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NUCLEON MOLECULAR ORBITALS AND THE TRANSITION MECHANISM  
BETWEEN MOLECULAR ORBITALS IN NUCLEUS-NUCLEUS COLLISIONS<sup>†</sup>

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in Tandem Energy Region.

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## abstract:

The molecular orbitals of the nucleon(s) in nucleus-nucleus collisions are dynamically defined as a linear combination of nucleon single-particle orbits (LCNO) in a rotating frame by using the coupled-reaction-channel (CRC) theory. Nucleon molecular orbitals and the promotions of nucleon, — especially due to the Landau-Zener radial coupling are discussed with the method above mentioned.

## 1. Introduction

The formation of the molecular orbitals of nucleons in heavy-ion collision processes has been the subject of various studies since for about thirty years [1-4]. The investigation of this problem was started in close to analogy to the molecular orbitals of electrons in atomic collisions. Nucleon molecular orbitals, however, are clearly different from the electron molecular orbitals in that they are strongly affected in the dynamical situation of the collisions and are to be treated completely in a quantum mechanical way at least for light heavy-ion systems. Recent progress, both from the experimental and theoretical side give evidence that at energies close to the Coulomb barrier strong coupling effects (9) and formation of molecular orbital formation can be observed (see ref.10,11).

Here we briefly show the main features of the theory [3] and the calculation of the molecular orbitals for the systems of light heavy-ions, and discuss the transition mechanism in the collision processes. Special attention is paid on the dynamical effects of the heavy-ion collisions on the formation of molecular orbitals and the nucleon promotion phenomena.

## 2. Sketch of the treatment of nucleon molecular orbitals

We assume that the system consists of two inert cores and the valence nucleon(s), which forms molecular orbitals around the core nuclei. Also, it is assumed that the molecular orbitals can be expanded by the eigen functions of

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bound/resonance states of the fragments of the collision processes (two fragments)[2];

$$M\Psi = \text{linear combination of nucleon orbitals (LCNO), } \psi_{\alpha}, \quad (1)$$

where M is the projection operator ( $M^2 = M$ ) of the truncation of nucleon molecular orbitals concerned. The wave function  $M\Psi$  obeys the equation,

$$M(E - H_{\text{eff}})M\Psi = 0. \quad (2)$$

The operator  $H_{\text{eff}}$  is the effective total Hamiltonian of the system. The wave function  $\psi_{\alpha}(R_{\alpha}, C_1, C_2)$  is the eigen function of the intrinsic Hamiltonian  $H^{\alpha}$  of the two fragment nuclei,

$$H^{\alpha}\psi_{\alpha}(R_{\alpha}, C_1, C_2) = \epsilon_{\alpha}\psi_{\alpha}(R_{\alpha}, C_1, C_2), \quad (3)$$

and they are not necessarily orthogonal to each other.

The orthogonal basis functions  $\phi_{\alpha}^{JM\Pi}$  are constructed as the eigen functions of the total angular momentum J and the parity  $\Pi$  by orthogonalizing the channel wave functions,  $\{\hat{\phi}_{\alpha}^{JM\Pi}\}$ , which include the angular part of the relative motion as well as the wave functions  $\psi_{\alpha}$ , mentioned above.

By using the orthogonal set  $\{\phi_{\alpha}^{JM\Pi}\}$ , we can make the expansion,

$$M^{JM\Pi}\psi^{JM\Pi} = \sum_{\alpha} \phi_{\alpha}^{JM\Pi} u_{\alpha}^{JM\Pi}(r)/r. \quad (4)$$

Hereafter we drop the superscript (JM $\Pi$ ) as far as there is no source of confusion. Inserting the above equation into eq.(2), we get the radial CRC equation for the radial relative wave function  $u(r) = (u_1(r), u_2(r), \dots, u_n(r))$ ,

$$\begin{aligned} & [E - (-\frac{\hbar^2}{2\mu_{\alpha}} \frac{d^2}{dr_{\alpha}^2} + \frac{\hbar^2}{2\mu_{\alpha}} \frac{L^2(\hat{r}_{\alpha})}{r_{\alpha}^2} + \epsilon_{\alpha})] u_{\alpha}(r_{\alpha}) = \\ & = \sum_{\beta} \int dr_{\beta} (U_{\alpha\beta}^D(r_{\alpha}) \delta(r_{\alpha} - r_{\beta}) + K_{\alpha\beta}^t(r_{\alpha}, r_{\beta}) + \Delta M_{\alpha\beta}(r_{\alpha}, r_{\beta})) u_{\beta}(r_{\beta}), \end{aligned} \quad (5)$$

or in matrix form,

$$(E - (T + R + \epsilon + U^D + K^t + \Delta M))u = 0, \quad (6)$$

where  $T$  is the operator of the radial kinetic energy and  $R$  the operator of the angular part of the relative motion. The interaction  $U^D$  is the effective interactions responsible for the "direct processes" and the  $K^t$  and  $\Delta M$  the effective interaction responsible for the "transfer processes". The  $K^t$  and  $\Delta M$  also generate the direct processes. The operator  $K^t$  and  $\Delta M$  is given, with the use of the transition operator  $K_{\alpha\beta} = \langle \hat{\phi}_\alpha, (V_{nC} + V_{CC}) \hat{\phi}_\beta \rangle$ , as,

$$K^t = \frac{1}{2\sqrt{N}} (K - NU^D + (K - NU^D)^T) \frac{1}{\sqrt{N}}, \quad (7)$$

$$\Delta M = \sum_{n=i}^{\infty} \frac{1}{n!} \frac{1}{2} \left(-\frac{1}{2}\right) \dots \left(\frac{1}{2} - n + 1\right) \sum_{k=0}^{n-1} N^{(1)k} [N^{-1/2}, \{K - NU^D - (K - NU^D)^T\}] N^{(1)n-k}, \quad (8)$$

where  $N$  is the overlap kernel  $N = \{N_{\alpha\beta}^{(1)}(r_\alpha, r_\beta)\}$  of the wave functions of the non-orthogonal system  $\{\hat{\phi}_\alpha\}$ , and  $N^{(1)} = N - I$ . The operator  $(K - NU^D)^T$  is the transposed operator of  $K - NU^D$ .

The most important feature of the above radial CRC equation is that there remain only interactions, which do not contain the kinetic energy operator  $T$ , or the total energy  $E$  in contrast to the CRC equation with the non-orthogonal system  $\{\hat{\phi}_\alpha\}$ , which is employed in usual treatment of the CRC theory [5]. We neglect the term  $\Delta M$ . This is because the overlap kernel  $N^{(1)}$  is small compared to unity in the grazing region.

The operator  $K^t$  contains so-called transfer form factors  $K$  and  $K^T$  of the post and prior forms "in a symmetric way" and is modified by the overlap kernel  $N$ . The most important problem on the treatment of the transfer interactions  $K$  and  $K^T$  is of the non-locality coming from the recoil effects of the transfer [5]. The non-locality causes not only the problem of the complexity of the treatment of the CRC equation but also the problem of the unique definition of the molecular axis of the system, which is needed in our discussion of molecular orbitals.

In our effective interaction  $K^t$ , however, this problem can be avoided at least at low energies, by employing a local approximation with  $r_\alpha \doteq r_\beta$ , because of the symmetric form of the  $K^t$  with respect to the  $K$ . The calculations with this approximation show almost the same results as the exact non-local calculation in the one-step DWBA.

Thus, we have a radial CRC equation, which contains "local" effective interaction  $U^{\text{tot}}$  alone,

$$U^{\text{tot}} = R + \epsilon + U^D + K^t. \quad (9)$$

The molecular orbital states  $\phi_p$  concerned here are defined with the diagonalization of the above interaction  $U^{\text{tot}}$  at each point of the relative radial distance  $r$ , and we obtain the adiabatic potential  $\mathcal{V}_p(r)$  for each state  $p$ ,

$$\mathcal{V}_p(r) = \{A^{-1}(r)U^{\text{tot}}(r)A(r)\}_{pp}, \quad (10)$$

and for the molecular orbitals

$$\phi_p = \sum_{\alpha} \phi_{\alpha} A_{\alpha p}(r). \quad (11)$$

The transformation matrix  $A(r)$  is equal to unit operator  $I$  at the infinity of  $r$ :

$$A(r) \rightarrow I. \quad (12)$$

In a second step, to obtain radial CRC equations with the use of the molecular orbital states  $\phi_p$  as the basis wave functions, we again expand the total wave function  $M\Psi$ ,

$$M\Psi = \sum_{p=1}^n \phi_p w_p(r)/r, \quad (13)$$

and get the following new CRC equation,

$$[E - (T + \mathcal{V}_p(r))]w_p(r) = \sum_q \Delta\mathcal{V}_{pq}(r)w_q(r), \quad (14)$$

with

$$\Delta\mathcal{V}_{qp}^{(1)}(r) = \Delta\mathcal{V}_{qp}^{(1)}(r) \frac{d}{dr} + \Delta\mathcal{V}_{qp}^{(2)}(r), \quad (15)$$

$$\Delta\mathcal{V}_{qp}^{(1)}(r) = -\frac{\hbar^2}{\mu} \left\{ A^{-1}(r) \frac{dA(r)}{dr} \right\}_{qp}, \quad (16)$$

$$\Delta\mathcal{V}_{qp}^{(2)}(r) = -\frac{\hbar^2}{2\mu} \left\{ A^{-1}(r) \frac{d^2 A(r)}{dr^2} \right\}_{qp}. \quad (17)$$

The adiabatic potentials  $\mathcal{V}_p(r)$  as well as the  $\phi_p$  and the radial couplings  $\Delta\mathcal{V}_{qp}(r)$  have been defined with the inclusion of the rotational operator  $R$ . Thus, these quantities depend on the total angular momentum  $J$  and the  $\phi_p$ 's are mixed states of the projection  $K$  on the molecular axis of the total angular momentum  $J$  in general (rotating molecular orbitals, RMO).

The  $S$ -matrix obtained from the above new CRC equation is identical to that obtained from the CRC equation with the original CRC-basis-function set

$\{\phi_\alpha\}$  (or  $\{\hat{\phi}_\alpha\}$ ), because they are equivalent to each other through the transformation matrix A in eq.(10). This CRC equation contains the concept of the molecular orbitals themselves, which enables us to discuss different phenomena.

### 3. Molecular orbital states and the transition mechanism

The transitions between rotating molecular orbital states used in our approach are generated by the radial coupling interactions  $\Delta V_{qp}(r)$  alone, by using the adiabatic potentials  $V_p(r)$  as the distorting potentials. This is in contrast to many other approaches where rotational coupling has to be considered explicitly for the transitions.

A particular transition mechanism between molecular orbitals, the Landau-Zener transition, attracts strong attention [6]. The Landau-Zener transition is generated by the radial coupling with a strong and sharp peak at a distance  $r (=r_0)$ , where two different adiabatic potentials cross each other [7-10] (avoided crossings).

In our model there appear three kinds of the crossings in general:

- i) crossing at small distance, where the Coriolis interaction, which is proportional to  $r^{-2}$ , plays the dominant role in the diagonalization (10).
- ii) crossings which occur in the nuclear interaction region.
- iii) crossings at distances larger than the grazing distance  $r_g$ , where again the Coriolis interaction becomes strong compared to the nuclear interaction.

The crossings at small distances are not so important because of the strong absorption effects and the formation of compound nucleus. The crossings in the grazing region are interesting and very important because transitions at these points are caused dominantly by nuclear interaction; they should be manifest in transfer and inelastic reactions.

At the distances larger than  $r_g$  the transitions between molecular-orbital states are strongly affected by the Coriolis interaction. Thus, the transition mechanism strongly depends on the total angular momentum J in general.

We consider the molecular orbitals of a neutron for the systems of core nuclei,  $^{12}\text{C}+^{12}\text{C}$ ,  $^{12}\text{C}+^{14}\text{C}$ ,  $^{12}\text{C}+^{16}\text{O}$  and  $^{16}\text{O}+^{16}\text{O}$ . We use as basis functions the single particle orbitals, 1p1/2, 2s1/2 and 1d5/2 in  $^{13}\text{C}$ , and 2s1/2 and 1d5/2 in  $^{15}\text{C}$  (or  $^{17}\text{O}$ ), which correspond to the states of  $^{15}\text{C}(\text{gr.}1/2^+, \text{ and } 0.90 \text{ MeV}, 5/2^+)$  (or  $^{17}\text{O}(\text{gr.}5/2^+, \text{ and } 0.87 \text{ MeV}, 1/2^+)$ ), respectively. In the

asymptotic region each molecular-orbital state approaches a sub-channel state in the original CRC basis.

In fig.1 the adiabatic potentials  $\sqrt{V}(r)$  and the radial couplings  $\Delta\sqrt{V}_{qp}^{(1)}(r)$  are shown for the state of  $J^\Pi = 1/2^+$  for the system  $^{13}\text{C}+^{14}\text{C}-^{12}\text{C}+^{15}\text{C}$ . The adiabatic potential for the lowest state of the molecular orbitals is strongly lowered from the original CRC diagonal potential (of the ground state) reflecting the strong coupled-channel effects.

The ground state of the molecular orbitals is a highly mixed state of  $k=1/2$  with components of the respective single-particle orbitals,  $2s1/2$ ,  $1d5/2$  of  $^{13}\text{C}$ ,  $2s1/2$ ,  $1d5/2$  of  $^{15}\text{C}$ , and  $1p1/2$  of  $^{13}\text{C}$ . This state takes the configuration of a covalent molecule, whose property is enhanced by the hybridization of the different-parity single-particle states of  $1p1/2$  and other  $sd$  orbitals [3].

In the collision transitions occur from the ground state of the molecular orbitals ( $p=1$ ) and to other states, especially to the state of  $p=2$ , at the distances  $r > r_g$ . The radial coupling  $\Delta\sqrt{V}_{12}(r)$  between the states of  $p = 1$  and  $2$  has a bump at  $r > r_g$ , suggesting the occurrence of the "Landau-Zener" like transition at  $r = r_1$  (see fig.1).

The same situation is found in the system  $^{12}\text{C}+^{13}\text{C}$  [3], in states of positive total parity  $\Pi=+$ . Compared with the coupling interaction between the original CRC basis functions corresponding to the  $p = 1$  and  $2$ , the radial coupling  $\Delta\sqrt{V}_{21}(r)$  is very strong at  $r > r_g$ , i.e., outside of the potential barrier. Thus, we have strong enhancement of the transition amplitudes between the states  $p = 1$  and  $2$  at energies lower than the Coulomb barrier. This is seen in fig.2, where the interaction  $\Delta\sqrt{V}_{12}(r)$  generating the inelastic scattering  $^{13}\text{C}(^{12}\text{C}, ^{12}\text{C})^{13}\text{C}^*(1/2^+)$  is shown.

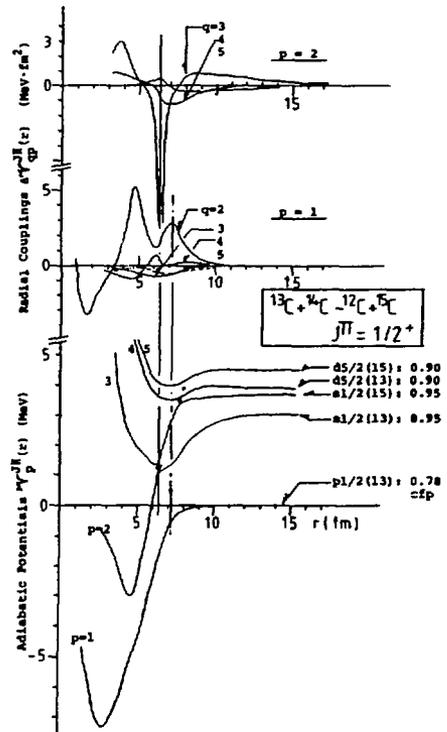


Fig.1. Adiabatic potentials and the radial couplings for the system  $^{13}\text{C}+^{14}\text{C}-^{12}\text{C}+^{15}\text{C}$  in  $J^\Pi = 1/2^+$ .

In the system  $^{12}\text{C}+^{13}\text{C}$  for the state of the total negative parity  $\Pi=-$  the behaviour of the radial coupling  $\Delta V_{12}(r)$  is different from those mentioned above, that is, the avoided crossing is located just behind the potential barrier, and  $\Delta V_{12}(r)$  has a very sharp peak at  $r=r_1$  (see fig.2), however, it almost vanishes outside the barrier.

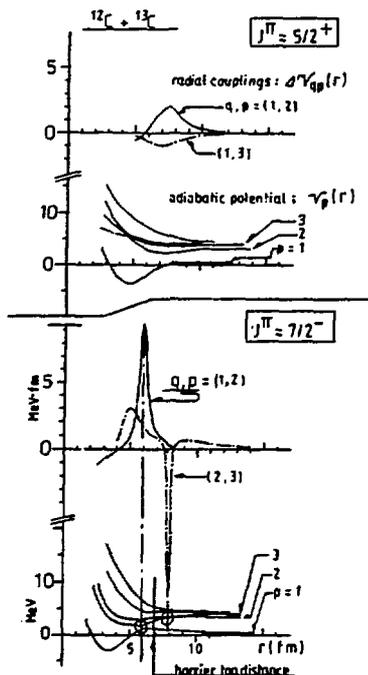


Fig.2. Adiabatic potentials and the radial couplings of the system  $^{12}\text{C}+^{13}\text{C}$  in the states of  $J^{\Pi} = 5/2^{+}$  and  $7/2^{-}$ .

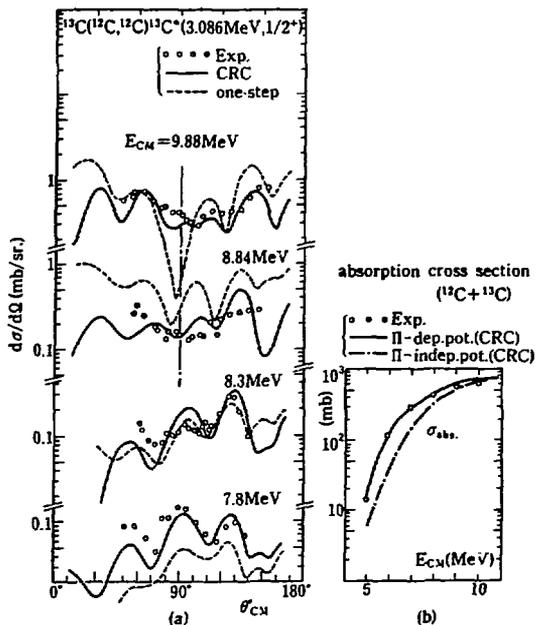


Fig.3. (a) Differential cross sections of  $^{13}\text{C}(^{12}\text{C}, ^{12}\text{C})^{13}\text{C}^*(1/2^{+})$  and (b) the absorption cross sections of the elastic scattering of  $^{13}\text{C}$  on  $^{12}\text{C}$ .

This coupling discussed above induces fast changes in the angular distributions of the inelastic scattering  $^{13}\text{C}(^{12}\text{C}, ^{12}\text{C})^{13}\text{C}^*(1/2^{+})$  with the change of energy close to the Coulomb barrier [9]. This radial coupling does not affect the incident wave in the state of  $\Pi = -$ , until it surpasses the potential barrier. Thus, the transition is almost inhibited at energies lower than the barrier top. On the other hand, in the states of  $\Pi = +$  the transition is strongly enhanced at these energies. Therefore, at the lowest energies only the  $\Pi = +$  amplitudes contribute to the cross section. This results in a angular distribution, which is symmetric with respect to  $90^{\circ}$

reaction angle. Once the energy is larger than the barrier top the radial couplings  $\Delta V_{21}(r)$  in the states of  $\Pi = -$  cause the nucleon promotion from the state  $p=1$  to the  $p=2$ . Thus, the amplitudes of  $\Pi = -$  states interfere with those of  $\Pi = +$  and the angular distribution loses its  $90^\circ$  symmetry with the increase of the energy. In fig.3 the calculation reproduces the rapid change of the angular distribution, because the minus parity contribution to the cross section rapidly increases with the energy.  $^{16}\text{O}+^{17}\text{O}$

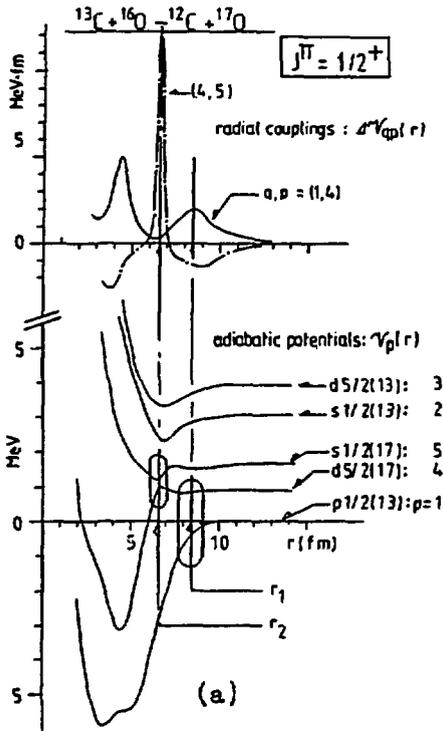


Fig.4. Adiabatic potentials and the radial couplings of the system  $^{13}\text{C}+^{16}\text{O}-^{12}\text{C}+^{17}\text{O}$  in the state of  $J^\Pi = 1/2^+$ .

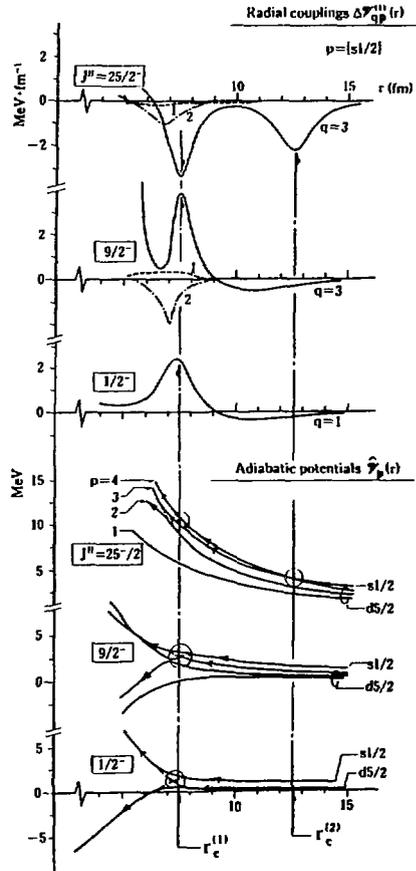


Fig.5. Adiabatic potentials and the radial couplings of the system  $^{16}\text{O}+^{17}\text{O}$  in the state of  $J^\Pi = 1/2^-, 9/2^-$  and  $25/2^-$ .

One of the characteristic features of the radial couplings between molecular orbitals is that generally large values are observed for molecular orbitals which are close to each other in the adiabatic potentials.

In the system  $^{13}\text{C}+^{16}\text{O}+^{12}\text{C}+^{17}\text{O}$  we find a crossing at  $r=r_1$  between the states  $p = 2$  and  $3$  as shown in fig.4. The radial coupling  $\Delta V_{23}^{(1)}(r)$  shows a

prominent peak at that point, suggesting the occurrence of the Landau-Zener transition. This crossing is the same as pointed out by Park, Scheid and Greiner in their calculation [7] with the two-center shell model (TCSM) and also by Milek and Reif [10] in their Woods-Saxon-TCSM calculation. The distance,  $r_1$ , obtained here is just the same as obtained by Milek and Reif. This crossing has attracted special attention because it has been considered to play an essential role in the inelastic scattering  $^{17}\text{O}(^{12}\text{C}, ^{12}\text{C})^{17}\text{O}^*(0.87\text{MeV}, 1/2^+)$ .

The same situation for rotational coupling as mentioned above occurs in the inelastic scattering  $^{17}\text{O}(^{16}\text{O}, ^{16}\text{O})^{17}\text{O}^*(1/2^+)$  [11] which will be discussed in the following. The adiabatic potential and the radial couplings are shown in fig.5 for this system; the crossing at  $r=r_1$  corresponds to that at  $r=r_2$  for the system  $^{13}\text{C}+^{16}\text{O}-^{12}\text{C}+^{17}\text{O}$ . With the increase of the  $J$  a crossing appears at

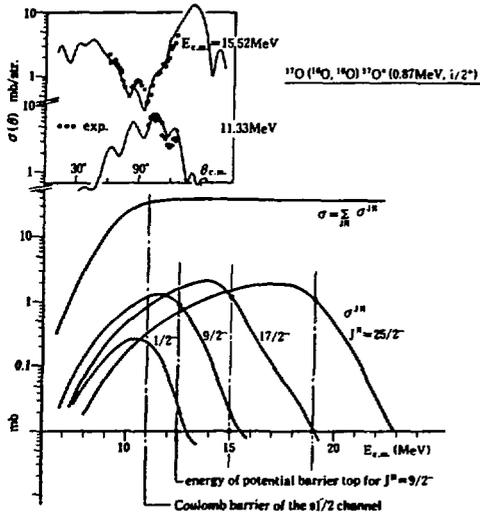


Fig. 6. Cross sections of the inelastic scattering  $^{17}\text{O}(^{16}\text{O}, ^{16}\text{O})^{17}\text{O}^*(0.87\text{MeV}, 1/2^+)$

$r=r_2$ , which is caused by the rotational coupling. At  $r_2$  the radial coupling shows the form of Landau-Zener type interaction, the corresponding transition around  $r_2$  has its origin in the effective long-range nuclear interaction, which is caused by the long-range tail of the  $2s_{1/2}$  single-particle wave function in  $^{17}\text{O}$ . Such a long-range property of the effective nuclear interaction has also been observed in the behaviour of the radial couplings for "lower"  $J$ .

At the  $r_2$  the potential energy  $E_c^{(2)}$  is clearly lower than the barrier-top  $E_B$  of the potential because of  $r_2 > r_g$ , therefore, the transition at the  $r_2$  occurs at

bombarding energies much lower than the effective barrier  $E_B$ , as long as the incident wave reaches the distance  $r_2$ . Thus, the partial cross section  $\sigma^{J\pi}$  starts to rise from the energy  $E_c^{(2)}$  and slowly increases until the bombarding energy reaches the energy  $E_B$ . Once the energy surpasses  $E_B$ , absorption occurs within the potential pocket and  $\sigma^{J\pi}$  decreases. A characteristic property of the new crossing is that the energy  $E_c^{(2)}$  is almost constant ( $\sim 12$  MeV) for all  $J$ -values, whereas the effective barrier  $E_B$  increases with  $J$ . Thus, the width,

$\Delta E = E_B - E_C^{(2)}$ , of the bump of  $\sigma^{JII}$  becomes broader and broader with increasing  $J$  (see fig.6).

In conclusion we summarize the following:

- 1) We have developed a molecular-orbital theory for rotating molecular-orbitals (RMO) based on the coupled-reaction-channel (CRC) method by using a linear combination of nucleon orbitals (LCNO). The RMO's are dynamically defined with the inclusion of the recoil effects (to first order) and the rotational coupling effects. Therefore, the RMO's depend on the total angular momentum  $J$ .
- 2) Covalent molecules with a spin projection of  $k=1/2$  are formed as the ground state of the molecular orbitals in collision processes. Hybridization of the  $1p_{1/2}$  and  $s$ - $d$  single-particle orbitals plays an essential role in this formation.
- 3) The existence of the Landau-Zener transition is pointed out in the inelastic scattering  $^{13}C(^{12}C, ^{12}C)^{13}C^*(3.09MeV, 1/2^+)$ . This is observed as the fast change of the angular distribution with the energy just above the Coulomb barrier.
- 4) The dynamical effects — the rotational coupling effects in particular, are very important especially at the distances larger than the grazing distance. The distance of the crossing points and even the number of crossings depend on the total angular momentum  $J$ .

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