

**$\alpha$ - $\alpha$  scattering in the generator-coordinate formalism**

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In the generator-coordinate formalism we calculate the phase shifts for  $\alpha$ - $\alpha$  scattering by solving the Hill-Wheeler equation in the continuum. The Pauli principle is exactly taken into account for the nuclear potential term. The Coulomb interaction is introduced under a long-range assumption. The results are compared to the experimental values.

[ NUCLEAR REACTIONS  $\alpha$ - $\alpha$  elastic scattering. Calculated phase shifts. ]

## I. INTRODUCTION

One can easily describe the ground state and the low-energy excited states of nuclei by use of the shell model. This model may then be refined by enlarging the configuration space in order to include particle-hole excitations. This procedure leads to large dimension problems, but the major objection is that our knowledge of the nucleon-nucleon force is still incomplete.

Other models are presented as alternatives to the shell model and in particular the  $\alpha$ -particle model. This model—in fact anterior to the shell model—was proposed in 1937 by Wefelmeier<sup>1</sup> and is founded on the exceptional stability of the  $\alpha$  particles. Indeed, the  $\alpha$  particles being very stable, one can assume that this stability persists when they are in groups in the nuclei, above all the light nuclei where the *LS* scheme seems to be valid and is well adapted to a conservation of the  $\alpha$  particles. For each light  $N=Z$  nucleus whose mass is four times that of the nucleon mass, it is then possible to use the  $\alpha$ -particle model.

The generator coordinate method (GCM) is a very powerful tool for the study of this model. The method originated by Hill, Wheeler, and Griffin<sup>2</sup> for the purpose of fission has been successful in the study of nuclear rotations<sup>3</sup> and collective motion in the light nuclei.<sup>4</sup> Recent studies by Brink,<sup>5</sup> Brink and Weiguny,<sup>6</sup> and C. W. Wong<sup>7</sup> have revived the question, and the formalism has been extended to deal with scattering phenomena.<sup>8</sup> This extension which was done with the aid of a schematic model (dineutron) is taken up again here in the realistic case of  $\alpha$ - $\alpha$  elastic scattering. We have chosen this case on one hand for its simplicity because there are only two interacting fragments and, on the other hand, because a great deal of experimental work is available to test the consistency of the generator coordinate method.

Two problems arise when working with GCM: how to choose the generator coordinates and how

to solve the equations obtained. In Sec. II briefly we describe the generator coordinate method and the choice of our generator coordinate while in Sec. III we show how to solve the Hill-Wheeler equation in the case of scattering. Finally, in Sec. IV we present and discuss the results obtained.

II. GENERATOR COORDINATE METHOD APPLIED TO THE  $\alpha$ - $\alpha$  SYSTEM

In this section we follow the development given in Ref. (8). In order to simplify the calculations all the nucleons are assumed to move on the 0S orbitals of an harmonic oscillator and no deformation of the  $\alpha$  particles during the collision is taken into account.

## A. Choice of base and Hill-Wheeler equation

In a collision problem, the relative distance between the interacting nuclei is the most important degree of freedom. This will fix our generator coordinate. Let us consider two  $\alpha$  particles (*A*) and (*B*), centered a  $+\frac{1}{2}\bar{r}$  and  $-\frac{1}{2}\bar{r}$  with respect to an arbitrary origin 0. The coordinates (of space, spin, and isospin) of (*A*) are labeled  $r_1, r_2, r_3,$  and  $r_4$  with respect to this origin. Those of the nucleons of (*B*) are labeled  $r_5, r_6, r_7,$  and  $r_8$ . The antisymmetrized wave function for the total system is thus written as

$$\Phi_{\bar{r}} = \mathcal{Q} \left\{ \varphi(r_1 - \frac{1}{2}r) \varphi(r_2 - \frac{1}{2}r) \varphi(r_3 - \frac{1}{2}r) \varphi(r_4 - \frac{1}{2}r) \right. \\ \left. \times \varphi(r_5 + \frac{1}{2}r) \varphi(r_6 + \frac{1}{2}r) \varphi(r_7 + \frac{1}{2}r) \varphi(r_8 + \frac{1}{2}r) \right\} \quad (1)$$

with

$$\varphi(x) = \pi^{-3/4} b^{-3/2} \exp[-(\bar{x})^2/2b^2] \bar{\chi}_i \bar{\tau}_i,$$

where  $\mathcal{Q}$  represents the antisymmetrization operator,  $b$  the harmonic oscillator parameter,  $\bar{\chi}_i$  and  $\bar{\tau}_i$  the spin and isospin variables. The values taken on by  $\bar{\chi}_i$  and  $\bar{\tau}_i$  are  $+\frac{1}{2}$  and  $-\frac{1}{2}$ .

In other words we represent the system of two

$\alpha$  particles by Slater determinants. But these determinants are not entirely satisfactory as they fix the mean positions of the centers of the clusters and consequently do not allow the true dynamical behavior of the structure to occur. Moreover, they are not eigenstates of the total angular momentum. One can obtain a more satisfactory wave function by taking linear combinations of all the Slater determinants, which, in the frame of the present problem, amounts to taking a coherent sum over all the positions that one can obtain by allowing  $\bar{r}$  to vary.

The set of the base functions  $\Phi_{\bar{r}}$  when  $\bar{r}$  takes all the possible values generates the wave function

$$\psi = \int d\bar{r} f(\bar{r}) \Phi_{\bar{r}}. \quad (2)$$

In this expression  $f(\bar{r})$  is the amplitude of the mixing of configurations which depend on a continuous vector labeled  $\bar{r}$ . This amplitude is closely related to the scattering wave function. As we shall see presently the explicit determination of  $f(\bar{r})$  is not necessary but this amplitude will lead us to the phase shifts describing the collision.

Let us call  $\mathcal{H}$  the  $N$ -body Hamiltonian of the problem. The wave function  $\psi$  is an approximate solution of the Schrödinger equation

$$\mathcal{H}\psi = E\psi. \quad (3)$$

One determines the best wave function  $\psi$  possible by solving the Hill-Wheeler integral equation

$$\int [H(\bar{r}, \bar{r}') - EN(\bar{r}, \bar{r}')] f(\bar{r}') d\bar{r}' = 0, \quad (4)$$

where

$$H(\bar{r}, \bar{r}') = \langle \Phi_{\bar{r}} | \mathcal{H} | \Phi_{\bar{r}'} \rangle \quad (5a)$$

and

$$N(\bar{r}, \bar{r}') = \langle \Phi_{\bar{r}} | \Phi_{\bar{r}'} \rangle. \quad (5b)$$

#### B. Relation with the resonating group formalism

As originated by Wheeler,<sup>9</sup> the resonating group method (RGM) has been the starting point of  $\alpha$ -cluster model calculations. For a composite system one writes the total wave function as a combination of antisymmetrized partial wave functions corresponding to the different possibilities of the neutron and proton distributions in the composite system in groups such as dineutrons,  $\alpha$  particles, lighter nuclei, etc. By using a variational procedure one determines the dependence of the total wave function with respect to the relative distances between the substructures, and this procedure leads to the resolution of an integro-differential equation.

The RGM is formally equivalent to the GCM.

Let us consider only the nonantisymmetrized spatial part of the base functions  $\Phi_{\bar{r}}$ :

$$\begin{aligned} \Phi_{\bar{r}} = & \prod_{i=1}^4 [\pi^{-3/4} b^{-3/2} e^{-(\bar{r}_i - \frac{1}{2}\bar{r})^2/2b^2}] \\ & \times \prod_{j=5}^8 [\pi^{-3/4} b^{-3/2} e^{-(\bar{r}_j + \frac{1}{2}\bar{r})^2/2b^2}], \end{aligned} \quad (6)$$

we can express  $\Phi_{\bar{r}}$  in the coordinate system where the center-of-mass coordinate, the relative coordinate, and the internal coordinates of the  $\alpha$  particles appear.

By performing a change of coordinate in  $\Phi_{\bar{r}}$ , calling  $\bar{R}_A = \frac{1}{4} \sum_{i=1}^4 \bar{r}_i$  and  $\bar{R}_B = \frac{1}{4} \sum_{j=5}^8 \bar{r}_j$ , the center of mass of the  $\alpha$  particles ( $A$ ) and ( $B$ ),  $\bar{R}_{c.m.} = \frac{1}{2}(\bar{R}_A + \bar{R}_B)$  the total center-of-mass coordinate, and  $\bar{R} = \bar{R}_A - \bar{R}_B$  the relative coordinate, we obtain

$$\begin{aligned} \Phi_{\bar{r}} = & [\pi^{-3/4} (b/2\sqrt{2})^{-3/2} e^{-4R_{c.m.}^2/b^2}] \\ & \times \Gamma(\bar{r}, \bar{R}) \psi_{\text{int}}(A) \psi_{\text{int}}(B), \end{aligned} \quad (7)$$

where  $\psi_{\text{int}}(A)$  and  $\psi_{\text{int}}(B)$  are the internal wave functions for the  $\alpha$  clusters ( $A$ ) and ( $B$ ), and

$$\Gamma(\bar{r}, \bar{R}) = \pi^{-3/4} (b/\sqrt{2})^{-3/2} \exp[-(\bar{r} - \bar{R})^2/b^2]. \quad (8)$$

We notice that the center-of-mass motion is factorized. Since the formalism is invariant by Galilean transformation, we shall ignore this center-of-mass motion in the remainder of the discussion. By inserting Eq. (7) in Eq. (2) the  $\alpha$ - $\alpha$  system wave function now reads

$$\psi = \mathcal{G} \psi_{\text{int}}(A) \psi_{\text{int}}(B) g(\bar{R}), \quad (9)$$

where

$$g(\bar{R}) = \pi^{-3/4} (b/\sqrt{2})^{-3/2} \int \exp[-(\bar{r} - \bar{R})^2/b^2] f(\bar{r}) d\bar{r}. \quad (10)$$

The expression given in Eq. (9) is precisely the expression of the wave function used in the resonating group method where the unknown function is  $g(\bar{R})$ . As Eq. (9) also represents the wave function used in GCM where the unknown function is  $f(\bar{r})$ , the connection between the two methods becomes evident and we may write the fundamental Eq. (10) formally

$$g = \Gamma \otimes f, \quad (10')$$

where the symbol  $\otimes$  denotes a convolution product.

#### C. Hill-Wheeler equation in coordinate space

It is easier to obtain the kernels of the Hill-Wheeler integral if one expresses  $\Phi_{\bar{r}}$  [Eq. (1)] in

second quantization:

$$|\Phi_{\bar{r}}\rangle = a_p^\dagger(\frac{1}{2}\bar{r})a_p^\dagger(\frac{1}{2}\bar{r})a_p^\dagger(-\frac{1}{2}\bar{r})a_p^\dagger(-\frac{1}{2}\bar{r})a_n^\dagger(\frac{1}{2}\bar{r})a_n^\dagger(\frac{1}{2}\bar{r})a_n^\dagger(-\frac{1}{2}\bar{r})a_n^\dagger(-\frac{1}{2}\bar{r})|0\rangle, \quad (11)$$

where  $|0\rangle$  represents the vacuum,  $a_p^\dagger$  ( $a_n^\dagger$ ) the creation operator for a proton of spin  $+\frac{1}{2}$  ( $-\frac{1}{2}$ ) and  $a_n^\dagger$  ( $a_p^\dagger$ ) the creation operator for a neutron of spin  $+\frac{1}{2}$  ( $-\frac{1}{2}$ ). These operators obey ordinary commutation rules and allow the use of the Lowdin's technique.<sup>10</sup>

The Hamiltonian  $\mathcal{H}$  of the system contains: (a) The kinetic energy of all the nucleons

$$\mathcal{T} = \sum_{i=1}^A \left[ -\frac{\hbar^2}{2M} \nabla_i^2 \right],$$

where  $M$  is the nucleon mass; (b) a two body potential energy term of general form

$$V_{ij} = V_0 e^{-(\bar{r}_i - \bar{r}_j)^2 / \mu^2} (A + BP_\sigma + CP_\tau + DP_\sigma P_\tau), \quad (12)$$

where  $V_0$  represents the depth and  $\mu$  the range of the potential,  $P_\sigma$  and  $P_\tau$  are the spin and isospin exchange operators, and  $A$ ,  $B$ ,  $C$ , and  $D$  are the coefficients of the mixture; (c) a Coulomb interaction term which is discussed in Sec. III F. We can now calculate the quantities useful for the problem. For the overlap  $N(\bar{r}, \bar{r}')$  we obtain

$$N(\bar{r}, \bar{r}') = \left\{ \exp[-(\bar{r} - \bar{r}')^2 / 8b^2] - \exp[-(\bar{r} + \bar{r}')^2 / 8b^2] \right\}^4. \quad (13)$$

a potential energy kernel

$$T(\bar{r}, \bar{r}') = \hbar \omega \left( \left( \frac{3}{4} - \frac{r^2 + r'^2}{4b^2} \right) N(\bar{r}, \bar{r}') + N^{3/4}(\bar{r}, \bar{r}') \cdot \frac{\bar{r}\bar{r}'}{2b^2} \cdot \left\{ \exp\left[-\frac{(\bar{r} - \bar{r}')^2}{8b^2}\right] + \exp\left[-\frac{(\bar{r} + \bar{r}')^2}{8b^2}\right] \right\} \right), \quad (14)$$

$$\begin{aligned} V(\bar{r}, \bar{r}') &= \frac{4V_0\mu^3}{(2b^2 + \mu^2)^{3/2}} \exp\left(-\frac{r^2 + r'^2}{2b^2}\right) \left[ \exp\left(\frac{\bar{r}\bar{r}'}{2b^2}\right) + \exp\left(-\frac{\bar{r}\bar{r}'}{2b^2}\right) - 2 \right] \\ &\times \left( 2(G - S) \left\{ \exp\left[-\frac{r^2}{4(2b^2 + \mu^2)}\right] + \exp\left[-\frac{r'^2}{4(2b^2 + \mu^2)}\right] - 1 \right\} \right. \\ &\left. - \exp\left[-\frac{(\bar{r} + \bar{r}')^2}{4(2b^2 + \mu^2)}\right] \left[ G - S \exp\left(\frac{\bar{r}\bar{r}'}{2b^2}\right) \right] - \exp\left[-\frac{(\bar{r} - \bar{r}')^2}{4(2b^2 + \mu^2)}\right] \left[ G - S \exp\left(-\frac{\bar{r}\bar{r}'}{2b^2}\right) \right] \right) \end{aligned} \quad (15)$$

with  $G = A + 2B + 2C + 4D$  and  $S = 4A + 2B + 2C + D$ .

### III. RESOLUTION OF HILL-WHEELER EQUATION

#### A. Difficulties in solving the equation in coordinate space

We write Eq. (4) in operator form:

$$(H - EN)f = 0.$$

We can reduce it to a diagonalization problem by multiplying it on the left by  $N^{-1/2}$  (provided

Asymptotically ( $r$  or  $r'$  large) we notice that

$$N \approx \Gamma \otimes \Gamma,$$

where  $\Gamma$  is the operator defined by Eq. (8). This result will be used later.

The interesting quantity in our problem is the relative energy between the  $\alpha$  particles. We must therefore take into account (i) the kinetic energy of the center-of-mass motion  $T_{\text{c.m.}} = 3\hbar\omega/4$ , (ii) the internal kinetic energy of each  $\alpha$  cluster  $T_{\text{int}} = 3(3\hbar\omega/4)$  where  $\hbar\omega = \hbar^2/Mb^2$ , and (iii) the internal potential energy of the two  $\alpha$  particles,

$$V_{\text{int}} = \frac{4\mu^3(S - G)V_0}{(2b^2 + \mu^2)^{3/2}} N(\bar{r}, \bar{r}').$$

Once we have subtracted

$$(2T_{\text{int}} + T_{\text{c.m.}} + V_{\text{int}})N(\bar{r}, \bar{r}')$$

from  $H(\bar{r}, \bar{r}')$ , we get the kernel of a Hill-Wheeler equation related to the relative motion of two  $\alpha$  particles of relative kinetic energy at infinity:

$$\hbar^2 k^2 / 2m,$$

where  $m = 2M$  is the reduced mass, and the wave number  $k$  is the asymptotic wave number of the relative motion. Hence we obtain a kinetic and

$N^{-1/2}$  exists)

$$(N^{-1/2} H N^{-1/2} - E)(N^{1/2} f) = 0,$$

and solve this eigenvalue problem for an integration mesh  $q_i$ , correctly chosen.

There is, however, a problem which renders the use of this method difficult: the values obtained at the points  $q_i$  do not generate a stable function  $f(q_i)$  when we change the integration

mesh. The closer the points, the more violently the function  $f(q_i)$  oscillates. These oscillations can be explained if we look at  $\Gamma(\bar{q}, \bar{q}')$ , the Fourier transform of  $\Gamma(\bar{r}, \bar{R})$  defined at Eq. (8):

$$\Gamma(\bar{q}, \bar{q}') = (2\pi)^{3/4} b^{3/2} e^{-b^2 q^2/4} [\delta(\bar{q} - \bar{q}') + \delta(\bar{q} + \bar{q}')] \quad (16)$$

which, when we call  $f(\bar{q})$  and  $g(\bar{q})$  the Fourier transforms of  $f(\bar{r})$  and  $g(\bar{r})$ , leads to

$$f(\bar{q}) = (2\pi)^{-3/4} b^{-3/2} e^{b^2 q^2/2} g(\bar{q}). \quad (17)$$

The function  $g(\bar{q})$  is a scattering function which decreases to 0 when  $q$  tends to infinity. However, this decrease is not in general fast enough to compensate for the quadratic exponential which figures in Eq. (17). Consequently, the inverse Fourier transform which leads from  $f(\bar{q})$  to  $f(\bar{r})$  diverges at high frequency and this explains the

violent oscillations of  $f(\bar{r})$  when the mesh points become closer.

#### B. Representation in momentum space

For solving the Hill-Wheeler equation for the continuous spectrum it is convenient to take  $g$  as the unknown function obeying the equation

$$\Gamma^{-1}(H - EN)\Gamma^{-1}g = 0 \quad (18)$$

and to solve it in momentum space.

We shall see later that this equation is a Schrödinger equation or more exactly a Lippmann-Schwinger equation, as it is solved in momentum space representation. As a matter of fact, the inversion of  $\Gamma$  in coordinate space is not an operation as easy as it is in momentum space. However, the divergence of  $\Gamma^{-1}$  at high frequency is compensated by the fast exponential decrease of the kernels  $N$ ,  $T$ , and  $V$  as one can see on the

#### Fourier transforms

$$N(\bar{q}, \bar{q}') = (2\pi)^{3/2} b^3 \exp\left[-\frac{1}{2}b^2 q^2\right] [\delta(\bar{q} - \bar{q}') + \delta(\bar{q} + \bar{q}')] + 6b^6 \exp\left[-\frac{1}{2}b^2(q^2 + q'^2)\right] - \frac{32}{3^{3/2}} b^6 \exp\left[-\frac{2b^2}{3}(q^2 + q'^2)\right] \left[ \exp\left(\frac{2b^2}{3}\bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2}{3}\bar{q}\bar{q}'\right) \right], \quad (19)$$

$$T(\bar{q}, \bar{q}') = \hbar\omega \left\{ (2\pi)^{3/2} \frac{1}{4} b^5 q^2 \exp\left[-\frac{1}{2}b^2 q^2\right] [\delta(\bar{q} + \bar{q}') + \delta(\bar{q} - \bar{q}')] - \frac{3}{2} b^6 \exp\left[-\frac{1}{2}b^2(q^2 + q'^2)\right] [3 - b^2(q^2 + q'^2)] + \frac{2^3}{3^{3/2}} b^6 \exp\left[-\frac{2b^3}{3}(q^2 + q'^2 + \bar{q}\bar{q}')\right] \left[ 3 - \frac{4b^2}{3}(q^2 + q'^2 + \bar{q}\bar{q}') \right] + \frac{2^3}{3^{3/2}} b^6 \exp\left[-\frac{2b^2}{3}(q^2 + q'^2 - \bar{q}\bar{q}')\right] \left[ 3 - \frac{4b^2}{3}(q^2 + q'^2 - \bar{q}\bar{q}') \right] \right\}. \quad (20)$$

The corresponding expression for  $V(\bar{q}, \bar{q}')$  is easily obtained. As it is rather cumbersome, we present it in Appendix A [Eq. (A1)].

#### C. Treatment of the divergences

After the application of the operator  $\Gamma^{-1}(\bar{q}, \bar{q}')$  no exponential divergences remain in the kernels  $n = \Gamma^{-1}N\Gamma^{-1}$ ,  $t = \Gamma^{-1}T\Gamma^{-1}$ , and  $v = \Gamma^{-1}V\Gamma^{-1}$ . One finds for  $n$  and  $t$  [the corresponding formula for  $v$  is given in Appendix A, Eq. (A2)]:

$$n(\bar{q}, \bar{q}') = \frac{1}{2} [\delta(\bar{q} + \bar{q}') + \delta(\bar{q} - \bar{q}')] + \frac{3b^3}{(2\pi)^{3/2}} \exp\left[-\frac{1}{4}b^2(q^2 + q'^2)\right] - \frac{16b^3}{3^{3/2}(2\pi)^{3/2}} \exp\left[-\frac{5b^2}{12}(q^2 + q'^2)\right] \left[ \exp\left(\frac{2b^2}{3}\bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2}{3}\bar{q}\bar{q}'\right) \right], \quad (21)$$

$$t(\bar{q}, \bar{q}') = \frac{1}{6} (\hbar\omega b^2) q^2 [\delta(\bar{q} - \bar{q}') + \delta(\bar{q} + \bar{q}')] + \frac{\hbar\omega}{(2\pi)^{3/2}} \left( -\frac{3}{4} b^3 \exp\left[-\frac{1}{4}b^2(q^2 + q'^2)\right] [3 - b^2(q^2 + q'^2)] + \frac{4b^3}{3^{3/2}} \exp\left[-\frac{5b^2}{12}(q^2 + q'^2)\right] \left\{ \left[ 3 - \frac{4b^2}{3}(q^2 + q'^2) \right] \left[ \exp\left(\frac{2b^2}{3}\bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2}{3}\bar{q}\bar{q}'\right) \right] + \frac{4b^2}{3}\bar{q}\bar{q}' \left[ \exp\left(\frac{2b^2}{3}\bar{q}\bar{q}'\right) - \exp\left(-\frac{2b^2}{3}\bar{q}\bar{q}'\right) \right] \right\} \right). \quad (22)$$

## D. Projection onto even waves

It now remains to project  $n$ ,  $t$ , and  $v$  onto even waves, as the Pauli principle excludes the odd waves. Denoting  $l$  the partial wave index, we find

$$n_l(q, q') = \frac{\delta(q - q')}{q^2} + \nu_l(q, q'), \quad (23)$$

$$\nu_l(q, q') = \left(\frac{2}{\pi}\right)^{1/2} \left\{ 3\sqrt{2} b^3 \exp\left[-\frac{b^2}{4}(q^2 + q'^2)\right] \delta_{l,0} - \frac{32\sqrt{2}b^3}{3^{3/2}} \exp\left[-\frac{5b^2}{12}(q^2 + q'^2)\right] i_l\left(\frac{2b^2}{3}qq'\right) \right\}, \quad (24)$$

$$t_l(q, q') = \frac{\hbar^2}{4M} \delta(q - q') + \theta_l(q, q'), \quad (25)$$

$$\begin{aligned} \theta_l(q, q') = \left(\frac{2}{\pi}\right)^{1/2} \frac{\hbar^2}{M} & \left( -\frac{9b}{4} \exp\left[-\frac{b^2}{4}(q^2 + q'^2)\right] \delta_{l,0} + \frac{3b^3}{4}(q^2 + q'^2) \exp\left[-\frac{b^2}{4}(q^2 + q'^2)\right] \delta_{l,0} \right. \\ & + \frac{4b}{3^{3/2}} \exp\left[\frac{5b^2}{12}(q^2 + q'^2)\right] \left\{ \left[6 - \frac{8b^2}{3}(q^2 + q'^2)\right] i_l\left(\frac{2b^2}{3}qq'\right) \right. \\ & \left. \left. + \frac{8b^2}{3(2l+1)} qq' \left[ l i_{l-1}\left(\frac{2b^2}{3}qq'\right) + (l+1) i_{l+1}\left(\frac{2b^2}{3}qq'\right) \right] \right\} \right), \end{aligned} \quad (26)$$

where  $i_l(x)$  represents the modified spherical Bessel function.

The equivalent expression for  $\nu_l(q, q')$  is given in Appendix A [Eq. (A3)]. Since the phase space in partial waves is  $q^2 dq$ , the equation

$$(t_l + v_l - En_l)g_l$$

contains in particular a term  $(q^2 - E)g_l(q)$  which is nothing but the characteristic term of a Lippmann-Schwinger equation. This justifies what has previously been stated about the reduction of a Hill-Wheeler equation to a Schrödinger equation.

## E. Role of the Pauli principle

Not only are the odd waves not present in the system, as the  $\alpha$  particles behave as bosons at long range, but, moreover, it is well known that at short range the Pauli principle imposes a change of four  $S$  orbits in  $P$  orbits (see Ref. 5).

The result is that the relative motion  $g_l(q)$  or  $g_l(r)$  in the  $S$  wave cannot contain any component on the  $0S$  and  $1S$  wave. In the same way, the relative motion in the  $D$  wave cannot contain any component on the  $0D$  wave. In fact, due to the numerical approximations that we shall allow, some spurious mixing of these  $0S$ ,  $1S$ , and  $1D$  states can be present. Since they do not change the wave function at long range, they do not change in principle the phase shifts. We shall verify after calculations that the numerical solutions are not perturbed by the eventual presence of these spurious components.

## F. Treatment of the Coulomb interaction

For the Coulomb interaction we make an approximation related to the long range of this

potential. In fact, when the two  $\alpha$  particles are far enough from each other, that is to say when the Pauli principle does not play an important role, the leading terms are those of the direct term and total exchange term.

We directly introduce the Coulomb potential in momentum representation. For this purpose we restrict ourselves for the moment to the case of the Coulomb potential  $v_c = z^2 e^2/R$ . Following, for instance, Ref. 11 we write

$$Eg(\bar{q}) = \frac{\hbar^2 q^2}{2m} g(\bar{q}) + \int v_c(\bar{q} - \bar{q}') g(\bar{q}') d\bar{q}', \quad (27)$$

$$v_c(\bar{q} - \bar{q}') = \frac{1}{(2\pi)^3} \int e^{i(\bar{q} - \bar{q}')\bar{R}} v_c(\bar{R}) d\bar{R},$$

which after projection on partial waves leads to

$$(k^2 - q^2)g_l(q) = \frac{2}{\pi} \frac{2m}{\hbar^2} \int_0^\infty I_l(q, q') q'^2 g_l(q') dq' \quad (28)$$

and

$$I_l(q, q') = \int_0^\infty j_l(qR) j_l(q'R) v_c(R) R^2 dR, \quad (29)$$

where  $j_l(x)$  is the spherical Bessel function of order  $l$ .

There is no closed formula for the integral  $I_l(q, q')$  if  $v_c(R)$  is truncated, and this will be the case. Due to the presence of the Bessel functions it cannot be calculated by general integration methods. In order to obtain it numerically we establish in Appendix B some of its properties and in particular a recursion formula which  $I_l(q, q')$  obeys.

We now come back to the complete equation

which contains the Coulomb term as well as the other terms deduced above from the transformation of the Hill-Wheeler equation:

$$(k^2 - q^2)g_l(q) = \frac{4M}{\hbar^2} \int_0^\infty W_l(q, q')g_l(q')q'^2 dq' \tag{30}$$

It looks like a Fredholm equation for the kernel

$$W_l(q, q') = \theta_l(q, q') + v_l(q, q') - E v_l(q, q') + \frac{2}{\pi} I_l(q, q'), \tag{31}$$

which plays the role of a nonlocal pseudopotential.

G. Method for calculating the phase shifts

We are only interested in the phase shifts generated by the equation shown above. To calculate the phase shifts we have thus chosen the Fredholm method as it was developed by Schwinger<sup>12</sup> and Baker.<sup>13</sup> The determinant  $D(z) = \det[1 - G^0(z)W]$ , where  $G^0(z) = (z - T)^{-1}$ , is the Green function of the free particle, and contains all the information about the scattering. For a given partial wave  $l$ ,

the phase shift then reads:

$$\tan \delta_l(E) = - \frac{\text{Im}[D_l(E + i\epsilon)]}{\text{Re}[D_l(E + i\epsilon)]} \tag{32}$$

By using the identity between operators

$$\det A = \exp \text{tr} \ln A \tag{33}$$

we obtain the following development for  $D_l(z)$ :

$$D_l(z) = 1 - \int_0^\infty \frac{dE_1 W_{11}^l}{z - E_1} + \frac{1}{2!} \int_0^\infty \int_0^\infty \frac{dE_1 dE_2}{(z - E_1)(z - E_2)} \begin{vmatrix} W_{11}^l & W_{12}^l \\ W_{21}^l & W_{22}^l \end{vmatrix} + \dots, \tag{34}$$

where the  $W_{ij}$  are the matrix elements of the pseudopotential (31) in energy representation. In our case we only have to calculate the integral of  $(qq')^{1/2}W_l(q, q')$  to return to momentum representation.

When we calculate within  $\text{Im}[D_l(z)]$  and  $\text{Re}[D_l(z)]$  the integrals (which are principal part values) by use of an  $N$ -point  $q_i$  Gauss-Legendre quadrature method, we obtain the following expressions, in which  $\omega_i$  represents the weights associated with

the  $q_i$  points:

$$\text{Im}[D_l(E + i\epsilon)] = -\pi \begin{vmatrix} -W_{00}^l & -\frac{2W_{01}^l \omega_1 q_1}{k^2 - q_1^2} \dots - \frac{2W_{0N}^l \omega_N q_N}{k^2 - q_N^2} \\ \vdots & \text{Re}[D_l(E + i\epsilon)] \\ \vdots & \\ -W_{N0}^l & \end{vmatrix}, \tag{35a}$$

$$\text{Re}[D_l(E + i\epsilon)] = \begin{vmatrix} 1 - \frac{2W_{11}^l \omega_1 q_1}{k^2 - q_1^2} & -\frac{2W_{22}^l \omega_2 q_2}{k^2 - q_2^2} & \dots & -\frac{2W_{1N}^l \omega_N q_N}{k^2 - q_N^2} \\ -\frac{2W_{21}^l \omega_1 q_1}{k^2 - q_1^2} & 1 - \frac{2W_{22}^l \omega_2 q_2}{k^2 - q_2^2} & \dots & \\ \vdots & \vdots & \ddots & \\ \frac{2W_{N1}^l \omega_1 q_1}{k^2 - q_1^2} & \dots & \dots & \frac{2W_{NN}^l \omega_N q_N}{k^2 - q_N^2} \end{vmatrix}. \tag{35b}$$

The Fredholm method has already been employed in particular by Jost and Pais<sup>14</sup> and by Reinhardt and Szabo<sup>15</sup> for calculations on phase shifts of a particle by a potential.

IV. RESULTS AND DISCUSSION

A. Parameters of the problem

One of the aspects of this problem lies in the general absence of parametrization. The only

numerical constants present are the value of the harmonic oscillator parameter which is related to the  $\alpha$ -particle radius, and the mixture defining a nucleon-nucleon force.

*Harmonic oscillator parameter.* This parameter is obtained from the r.m.s. radius of an  $\alpha$  particle of which the center of mass is fixed:

$$\langle x_\alpha^2 \rangle = \frac{\int x^4 \rho(x) dx}{\int x^2 \rho(x) dx} = \frac{9}{8} b^2, \tag{36}$$

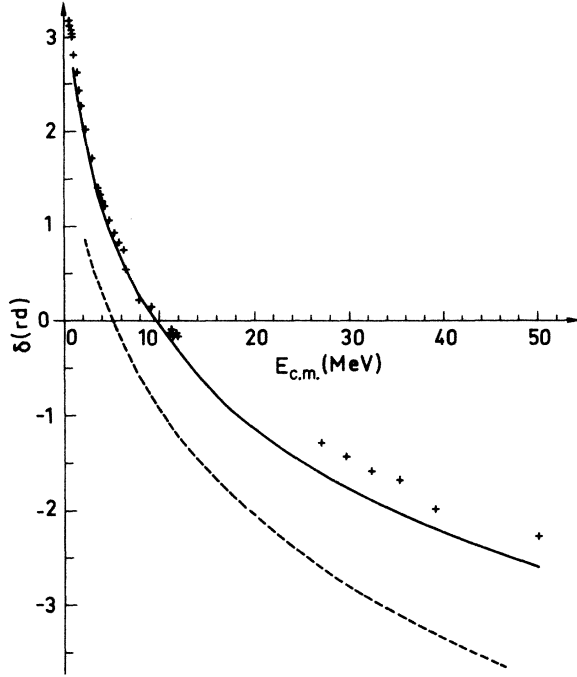


FIG. 1. The  $l=0$  phase shift. The full line curve represents the values obtained with the Volkov potential [Eq. (37)], the dashed curve represents the values obtained with the Brink  $B1$  potential [Eq. (38)]. The experimental points (+) are those listed in Ref. 16.

where

$$\rho(x) = \int \prod_{i=1}^4 (dx_i |e^{-x_i^2/2b^2}|^2) \delta(\bar{x} - \bar{x}_1) \delta\left(\sum_{j=1}^4 \bar{x}_j\right).$$

This leads to  $b = 1.36$  fm for the value<sup>16</sup>  $x_\alpha = 1.44$  fm of the  $\alpha$ -particle radius.

*Two-body potential.* We have used the soft repulsive core potentials of Volkov<sup>17</sup>

$$V(x) = (0.44 + 0.56P_x)(-60 e^{-(x/1.80)^2} + 60 e^{-(x/1.01)^2}) \quad (37)$$

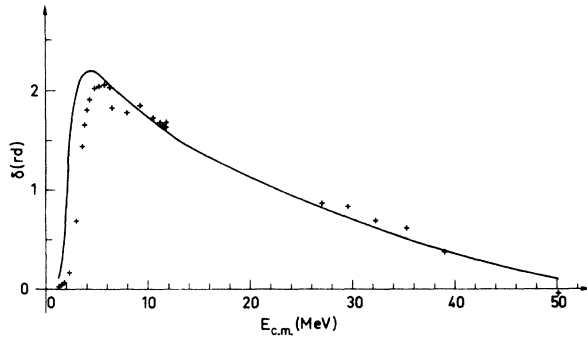


FIG. 2. The  $l=2$  phase shift obtained with the Volkov potential. The experimental points (+) are those listed in Ref. 16.

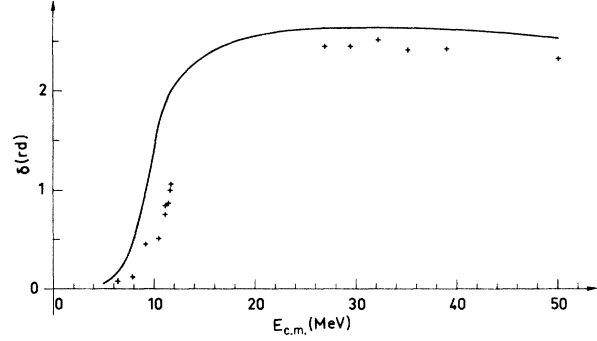


FIG. 3. The  $l=4$  phase shift obtained with the Volkov potential. The experimental points (+) are those listed in Ref. 16.

and of Brink and Boeker<sup>18</sup>  $B_1$

$$V(x) = -140.6 e^{-(x/1.4)^2} (0.51 + 0.49P_x) + 389.5 e^{-(x/0.7)^2} (1.53 - 0.53P_x). \quad (38)$$

*Coulomb potential.* The determinantal method described above holds only if the radial part of the potentials tends to 0 faster than  $1/\gamma$  when  $\gamma \rightarrow \infty$ . We have adopted the truncated Coulomb potential

$$v_c(R) = z^2 e^2 / R \quad \text{if } R \leq R_0, \\ = 0 \quad \text{if } R > R_0. \quad (39)$$

We replace, after  $R_0$ , the Coulomb potential by the correction

$$\gamma \ln(2kR_0),$$

where

$$\gamma = z^2 e^2 / \hbar v$$

and  $v$  is the velocity of the incident particle.

We choose  $R_0 = 30$  fm and we have checked that the Coulomb phase shifts  $\sigma_l$  obtained by resolution of the equations containing only the Coulomb term

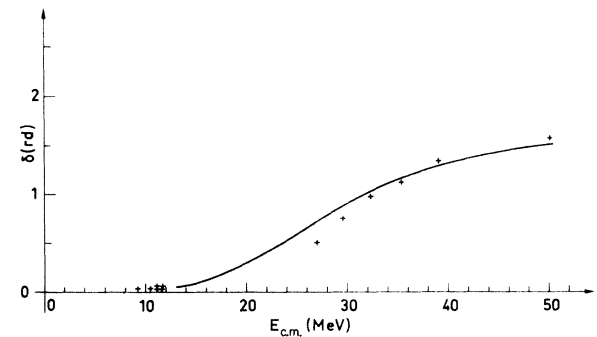


FIG. 4. The  $l=6$  phase shift obtained with the Volkov potential. The experimental points (+) are those listed in Ref. 16.

gives the well-known result

$$\sigma_l = \Gamma(l+1 + i\gamma), \quad (40)$$

where  $\Gamma$  represents here the Euler function and  $l$  is the  $l$ th partial wave.

Finally, in order to take into account the gross features of the exchange effects, we have also replaced the expression given in Eq. (39) by the following one:

$$\begin{aligned} v_c(R) &= \frac{z^2 e^2}{2R} \left( 3 - \frac{R^2}{x_\alpha^2} \right) \quad 0 \leq R \leq 2x_\alpha, \\ &= \frac{z^2 e^2}{R} \quad 2x_\alpha < R \leq R_0, \\ &= 0 \quad R > R_0. \end{aligned} \quad (41)$$

The results for the  $\delta_l$  phase shifts have not been significantly modified.

*Integration mesh.* We use a Gauss-Legendre method in order to perform the integrals in the determinants defined in Eqs. (35a) and (35b). The mesh is the following: a 12 point method between 0 and 1 fm, a 12 point method between 1 and 2 fm, and an 8 point method between 2 and 30 fm.<sup>19</sup>

We have also used a 32 point method preceded by the change of variable

$$q_i = k \tan\left[\frac{1}{4}\pi(1 + x_i)\right],$$

the  $x_i$  denoting the Gauss-Legendre points. The two methods give the same results.

## B. Results

We have represented in Fig. 1 the results of the phase shifts obtained for the S wave with a Volkov [Eq. (37)] and Brink B1 [Eq. (38)] interaction. Both the two forces give correct results but the Volkov one is closer to the experimental results. We have also used all the other B and C forces listed in the Brink and Boeker<sup>18</sup> paper. All the results are distributed around B1 and are not shown here. In Figs. 2, 3, and 4 are given the  $l=2, 4,$  and  $6$  phase shifts, respectively. The agreement with experiment is rather good.

The same results have already been reported by several authors, namely Okai and Park<sup>20</sup> and Federsel *et al.*,<sup>21</sup> by use of the resonating group method. All these calculations show the equivalence between the RGM and GCM. The flexibility of the GCM in particular could be useful to calculate an effective  $\alpha$ - $\alpha$  potential.

There is, however, another method due to de Takacsy<sup>22</sup> to obtain the phase shifts. Essentially in this method the Hill-Wheeler integral is solved in coordinate space and the integral from 0 to  $\infty$  is replaced by an integral from 0 to an arbitrary cutoff  $S_0$ . The part from  $S_0$  to infinity of the integral is replaced by something else where the unknown function  $f(r)$  is replaced by the asymptotic scattering function. de Takacsy with less integration points shows nuclear phase shifts.

The drawback of this method is that this arbitrary cutoff in the Hill-Wheeler integral introduces an additional parameter, and there is no proof that if  $S_0$  is increased the solution remains stable. This objection has already been pointed out by Horiuchi<sup>23</sup> in his calculations in coordinate space, since he was obliged to define for each partial wave a different "channel radius" in order to fit the experimental results.

To conclude, we note that our microscopic theory is free of parametrization. Except for the Coulomb interaction, the Pauli principle is correctly taken into account and the Coulomb force is introduced without use of the usual parametrizations, leading to a rather good description of  $\alpha$ - $\alpha$  scattering. This theory could be extended to heavier nuclei such as  $^{16}\text{O}$ - $^{16}\text{O}$  or  $^{16}\text{O}$ - $^{12}\text{C}$  scattering, but then requires some additional approximations.

## ACKNOWLEDGMENTS

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## APPENDIX A: DIFFERENT EXPRESSIONS FOR THE NUCLEAR POTENTIAL TERM

### A. Fourier transform of $V(\vec{r}, \vec{r}')$

$$\begin{aligned} V(\vec{q}, \vec{q}') &= 16\mu^3 b^6 V_0 (G - S) \left( -\frac{4}{3^{3/2}(2b^2 + \mu^2)^{3/2}} \exp\left[-\frac{2b^2}{3}(q^2 + q'^2)\right] \left[ \exp\left(\frac{2b^2}{3}\vec{q}\vec{q}'\right) + \exp\left(-\frac{2b^2}{3}\vec{q}\vec{q}'\right) \right] \right. \\ &\quad + \frac{4}{(8b^2 + 3\mu^2)^{3/2}} \left. \left\{ \exp\left[-\frac{(5b^2 + 2\mu^2)b^2 q'^2 + (4b^2 + 2\mu^2)b^2 q^2}{8b^2 + 3\mu^2}\right] \right. \right. \\ &\quad \left. \left. + \exp\left[-\frac{(5b^2 + 2\mu^2)b^2 q^2 + (4b^2 + 2\mu^2)b^2 q'^2}{8b^2 + 3\mu^2}\right] \right\} \right. \\ &\quad \left. \times \left\{ \exp\left[\frac{(4b^2 + 2\mu^2)b^2 \vec{q}\vec{q}'}{8b^2 + 3\mu^2}\right] + \exp\left[-\frac{(4b^2 + 2\mu^2)b^2 \vec{q}\vec{q}'}{8b^2 + 3\mu^2}\right] \right\} \right. \end{aligned}$$



$$\begin{aligned}
& -\frac{2^{3/2}}{(5b^2+2\mu^2)^{3/2}} \left[ \exp\left(-\frac{b^2q^2}{2}\right) \exp\left(-\frac{2b^2+\mu^2}{5b^2+2\mu^2} b^2q'^2\right) \right. \\
& \quad \left. + \exp\left(-\frac{b^2q'^2}{2}\right) \exp\left(-\frac{2b^2+\mu^2}{5b^2+2\mu^2} b^2q^2\right) \right] + \frac{1}{(2b^2+\mu^2)^{3/2}} \exp\left[-\frac{b^2}{2}(q^2+q'^2)\right] \\
& -32\mu^3b^6V_0(G+2S) \frac{1}{(12b^2+3\mu^2)^{3/2}} \exp\left[-\frac{b^2(5b^2+2\mu^2)(q^2+q'^2)}{12b^2+3\mu^2}\right] \\
& \times \left[ \exp\left(\frac{2b^2+2\mu^2}{12b^2+3\mu^2} b^2\bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2+2\mu^2}{12b^2+3\mu^2} b^2\bar{q}\bar{q}'\right) \right] \\
& +4\mu^3b^6V_0(S+2G) \frac{1}{(3b^2+\mu^2)^{3/2}} \exp\left[-\frac{b^2(5b^2+2\mu^2)}{12b^2+4\mu^2}(q^2+q'^2)\right] \\
& \times \left[ \exp\left(\frac{b^2}{6b^2+2\mu^2} b^2\bar{q}\bar{q}'\right) + \exp\left(-\frac{b^2}{6b^2+2\mu^2} b^2\bar{q}\bar{q}'\right) \right] \\
& -32\mu^3b^6V_0G \frac{1}{(8b^2+3\mu^2)^{3/2}} \exp\left[-\frac{b^2(5b^2+2\mu^2)}{8b^2+3\mu^2}(q^2+q'^2)\right] \left[ \exp\left(\frac{6b^2+2\mu^2}{8b^2+3\mu^2} b^2\bar{q}\bar{q}'\right) + \exp\left(-\frac{6b^2+2\mu^2}{8b^2+3\mu^2} b^2\bar{q}\bar{q}'\right) \right] \\
& +4\mu^3b^6V_0S \frac{1}{(2b^2)^{3/2}} \exp\left[-\frac{5b^2+2\mu^2}{8}(q^2+q'^2)\right] \left[ \exp\left(\frac{3b^2+2\mu^2}{4}\bar{q}\bar{q}'\right) + \exp\left(-\frac{3b^2+2\mu^2}{4}\bar{q}\bar{q}'\right) \right],
\end{aligned}$$

with  $G = A + 2B + 2C + 4D$  and  $S = 4A + 2B + 2C + D$ .

(A1)

#### B. Treatment of the divergences

$$\begin{aligned}
v(\bar{q}, \bar{q}') &= \frac{8\mu^3b^3V_0(G-S)}{(2\pi)^{3/2}} \left\{ \frac{4}{(8b^2+3\mu^2)^{3/2}} \left[ \exp\left(-\frac{b^2}{4} \frac{12b^2+5\mu^2}{8b^2+3\mu^2} q'^2\right) \exp\left(-\frac{b^2}{4} \frac{8b^2+5\mu^2}{8b^2+3\mu^2} q^2\right) \right. \right. \\
& \quad \left. \left. + \exp\left(-\frac{b^2}{4} \frac{12b^2+5\mu^2}{8b^2+3\mu^2} q^2\right) \exp\left(-\frac{b^2}{4} \frac{8b^2+5\mu^2}{8b^2+3\mu^2} q'^2\right) \right] \right. \\
& \quad \times \left[ \exp\left(\frac{2b^2(2b^2+\mu^2)}{8b^2+3\mu^2} \bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2(2b^2+\mu^2)}{8b^2+3\mu^2} \bar{q}\bar{q}'\right) \right] \\
& -\frac{2^{3/2}}{(5b^2+2\mu^2)^{3/2}} \left[ \exp\left(-\frac{b^2}{4} q^2\right) \exp\left(-\frac{b^2}{4} \frac{3b^2+2\mu^2}{5b^2+2\mu^2} q'^2\right) \right. \\
& \quad \left. + \exp\left(-\frac{b^2}{4} q'^2\right) \exp\left(-\frac{b^2}{4} \frac{3b^2+2\mu^2}{5b^2+2\mu^2} q^2\right) \right] \\
& -\frac{4}{3^{3/2}(2b^2+\mu^2)^{3/2}} \exp\left[-\frac{5b^2}{12}(q^2+q'^2)\right] \left[ \exp\left(\frac{2b^2}{3}\bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2}{3}\bar{q}\bar{q}'\right) \right] \\
& \quad \left. + \frac{1}{(2b^2+\mu^2)^{3/2}} \exp\left[-\frac{b^2}{4}(q^2+q'^2)\right] \right\} \\
& -\frac{16\mu^3b^3V_0(G+2S)}{(2\pi)^{3/2}} \frac{1}{3^{3/2}(4b^2+\mu^2)^{3/2}} \exp\left[-\frac{b^2}{12} \frac{8b^2+5\mu^2}{4b^2+\mu^2}(q^2+q'^2)\right] \\
& \times \left[ \exp\left(\frac{2b^2}{3} \frac{b^2+\mu^2}{4b^2+\mu^2} \bar{q}\bar{q}'\right) + \exp\left(-\frac{2b^2}{3} \frac{b^2+\mu^2}{4b^2+\mu^2} \bar{q}\bar{q}'\right) \right] \\
& +\frac{2\mu^3b^3V_0(S+2G)}{(2\pi)^{3/2}} \frac{1}{(3b^2+\mu^2)^{3/2}} \exp\left[-\frac{b^2}{4} \frac{2b^2+\mu^2}{3b^2+\mu^2}(q^2+q'^2)\right] \\
& \times \left[ \exp\left(\frac{b^2}{2} \frac{b^2}{3b^2+\mu^2} \bar{q}\bar{q}'\right) + \exp\left(-\frac{b^2}{2} \frac{b^2}{3b^2+\mu^2} \bar{q}\bar{q}'\right) \right] \\
& -\frac{16\mu^3b^3V_0G}{(2\pi)^{3/2}} \frac{1}{(8b^2+3\mu^2)^{3/2}} \exp\left[-\frac{b^2}{4} \frac{12b^2+5\mu^2}{8b^2+3\mu^2}(q^2+q'^2)\right]
\end{aligned}$$

$$\begin{aligned} & \times \left\{ \exp \left[ \frac{2b^2(3b^2 + \mu^2)}{8b^2 + 3\mu^2} q \bar{q}' \right] + \exp \left[ - \frac{2b^2(3b^2 + \mu^2)}{8b^2 + 3\mu^2} q \bar{q}' \right] \right\} \\ & + \frac{2\mu^3 b^3 V_0 S}{(2\pi)^{3/2}} \frac{1}{(2b^2)^{3/2}} \exp \left[ - \frac{3b^2 + 2\mu^2}{8} (q^2 + q'^2) \right] \left[ \exp \left( \frac{3b^2 + 2\mu^2}{4} q \bar{q}' \right) + \exp \left( - \frac{3b^2 + 2\mu^2}{4} q \bar{q}' \right) \right]. \end{aligned} \quad (A2)$$

C. Projection on the multipoles

$$\begin{aligned} v_i(q, q') &= \left( \frac{2}{\pi} \right)^{1/2} 16\mu^3 b^3 V_0 (G - S) \left( \frac{4}{(8b^2 + 3\mu^2)^{3/2}} \left\{ \exp \left( - \frac{b^2}{4} \frac{12b^2 + 5\mu^2}{8b^2 + 3\mu^2} q^2 \right) \exp \left( - \frac{b^2}{4} \frac{8b^2 + 5\mu^2}{8b^2 + 3\mu^2} q'^2 \right) \right. \right. \\ & \quad \left. \left. + \exp \left( - \frac{b^2}{4} \frac{12b^2 + 5\mu^2}{8b^2 + 3\mu^2} q'^2 \right) \exp \left( - \frac{b^2}{4} \frac{8b^2 + 5\mu^2}{8b^2 + 3\mu^2} q^2 \right) \right\} \right. \\ & \quad \left. \times i_i \left[ \frac{2b^2(2b^2 + \mu^2)}{8b^2 + 3\mu^2} q \bar{q}' \right] \right\} \\ & \quad - \frac{2^{3/2}}{(5b^2 + 2\mu^2)^{3/2}} \left[ \exp \left( - \frac{b^2}{4} q^2 \right) \exp \left( - \frac{b^2}{4} \frac{3b^2 + 2\mu^2}{5b^2 + 2\mu^2} q'^2 \right) \right. \\ & \quad \left. + \exp \left( - \frac{b^2}{4} q'^2 \right) \exp \left( - \frac{b^2}{4} \frac{3b^2 + 2\mu^2}{5b^2 + 2\mu^2} q^2 \right) \right] \delta_{i,0} \\ & \quad - \frac{4}{3^{3/2}(2b^2 + \mu^2)^{3/2}} \exp \left[ - \frac{5b^2}{12} (q^2 + q'^2) \right] i_i \left( \frac{2b^2}{3} q q' \right) \\ & \quad + \frac{1}{(2b^2 + \mu^2)^{3/2}} \exp \left[ - \frac{b^2}{4} (q^2 + q'^2) \right] \delta_{i,0} \\ & - \left( \frac{2}{\pi} \right)^{1/2} 32\mu^3 b^3 V_0 (G + 2S) \frac{1}{3^{3/2}(4b^2 + \mu^2)^{3/2}} \exp \left[ - \frac{b^2}{12} \frac{8b^2 + 5\mu^2}{4b^2 + \mu^2} (q^2 + q'^2) \right] i_i \left[ \frac{2b^2(b^2 + \mu^2)}{12b^2 + 3\mu^2} q q' \right] \\ & + \left( \frac{2}{\pi} \right)^{1/2} 4\mu^3 b^3 V_0 (2G + S) \frac{1}{(3b^2 + \mu^2)^{3/2}} \exp \left[ - \frac{b^2}{4} \frac{2b^2 + \mu^2}{3b^2 + \mu^2} (q^2 + q'^2) \right] i_i \left( \frac{b^2}{2} \frac{b^2}{3b^2 + \mu^2} q q' \right) \\ & - \left( \frac{2}{\pi} \right)^{1/2} 32\mu^3 b^3 V_0 G \frac{1}{(8b^2 + 3\mu^2)^{3/2}} \exp \left[ - \frac{b^2}{4} \frac{12b^2 + 5\mu^2}{8b^2 + 3\mu^2} (q^2 + q'^2) \right] i_i \left[ \frac{2b^2(3b^2 + \mu^2)}{8b^2 + 3\mu^2} q q' \right] \\ & + \left( \frac{2}{\pi} \right)^{1/2} 4\mu^3 b^3 V_0 S \frac{1}{(2b^2)^{3/2}} \exp \left[ - \frac{3b^2 + 2\mu^2}{8} (q^2 + q'^2) \right] i_i \left( \frac{3b^2 + 2\mu^2}{4} q q' \right). \end{aligned} \quad (A3)$$

APPENDIX B: PROPERTIES OF THE INTEGRAL

$$I_l(q, q') \text{ [Eq. (29)]}$$

In this Appendix, to shorten the notations, we omit the  $z^2 e^2$  factor appearing in the Coulomb potential defined in Eq. (39), and Eq. (29) becomes

$$I_l(q, q') = \int_0^{R_0} dR j_l(qR) j_l(q'R) R.$$

Let us work on a more general expression:

$$I_l^N(q, q') = \int_0^{R_0} dR j_l(qR) j_l(q'R) R^N. \quad (B1)$$

Applying

$$j_{l+1}(x) = \left( \frac{d}{dx} + \frac{l}{x} \right) j_l(x),$$

once to  $j_l(qR)$  and once to  $j_l(q'R)$ , we obtain by

summing the two expressions for  $I_l^N$ ,

$$\begin{aligned} 2l I_l^N &= q' \int_0^{R_0} R^{N+1} dR j_l(qR) j_{l+1}(q'R) \\ &+ q \int_0^{R_0} R^{N+1} j_{l+1}(qR) j_l(q'R) \\ &+ \int_0^{R_0} R^{N+1} d(j_l(qR) j_l(q'R)). \end{aligned}$$

We increase the order of  $j_l(qR)$  and  $j_l(q'R)$  and obtain, when integrating by parts and repeating the procedure, the final result

$$\begin{aligned} (2l + N - 1) I_l^N - (2l + 3) \frac{q^2 + q'^2}{qq'} I_{l+1}^N + (2l - N + 5) I_{l+2}^N \\ = R_0^{N+1} [j_l(qR_0) j_l(q'R_0) - j_{l+2}(qR_0) j_{l+2}(q'R_0)]. \end{aligned} \quad (B2)$$

We notice that

$$(2l+N-1)I_l^N - (2l+3)\frac{q^2+q'^2}{qq'}I_{l+1}^N + (2l-N+5)I_{l+2}^N = 0$$

is just the recursion relation for the Legendre polynomials  $P_l^\mu(X)$  and  $Q_l^\mu(X)$ , where  $\mu$  is related to  $N$  and

$$X = \frac{q^2 + q'^2}{2qq'}$$

Consequently the  $I_l^N$  have components on the  $Q_l$  and therefore one must start the calculation of the

$I_l^N$  by a decreasing recursion until the final result  $I_0^N$ . The consistency of the method depends on this value of  $I_0^N$  which always can be obtained by a direct calculation.

When  $q = q'$ , due to

$$\sum_{l=0}^{\infty} (2l+1)j_l^2(x) = 1,$$

we establish the following relation:

$$\sum_{l=0}^{\infty} (2l+1)I_l^N(q, q) = \frac{R_0^N + 1}{N+1}. \quad (\text{B3})$$

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