N^{15}$

Figure 2: Sketch of the adiabatic approximation in the scattering of heavy ions formed with a core plus valence nucleons.

a) incoming asymptotic state
b) intermediate state: molecular state (multi-step exchange)
c) d) asymptotic final states.

Figure 3: Diagram of the different variables used in the text. The letters B and C label the two cores, x the exchanged nucleon (or hole), G_D and G_A the centers of mass of the nuclei D and A and G_{BC} the center of mass of the two cores.

Figure 4: The different frame of references used in the model

a) The laboratory fixed frame (referred to as the fixed frame in the text) with the three axis labelled by X, Y, Z. In this frame the position of the two cores is given by the angles α and β and by their relative distance R; we have also indicated the position of the moving frame with the three axis.

b) The moving frame. This moving frame has its axis defined by the direction BC of the two cores; the axis is always in the plane XoY (see (a)), this means that the Euler angle γ is set equal to zero; we have sketched the vector r in this moving frame.

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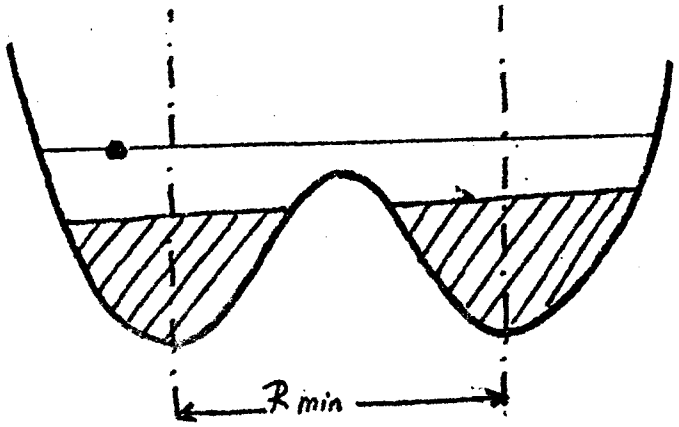
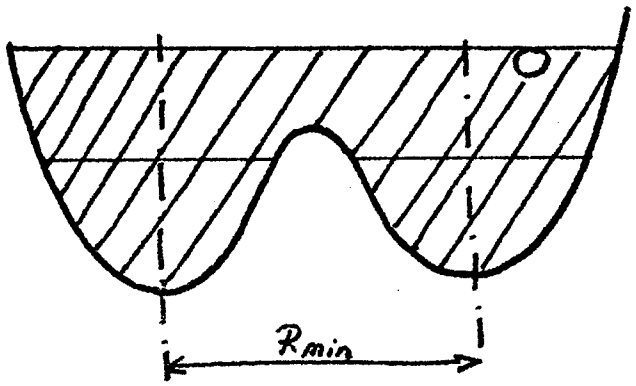


(a)

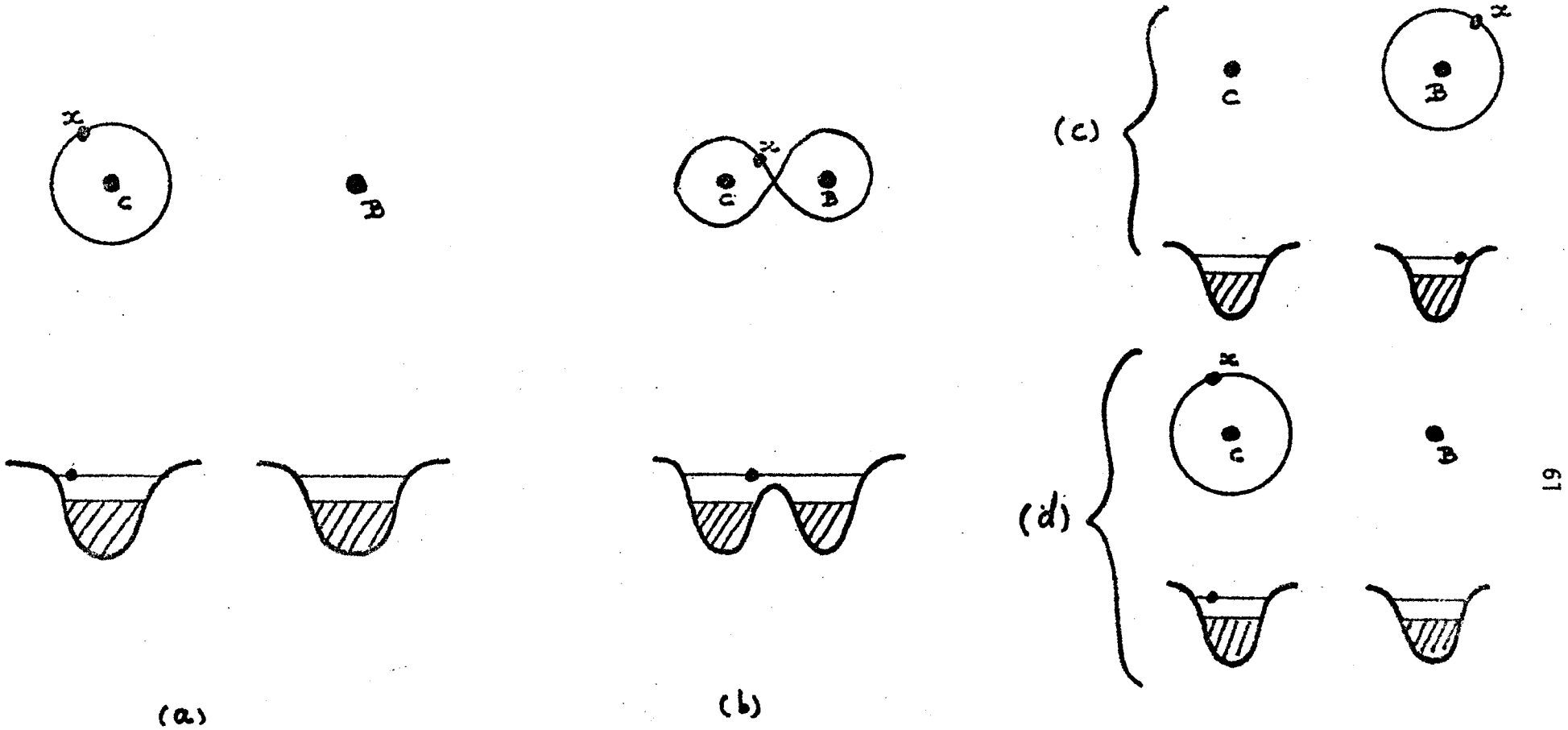


(b)

Ex: $^{16}O + {}^{17}O \rightarrow {}^{16}O + {}^{17}O$

Ex: $^{16}O + {}^{15}N \rightarrow {}^{16}O + {}^{15}N$

Figure 1



Sketch of the adiabatic approximation in the scattering of heavy ions formed of a core plus valence nucleons

a) incoming asymptotic state

b) intermediate state : "molecular state" (multistep exchange)

c)d) asymptotic final states

Figure 2

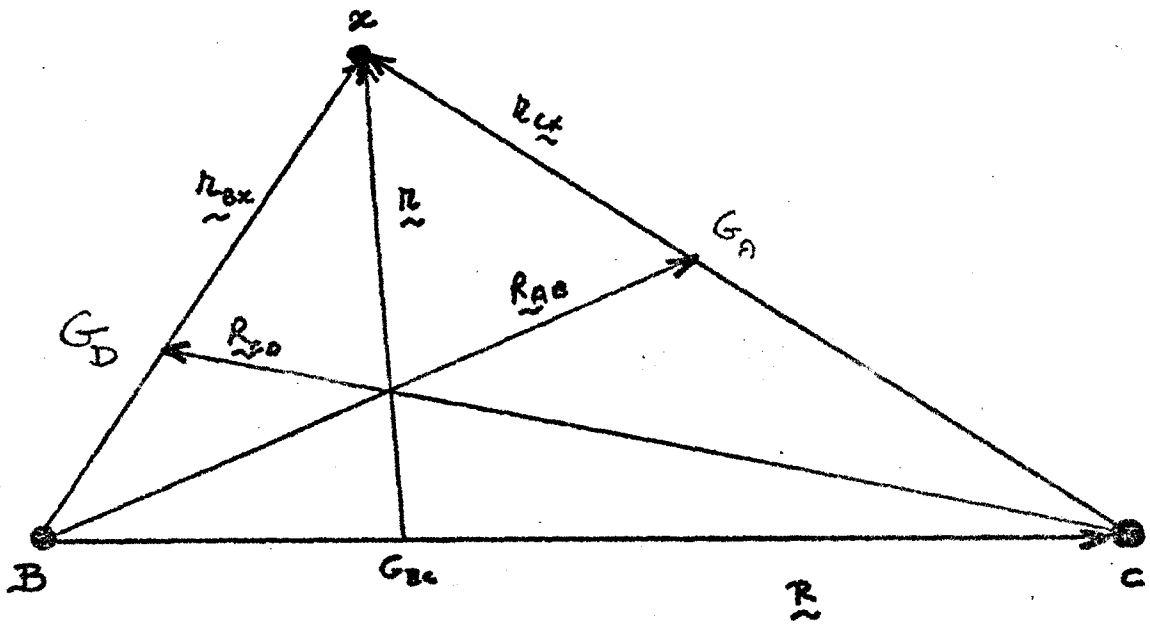


Figure 3

Fig. 4