

MICROSCOPIC R-MATRIX THEORY IN A GENERATOR COORDINATE BASIS

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1. Introduction. - The microscopic methods describing nuclear collisions, which make use of the generator coordinate formalism, may be classified into two categories. In the resonating group method (RGM), the RGM kernels are derived in a simpler way from the generator coordinate kernels. In the generator coordinate methods (GCM), the GCM kernels are used without any further integral transform. The microscopic R-matrix method (MRM) falls into the latter category. However, in this method, the scattering boundary conditions are imposed on the relative wave function in the configuration space like in the RGM and not in the generator coordinate space. The MRM thus combines the simplicity of calculation of the GCM kernels and the use of exact boundary conditions. In order to profit simultaneously by these properties, the configuration space is divided into two parts : the internal or interaction region and the external or asymptotic region. The R-matrix formalism¹⁾ provides a very convenient way of solving a single-channel or multichannel scattering problem in both regions.

The R-matrix formalism has been adapted to the theoretical study of nuclear reactions in several methods proposed by Tobocman and coworkers²⁾⁻⁵⁾ and by Lane and Robson⁶⁾. In 1970, Horiuchi applied the GCM and one of these methods²⁾ to the microscopic study of $\alpha - \alpha$ scattering. Below 20 MeV (c.m.) he obtained a good agreement with experimental data and RGM calculations but his results were dependent on a non-physical parameter : the radius of the interaction region (see subsect. 2.1). This dependence was showed by us⁸⁾ to be due to the use of an early version of the method proposed by Tobocman and Nagarajan. We have extended more elaborate versions of these methods^{4) 6)} to the use of a GCM basis⁸⁾. Calculations on $\alpha - \alpha$ scattering were shown to give accurate results

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with low computation times. This first version of the MRM is slightly different from the method which is presented in this talk. Simplifications were necessary to extend the method to heavy-ion scattering but they were made without any loss of accuracy ⁹⁾. The MRM is then easy to generalize to multichannel scattering ¹⁰⁾

In sect. 2, the R-matrix formalism is extended to the case of antisymmetrized wave functions. In sect. 3, the scattering problem is solved in R-matrix formalism. In sect. 4, the MRM is shown to be very similar to a number of other methods. In sect. 5, a choice for the parameter defining the interaction region is proposed. In sect. 6, elastic $\alpha - {}^{12}\text{C}$ phase shifts are presented. Conclusions are presented in sect. 7.

2. Extension of R-matrix formalism to antisymmetrized wave functions.-

2.1. Interaction and asymptotic regions. - Let us first neglect antisymmetrization. The philosophy of the R-matrix method is to divide into two parts the 3A-dimension configuration space of the colliding nuclei. In the internal (or interaction) region P, nuclear interactions between the nuclei are important. In the external (or asymptotic) region \bar{P} , both nuclei are separated by a distance which is larger than the range of nuclear forces ¹⁾. Regions P and \bar{P} are separated by the surface S.

We shall restrict our talk to the single-channel case, with zero spin nuclei. A straightforward generalization is presented in ref. ¹⁰⁾. In the external region, the scattering wave function may be approximated by its asymptotic form

$$\Psi_{\ell} \approx \frac{1}{\rho} (I_{\ell}(\rho) - U_{\ell} O_{\ell}(\rho)) \phi_1 \phi_2 Y_{\ell}^{\circ}(\Omega_{\rho}) \quad (1)$$

where ϕ_1 and ϕ_2 are antisymmetrized and normalized internal wave functions, ρ is the relative coordinate, I_{ℓ} and O_{ℓ} are Coulomb ingoing and outgoing wave functions and U_{ℓ} is the collision matrix. As usually, in R-matrix theories, three-and more-body channels are neglected.

The internal region is characterized by a parameter (denoted a) beyond which relation (1) becomes valid. This parameter is called the radius of the internal region. However, the definition we have given is not correct for an antisymmetrized wave function. We shall now extend it

to this case.

First, the relative coordinate $\underline{\rho}$ has to be defined more precisely, i.e.

$$\underline{\rho} = \frac{1}{A_1} \sum_{i=1}^{A_1} \underline{r}_i - \frac{1}{A_2} \sum_{i=1}^{A_2} \underline{r}_i \quad (2)$$

where \underline{r}_i is the individual coordinate of nucleon i and A_x is the number of nucleons of nucleus x . With an antisymmetrized basis, the definition of $\underline{\rho}$ is not unique. Other definitions are obtained by exchanging nucleons between both nuclei. Since the A nucleons are undistinguishable, there are

$$c = \frac{1}{1 - \delta_{A_1, A_2}} \frac{A!}{A_1! A_2!} \quad (3)$$

possible independent coordinates $\underline{\rho}_n$ which could be defined equivalently. Relation (1) should thus be replaced by

$$\Psi_2 \approx \mathcal{A} \frac{1}{c} (T_1(\underline{r}_1) - \dots - \dots) \Psi_1 \quad (4)$$

where \mathcal{A} is the antisymmetrization projector.

The external region is then defined as the region of the configuration space where relation (4) is valid, i.e. the region where at least one of the coordinates ρ_n is larger than a . The internal region P is thus defined by the conditions

$$\{ \rho_n < a \} \quad n = 1, \dots, c \quad (5)$$

All the relations (5) are satisfied simultaneously for points located inside the internal region.

To illustrate this on an example, consider the case of three one-dimensional nucleons ¹¹⁾ which is presented in fig. 1.

The possible relative and internal coordinates are

$$\begin{aligned} \rho_1 &= x_1 - \frac{x_2 + x_3}{2} & , \quad \bar{x}_1 &= x_2 - x_3 \\ \rho_2 &= x_2 - \frac{x_1 + x_3}{2} = \frac{3}{4} \bar{x}_1 - \frac{\rho_1}{2} & , \quad \bar{x}_2 &= x_3 - x_1 = -\rho_1 - \frac{\bar{x}_1}{2} \\ \rho_3 &= x_3 - \frac{x_1 + x_2}{2} = -\frac{1}{4} \bar{x}_1 - \frac{\rho_1}{2} & , \quad \bar{x}_3 &= x_1 - x_2 = -\rho_1 + \frac{\bar{x}_1}{2} \end{aligned} \quad (6)$$

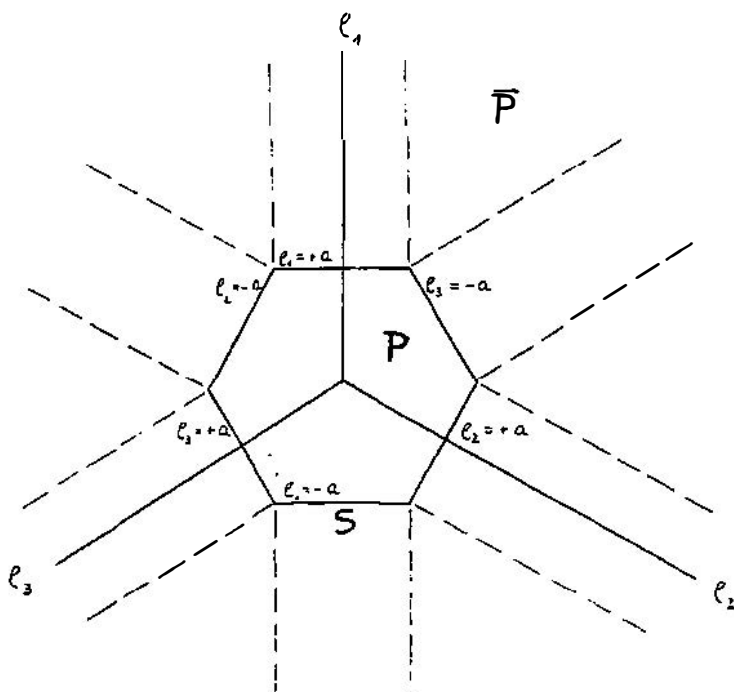


Fig. 1

The three conditions (5) intersect to give the hexagonal interaction region P. If one of the relative coordinates (say ρ_1) tends towards infinity, the corresponding internal coordinate $\bar{\rho}_1$ remaining small, the asymptotic form (4) of the scattering wave function becomes nearly identical to (1). The other terms of (4) are negligible because the square integrable wave functions Φ_1 and Φ_2 depend on ρ_1 (see relations (6)). This property is true in the two-body channels (dashed lines in fig. 1).

We have thus seen on this simple example that asymptotically, relation (4) is equivalent to \mathcal{C} relations (1) with ρ replaced by ρ_n . In order to have this equivalence in the whole external region \bar{P} , we now modify the definition of the internal region in the following way: the interaction region is defined by relation (5) where the radius a is sufficiently large so that, in the external region, (i) nuclear interactions between the nuclei are negligible and (ii) antisymmetrization

effects are negligible.

If the above conditions are satisfied, the results of R-matrix calculations should not depend on the value chosen for a .

2.2 Matrix elements in the interaction region. - In sect. 3, we shall solve the Schrödinger equation in the interaction region. We shall need matrix elements of the total Hamiltonian H calculated over this region.

The GCM wave functions Φ_L are linear combinations of L -projected Slater determinants. The individual orbitals are harmonic oscillator wave functions with the same size parameter $b = (\hbar / m\omega)^{1/2}$. The centre-of-mass wave function $\Phi_{c.m.}$ can be factorized exactly. In RGM notations, the GCM wave functions may be written as usually ⁷⁾

$$\Phi_L = \left(\frac{A!}{A_1! A_2!} \right)^{1/2} \Phi_{c.m.} \int_0^\infty \Gamma_L(\rho, z) \Phi_1 \Phi_2 Y_L^0(\Omega_\rho) \quad (7)$$

where ρ is the generator coordinate and

$$\Gamma_L(\rho, z) = 16 \pi^{3/4} (2L+1)^{-1/2} \left(\frac{\mu}{b^2} \right)^{3/4} e^{-\frac{\mu}{2b^2}(\rho^2 - z^2)} \mathcal{H}_L \left(\frac{\mu z \rho}{b^2} \right) \quad (8)$$

\mathcal{H}_L being a spherical Hankel function, and

$$\mu = A_1 A_2 / A \quad (9)$$

is the dimensionless reduced mass.

In the asymptotic region, one may neglect the exchanges of nucleons between the nuclei and Φ_L is approximated by

$$\Phi_L \approx (1 + \delta_{1,2})^{1/2} c^{-1/2} \Phi_{c.m.} \Gamma_L(\rho, z) \Phi_1 \Phi_2 Y_L^0(\Omega_\rho) \quad (\rho > a) \quad (10)$$

where $\delta_{1,2} = 1$ corresponds to identical nuclei.

Now, we are able to give an accurate approximate value for a matrix element over the interaction region P . We shall subtract from a matrix element calculated over the whole space an approximate value of the matrix element calculated over the external region \bar{P} . Neglecting in \bar{P} the three- and more-body channels, we only take into account the c regions of the configuration space where one of the coordinates ρ_n is larger than a (see ref. ¹¹⁾ for a more detailed discussion). In each of the two-body regions, the GCM wave function is approximated by its asymptotic form (10) and a corresponding approximation is made for the Hamiltonian. Using the fact that Φ_1 , Φ_2 and $\Phi_{c.m.}$ are normalized to unity, the matrix element

may be written

$$\langle \phi_e(r) | H - E | \phi_e(r') \rangle_P = H_e(r, r') - E N_e(r, r') \quad (11)$$

$$- (1 + \delta_{1,2}) \int_a^\infty \Gamma_e(\rho, r) \left\{ -\frac{\hbar^2}{2m\mu} \left(\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho} \frac{\partial}{\partial \rho} - \frac{l(l+1)}{\rho^2} \right) - \frac{Z_1 Z_2 e^2}{\rho} + E_1 + E_2 - E \right\} \Gamma_e(\rho, r') \rho^2 d\rho$$

where E_1 and E_2 are the internal energies of the colliding nuclei.

The l - projected GCM kernels

$$\begin{Bmatrix} H_e(r, r') \\ N_e(r, r') \end{Bmatrix} = \langle \phi_e(r); \begin{Bmatrix} H \\ 1 \end{Bmatrix}; \phi_e(r') \rangle \quad (12)$$

are calculated using usual projection techniques. The second term of the r.h.s. of (11) is simply evaluated by a numerical quadrature. This term is rather small but plays an important role. Its neglect was responsible for the dependence on a of Horiuchi's results on α - α scattering ⁷⁾ Let us also remark that, due to the kinetic energy, this second term and thus the matrix element over P is not symmetrical in r and r' .

2.3. Bloch operator. - The kinetic energy operator T is not hermitian over the interaction region. Using Green's theorem, it is easy to show that the non-hermitian part of T is a surface term. Bloch ¹²⁾ has introduced a surface operator \mathcal{L} which makes $H + \mathcal{L}$ hermitian. It is defined by

$$\begin{aligned} \langle \phi | H - H^\dagger | \psi \rangle_P &= \langle \phi | T - T^\dagger | \psi \rangle_S \\ &= \langle \phi | \mathcal{L}^\dagger - \mathcal{L} | \psi \rangle_S \end{aligned} \quad (13)$$

Restricting the surface S of the internal region to its interaction with the two-body channels, \mathcal{L} may be chosen as

$$\mathcal{L}^P = \frac{\hbar^2}{2m\mu} \sum_{n=1}^c \frac{1}{a} \delta(\rho_n - a) \frac{\partial}{\partial \rho_n} \rho_n \quad (14)$$

Using the equivalence of the coordinates ρ_n , the matrix elements of \mathcal{L}^\dagger are the same as the matrix elements of \mathcal{L} ⁸⁾

$$\mathcal{L} = c \frac{\hbar^2}{2m\mu} \frac{1}{a} \delta(\rho - a) \frac{\partial}{\partial \rho} \rho \quad (15)$$

from the r.h.s. of (20c) Lane and Robson have shown that the direct solution of equation (20c) may also be derived from a variational principle (see also refs. 13). The solution of eq. (20c) is thus in principle the best solution one can obtain from a Bloch-Schrödinger equation.

Under certain conditions, it is possible to prove the complete equivalence between the different solutions of equations (20c) (for any value of L) and (20b). These conditions are fulfilled in our calculations using the approximations defined in sect. 2. We shall thus restrict ourselves to the simplest equation, i.e. (20a). However, the same technique may be used for the other equations.

Equation (20a) presents a surface term in its r.h.s. To solve this equation, we replace Ψ_L in this term by its asymptotic form (1). The equation then becomes an inhomogeneous equation which can be solved approximately by expanding Ψ_L in a finite set of GCM wave functions.

Using

$$\Psi_L = \sum_n f_n \phi_L(x_n) \quad (21)$$

and projecting (20a) over $\Gamma_L(x_n)$ in the interaction region, one obtains

$$\sum_n f_n C_{mn} = (1 + \delta_{1,2})^{1/2} c^{-1/2} \frac{k^2 k a}{i \mu} \Gamma_L(a, r_n) \left(\Gamma_L(k a) - U_L O_L(k a) \right) \quad (22)$$

where the symmetrical matrix C is defined as

$$C_{mn} = \langle \phi_L(x_m), \hat{H} - \mathcal{L}(0) - E | \phi_L(x_n) \rangle_p \quad (23)$$

Matrix elements C_{mn} can be calculated from (11) and (16). The coefficients f_n can be calculated from (22) as a function of the collision matrix element U_L . Imposing the continuity of the wave function at the surface S and using (9), one has

$$c^{-1/2} (1 + \delta_{1,2})^{1/2} \sum_n f_n \Gamma_L(a, r_n) = \frac{1}{a} \left(\Gamma_L(k a) - U_L O_L(k a) \right) \quad (24)$$

Remark that it is not necessary to impose the continuity of the derivative of the wave function because the Bloch operator in eq. (20a) already contains a condition of continuity of the logarithmic derivative. Calculating the coefficients f_n from (22) and replacing in (23), one obtains

$$U_\ell = \frac{I_\ell(ka) - ka I'_\ell(ka) R_\ell}{O_\ell(ka) - ka O'_\ell(ka) R_\ell} \quad (25)$$

where the R-matrix R_ℓ is given by

$$R_\ell = (1 + \delta_{1,2}) \frac{\hbar^2 a}{2m\mu} \sum_{m,n} \Gamma_\ell(a, z_m) (C_1^{-1})_{mn} \Gamma_\ell(a, z_n) \quad (26)$$

Numerical calculations are extremely simple if one knows numerical values of the GCM kernels H_ℓ and N_ℓ at a number of discretization points. Relations (25) and (26) are easily extended to the multichannel scattering case¹⁰⁾.

4. Comparison with other GCM calculations. -

The present comparison is restricted to a number of methods which exhibit close similarities with the MRM, i.e. the methods of Mito and Kamimura¹⁴⁾ (MK), Canto and Brink^{15, 16)} (CB1 and CB2) and Nagata and Yamamoto¹⁷⁾ (NY). Method NY is identical to method CB2¹⁷⁾. These methods have in common the following features: (i) they only make use of the GCM kernels H_ℓ and N_ℓ calculated at a number of discretization points. There is thus no need for integral transforms like in the RGM - GCM. It is not necessary to know the analytical form of H_ℓ and N_ℓ .

(ii) the generating function

$f_\ell(r)$ is not present in the final formulae. The asymptotic form of $f_\ell(r)$ or the GC functions corresponding to the Coulomb wave functions have not to be known. This condition is not verified by the method of Mihailović et al¹⁸⁾.

In all the above-mentioned methods, an Ansatz is chosen for the RGM relative function $g_\ell(r)$. This Ansatz is used as a trial function in a variational principle (MK, CB2, NY) or is used to solve directly the Hill-Wheeler equation (CB1). The methods may be classified into two categories according to the way the Ansatz is defined (see Fig. 2). In two of them (CB2, NY), the Ansatz is defined in an "interaction region", i.e. for values of the relative coordinate smaller than a parameter R similar to radius a of the MRM. In the other two (MK, CB1), the Ansatz is defined for any value of r by adding to the short-range GCM terms a regulari-

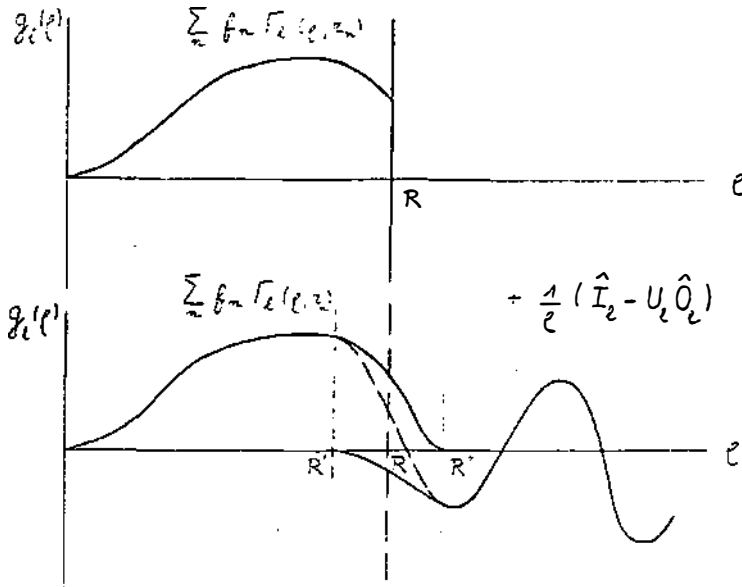


Fig. 2

zed asymptotic form $\frac{1}{\epsilon} (\hat{I}_2 - U_2 \hat{O}_2)$. This regularized term becomes negligible below a value of ϵ which is close to R . This is the main difference between these methods and the method of Mihailović et al where the regularized asymptotic term is significant for any value of ϵ . The technique of regularization is different in MK and CBl. In the MRM, CB2 and NY, there is no overlap between the short-range GCM terms and the asymptotic term.

Methods CB2 and NY can be shown to be exactly equivalent to our MRM. This is easily proved by comparing respectively relations (3.20) and (3.21) of ref. ¹⁵⁾ to relations (26) and (25) of the present talk. This exact equivalence allows us to make an accurate comparison between the results of the MRM and methods MK and CBl. For $\alpha - \alpha$ scattering, Nagata and Yamamoto have compared their results with those obtained with method MK using the same numerical conditions. With eight discretization points, both methods differ up to 60 MeV by less than 0.1 degree for $\mu = 0$, and 0.5 degree for $\mu = 4$. Canto and Brink ¹⁵⁾ find a similar agreement for the same collision between CBl and CB2 (and thus the MRM).

For $^{16}_O + ^{16}_O$, the phase shifts obtained with both methods are in agreement within two degrees ¹⁶⁾.

With a same number of discretization points, all the methods discussed here seem thus to give results in close agreement. The agreement with other GCM and RGM calculations is also found satisfying for all these methods.

5. Choice of the radius of the internal region. -

In the present section, we try to find a simple approximate law giving radius A (or parameter R of MK or CB) for a given scattering. We shall successively study values of the distance between the nuclei, beyond which antisymmetrization effects, parity dependence and nuclear interaction become negligible.

5.1. Range of antisymmetrization. - Since we are looking for an approximate law, we may simplify the problem as much as possible. We shall study the range of antisymmetrization on the non-projected GCM overlap kernel $N(\underline{r}, \underline{r}')$. The different terms of N may be classified according to their exponential factor,

$$\begin{array}{ll}
 \text{direct term} & e^{-\frac{\mu}{2b^2} (r - r')^2} \\
 \text{one-exchange term} & e^{-\frac{\mu}{2b^2} (r - r')^2 - \frac{1}{2b^2} r \cdot r'} \\
 \dots & \dots \\
 \nu\text{-exchange term} & e^{-\frac{\mu}{2b^2} (r - r')^2 - \frac{\nu}{2b^2} r \cdot r'}
 \end{array} \quad (27)$$

The coefficient of $\underline{r}, \underline{r}'$ is the number ν of nucleons exchanged between the colliding nuclei. The maximum value of ν is A_2 (say $A_1 \geq A_2$). Making $\underline{r} = \underline{r}'$, one sees that for large values of r , the one-exchange term is the largest term due to antisymmetrization (at this moment, we are neglecting the effects of parity projection).

Taking into account the highest power of r in its polynomial factor, this term may be written

$$C_{\nu} \left(\frac{r^2}{2b^2} \right)^{\nu_1 - \nu_2} e^{-\frac{r^2}{2b^2}} \quad (28)$$

where ν_1, ν_2 is the principal quantum number of the last oscillator shell to be filled. We shall consider antisymmetrization negligible if this term is smaller than a given small number ϵ . Assuming that C_{ν} does not depend much on the collision (which is easily checked for $\nu = \nu_1, \nu_2 = 16_0$

and $^{16}_0 - ^{16}_0$), the range R_{ϵ} of antisymmetrization is given by

$$\left(\frac{R_{\epsilon}^2}{2\epsilon^2}\right)^{n_1+n_2} e^{-\frac{R_{\epsilon}^2}{2\epsilon^2}} = \frac{\epsilon}{C_{\epsilon}} \quad (29)$$

Values of R_{ϵ}/ϵ obtained from (29) with two different choices for ϵ/C_{ϵ} , are given in table 1

A_1	A_2	n_1+n_2	$\epsilon/C_{\epsilon} = 10^{-3}$	$\epsilon/C_{\epsilon} = 10^{-4}$
4	4	0	3.72	4.29
16	4	1	4.27	4.83
16	16	2	4.87	5.40
40	4	2	4.87	5.40
40	16	3	5.48	5.98
40	40	4	6.10	6.55

Table 1

The results of table 1 can be approximately summarized by the relation

$$R_{\epsilon} \approx \epsilon \left\{ [2 \ln(C_{\epsilon}/\epsilon)]^{\frac{1}{2}} + 0.6(n_1+n_2) \right\} \quad (30)$$

5.2. Range of parity dependence. - The range of parity effects may be studied by making $\underline{x} = -\underline{x}'$ in (27). The leading term is now the maximum exchange term and is in most cases given by ¹⁹⁾

$$C_P \left(\frac{r^2}{2\epsilon^2}\right)^n e^{-\frac{r^2}{2\epsilon^2}} \quad (31)$$

where

$$y = (2\mu - A_2)^{-\frac{1}{2}} = \left(\frac{A_2(A_1 - A_2)}{A_1 + A_2}\right)^{-\frac{1}{2}} \quad (32)$$

Power n in (31) is rather complicated but can be determined from fig. 3 of ref. ¹⁹⁾. We eliminate the trivial case $A_1 = A_2$. Term (31) dominates term (28) if y is larger than unity. All the possible cases are

$$A_2 = A_1 - 1 \quad y = \left(2 + \frac{1}{A_2}\right)^{\frac{1}{2}} \geq 2^{\frac{1}{2}} \quad (33a)$$

$$A_2 = A_1 - 2 \quad y = \left(1 + \frac{1}{A_2}\right)^{\frac{1}{2}} \geq 1 \quad (33b)$$

$$A_2 = 1 \quad \gamma = \left(1 + \frac{2}{A_1 - 1}\right)^{\frac{1}{2}} \gtrsim 1 \quad (33c)$$

$$A_2 = 2, A_1 = 5 \quad \gamma = \left(\frac{7}{6}\right)^{\frac{1}{2}} \quad (33d)$$

Approximating power n in (31) by $n_1 + n_2$ (which is exact in cases (33a) and (33c)), we may replace in (30), the oscillator parameter b by γb when γ is larger than unity.

5.3. Range of nuclear interaction. - Assuming that this range is larger than the range of antisymmetrization, we only consider the direct nuclear term in the non-projected GCM kernel. For a gaussian potential $V_N \left[-\frac{(r_1 - r_2)^2}{\alpha^2}\right]$, it can be approximated by

$$V_N(r) \approx C_N \left(\frac{r^2}{2b^2}\right)^{n_1 + n_2} e^{-\frac{r^2}{\alpha^2 + 2b^2}} \quad (34)$$

Constant C_N is much more complicated than C_{st} but the power of $r^2/2b^2$ is the same as in (28). The range of the exponential factor in V_N is somewhat larger than in (28). Term V_N decreases thus slightly more slowly than the one-exchange term of the overlap kernel. Because of the similarity between (34) and (28) and because we search for a very simple approximation, we shall assume that law (30) also approximately holds for the range of the nuclear interaction.

5.4. Approximate law for the radius of the internal region. - Values of the ratio a/b (or R/b) which have actually been used in microscopic calculations, are shown in table 2

collision	MRM ^{8,9,20)}	MK ¹⁴⁾	CB ^{15, 16)}
$\infty - \infty$	4.0	4.2	4.5
$\infty - {}^{16}\text{O}$	4.5	4.4	-
${}^{16}\text{O} - {}^{16}\text{O}$	5.2	5.4	5.0

Table 2

With these values, we fit the parameter in equation (30), giving the approximate law

$$a = b \times \left(4.0 + 0.6(n_1 + n_2)\right) \times \max(1, \gamma) \quad (35)$$

The last factor in (35) may introduce an important correction if the masses of the nuclei differ by unity. In the case of $\alpha - {}^3\text{He}$ for example, (35) gives a $\approx 6b$ in place of a $\approx 4b$.

6. Applications. -

6.1. General remarks. - The MRM has already been applied to $\alpha - \alpha$ ⁸⁾, $\alpha - {}^{16}\text{O}$ ⁹⁾, ${}^{16}\text{O} - {}^{16}\text{O}$ ²⁰⁾ and ${}^{12}\text{C} - {}^{16}\text{O}$ ²¹⁾ scattering. The calculations in ref. ⁸⁾ were slightly different from the method presented here. The main difference is a more elaborate (and more difficult) method of calculating the matrix elements over the internal region and over its surface. However, with a slight increase of radius Ω , the results of ref. ⁸⁾ can be obtained with the formulae of the present talk.

In refs. ⁸⁾ and ⁹⁾, we have shown that a good accuracy is obtained with a small number of discretization points. For the heavier systems, the results have been obtained with about ten points. For all the above-mentioned collisions, we have checked that the phase shifts do not depend much on the value chosen for the radius of the internal region. We believe that the fluctuations of the phase shifts, when modifying a , (less than three degrees in general) may be considered as the accuracy of the calculation.

The MRM being very simple, most of the computational time is used to obtain values of the kernels H_ℓ and N_ℓ at the discretization points. Since the number of points is small, the MRM is a rather economical method. The numerical values of the matrix elements are calculated using the computer code WICK ²²⁾. This program performs the theoretical calculation of the kernels as a function of one-body and two-body matrix elements and then computes their numerical value. The Coulomb kernel is calculated exactly.

6.2. $\alpha - {}^{12}\text{C}$ scattering. - The $\alpha - {}^{12}\text{C}$ system has already been studied in a static approximation by Horiuchi ²³⁾ and by Suzuki ²⁴⁾. We present here a dynamical study of the elastic $\alpha - {}^{12}\text{C}$ scattering.

Like in ${}^{12}\text{C} - {}^{16}\text{O}$ scattering, one of the colliding nuclei is an open-shell nucleus. To describe the ${}^{12}\text{C}$ nucleus in its ground state, we use a linear combination of nineteen Slater determinants ²⁵⁾. The ℓ -projected energy curves

$$E_L(r) = H_L(r, r) / V_L(r, r) - H_L(0, \infty) / V_L(0, \infty) \quad (36)$$

are shown in fig. 3, using effective interactions B1²⁶⁾ with $b = 1.60$ fm and V2 ($M = 0.67$)²⁷⁾ with $b = 1.751$ fm which has already been used by Horiuchi²³⁾. Qualitatively, both set of curves present the same complicated shape. They have a common defect, the 0^+ potential well is too deep to describe correctly the energy of the ground state of ^{16}O . This is due to the fact that α and ^{16}O are better described than ^{12}C in the harmonic oscillator model. The 1^- curve is very different with both interactions.

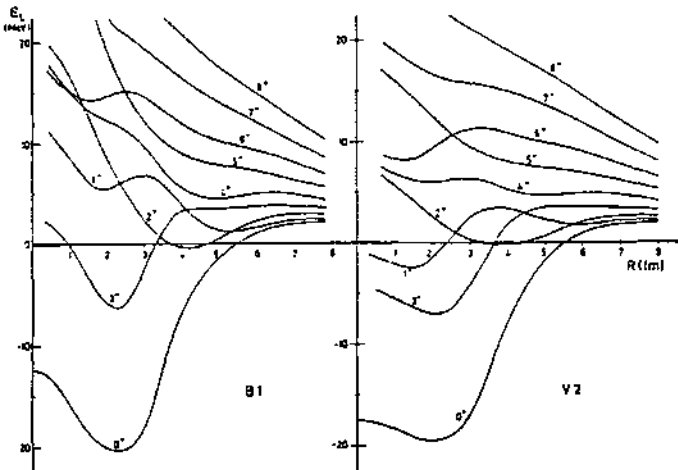


Fig. 3

Relation (35) gives $a = 4.6 b$, giving 7.4 fm with B1 and 8 fm with V2. We have used nine discretization points and $a = 7.8$ fm with B1 and ten discretization points and $a = 8.0$ fm with V2. The phase shifts obtained with B1 (dashed lines) and V2 (full lines) are shown in figs. 4 and 5 together with experimental results²⁸⁾.

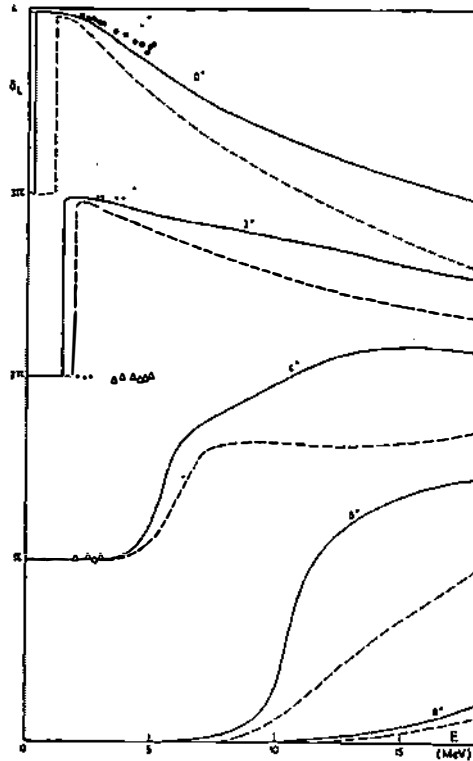


Fig. 4

The resonances which are obtained with both potentials are located at higher energies than the experimental ones and are thus much broader. The agreement is better with the potential proposed by Horiuchi. This is especially clear for the 1^- curve although the first 1^- state obtained with V_2 is still located above the $\alpha + {}^{12}\text{C}$ threshold. The agreement with experimental data is extremely poor for the 2^+ state where we find a resonance in place of the 6.92 MeV bound state and where the other resonances are missing. These resonances should be explained when introducing excited states of ${}^{12}\text{C}$ in a coupled-channel calculation²⁴⁾.

7. Conclusion. -

The MRM is a GCM which allows to study heavy-ion collisions in a very simple way. This simplicity comes from the fact that the method only

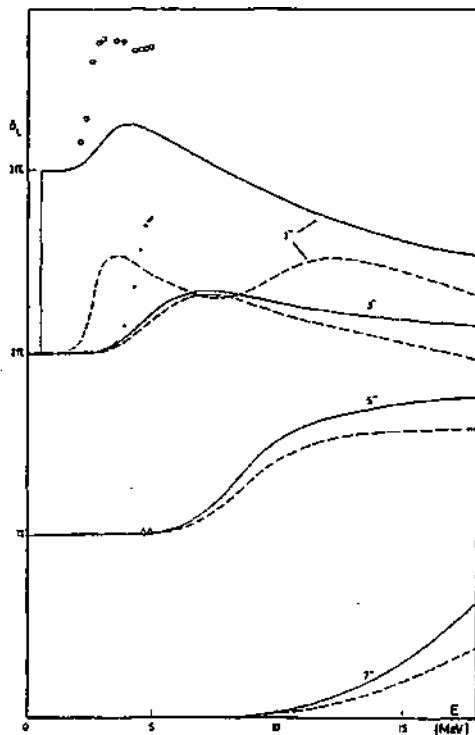


Fig. 5

requires numerical values of the GCM kernels.

The calculation of the GCM kernels is the common problem to all the RGM and GCM. In the MRM and in similar methods, there is no need for further integral transforms of these kernels. Moreover, it is possible to compute the Coulomb kernel without approximation. For high l -values, the accuracy of the MRM only depends on the accuracy of the GCM matrix elements.

Accurate results are obtained with a rather small number of discretization points, reducing the computation time. The MRM and the other methods discussed in sect. 4 appear to be a valuable alternative to RGM calculations. The extension of the MRM to multi-channel scattering is straightforward. Calculations are in progress on the inelastic $^{12}\text{C}(^{16}\text{O}, ^{16}\text{O})^{12}\text{C}(2^+)$ scattering²⁹⁾.

References

- 1) A.M. Lane and R.G. Thomas, Rev. Mod. Phys. 30 (1958) 257.
- 2) W. Tobocman and M.A. Nagarajan, Phys. Rev. 138 (1965) B1351.
- 3) M.A. Nagarajan, S.K. Shah and W. Tobocman, Phys. Rev. 140 (1965) B63.
- 4) L. Garside and W. Tobocman, Phys. Rev. 173 (1968) 1047.
- 5) F. Schmittroth and W. Tobocman, Phys. Rev. C3 (1971) 1010.
- 6) A.M. Lane and D. Robson, Phys. Rev. 178 (1969) 1715.
- 7) H. Horiuchi, Prog. Theor. Phys. 43 (1970) 375.
- 8) D. Baye and P.-H. Heenen, Nucl. Phys. A233 (1974) 304.
- 9) P.-H. Heenen, Nucl. Phys. A272 (1976) 399 .
- 10) D. Baye, P.-H. Heenen and M. Libert-Heinemann, Nucl. Phys. A, in press.
- 11) D. Baye and P.-H. Heenen, Bull. Cl. Sc. Acad. Roy. Belg. 60 (1974) 444.
- 12) C. Bloch, Nucl. Phys. 4 (1957) 503.
- 13) R.A. Chatwin, Phys. Rev. C2 (1970) 1167.
W. Mac Donald and R. Raphael, Phys. Rev. C14 (1976) 2044.
- 14) Y. Mito and M. Kamimura, Prog. Theor. Phys. 56 (1976) 583.
- 15) L.F. Canto and D.M. Brink, Nucl. Phys. A279 (1977) 85.
- 16) L.F. Canto, Nucl. Phys. A279 (1977) 97.
- 17) S. Nagata and Y. Yamamoto, Prog. Theor. Phys. 57 (1977) 1088.
- 18) M.V. Mihailowić, L.J.B. Goldfarb and M.A. Nagarajan, Nucl. Phys. A273 (1976) 207.
- 19) D. Baye, J. Deenen and Y. Salmon, Nucl. Phys. A, in press.
- 20) D. Baye and P.-H. Heenen, Nucl. Phys. A276 (1977) 354.
- 21) D. Baye and P.-H. Heenen, Nucl. Phys. A283 (1977) 176.
- 22) D. Baye, 1974 , unpublished.
- 23) H. Horiuchi, Intern. Symposium on cluster structure of nuclei, Tokyo , 1975, p. 41.
- 24) Y. Suzuki, Prog. Theor. Phys. 55 (1976) 1751.
- 25) D. Baye, Nucl. Phys. A272 (1976) 445.
- 26) D.M. Brink and E. Boeker, Nucl. Phys. A91 (1967) 1.
- 27) A.B. Volkov, Nucl. Phys. 74 (1965) 33.
- 28) G.J. Clark, D.J. Sullivan and P.B. Treacy, Nucl. Phys. A110 (1968) 481.
- 29) D. Baye , P.-H. Heenen and M. Libert-Heinemann, contribution to the conference.

DISCUSSION

H. Horiuchi: I calculated also the $^{12}\text{C} + \alpha$ system in the RGM framework using the harmonic oscillator basis. I found that the choice of the suitable two-nucleon force is very important for the microscopic description of inter-cluster interactions. Usual effective two-nucleon interactions which fit the α and ^{16}O binding energies give too shallow binding energy for ^{12}C . This means a too strong binding between α and ^{12}C . You mentioned in your talk two systems $\alpha + ^{12}\text{C}$ and $^{16}\text{O} + ^{12}\text{C}$ which include ^{12}C cluster. I would like to hear your comment on the choice of the two-nucleon force which may cause bad effect on the inter-cluster force derived microscopically.

D. Baye: Any microscopic interaction will give a too strong binding energy for $\alpha + ^{12}\text{C}$. I believe this is a problem of wave function and not a problem of interaction. The ^{12}C nucleus is not well described and, as you said, its binding energy is too much underestimated, compared to the binding energies of the closed-shell nuclei and ^{16}O . For non-zero values of the angular momentum, interaction V2 with $M = 0.67$ seems to give the best results. For $^{12}\text{C} + ^{16}\text{O}$, the situation is different. The underestimation of the total energy of the system seems to remain nearly constant when the distance between the colliding nuclei decreases. The $^{12}\text{C} + ^{16}\text{O}$ interaction is thus much more realistic since it is the difference between two nearly equally underestimated energies.

Y.C. Tang: Is your method restricted to the case where the cluster internal functions are harmonic-oscillator wave functions of the same width parameter?

D. Baye: Until now, our calculations are restricted to this case. This is due to the fact that we compute the GCM matrix elements with identical width parameters in order to avoid centre-of-mass problems. However, the MRM could be extended to the more general case of different parameters. Then we should have to introduce a projection on the centre-of-mass

motion in our calculation of the GCM matrix elements. The calculation would become then much more tedious.

B.Giraud: Does your continuity equation guarantee convergence if the basis on which the R matrix is calculated is enriched?

D. Baye: The continuity conditions are correctly fulfilled at the surface of the interaction region. The Bloch operator in the Bloch-Schrödinger equation contains a condition of continuity of the logarithmic derivative of the wave function. With our continuity relation, we thus obtain both the continuity of the wave function and of its first derivative. This should not introduce a problem of convergence in our method, but I must say that the convergence has not been studied theoretically.

K. Dietrich: In the interior region the system will try to avoid density distributions which locally exceed the saturation value. Does your system of basis functions provide a convenient description of this effect or do you have to incorporate many excited configurations for realistic calculations?

D. Baye: First, I must say that we do not have much freedom in choosing the basis of wave functions. The generator coordinate treatment requires the use of harmonic oscillator single particle states. The only parameter which can be modified is the size parameter of these states. Moreover, the calculations are quite difficult and it is difficult to extend the basis to many excited states. However, the GCM basis should provide a good description of the saturation effect due to the Pauli principle.