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B. Barsella and S. Rosati : CALCULATIONS WITH CENTRAL FIELD WAVE FUNCTIONS FOR s-SHELL NUCLEI. -

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SUMMARY. -

The Hartree-Fock method and one of its modification have been applied to the nuclei with $A = 3, 4$. The modified Hartree-Fock method results more efficient and, in case of not too repulsive nucleon--nucleon potentials, gives acceptable values for the binding energies and nearly correct mass distributions.

1. - INTRODUCTION. -

In the last few years many Hartree-Fock (HF) calculations have been made for light and medium-light nuclei using two-body interactions which fit scattering data with reasonable accuracy. Recently Gibson et al.[1] have studied the specific case of ^{4}He with Volkov[2] two-body potentials using the HF method or the limited Hartree-Fock (LHF) method where a trial radial function is assumed, and they conclude that there are no remarkable differences between the results of the two methods. The basic assumptions commonly adopted, are that the hamiltonian is a sum of one-body (kinetic energy) and two-body operators[3] and that the wave function is well approximated by a Slater determinant of single-particle orbitals. The second assumption can however be dropped with no substantial increase in the calculations considering radial functions depending only on the modules of the distances of the particles from a center: we shall call this method the extended Hartree-Fock (EHF) method.

In the present paper we discuss a set of HF and EHF calculations with aim at (i) improving the results given by Slater-type wave

functions and (ii) setting a basis for further applications to p-shell nuclei. It will be shown that the EHF procedure gives better results than the HF one provided that simple but conveniently chosen trial wave functions be used. Moreover with realistic soft-core nucleon-nucleon potentials it is necessary to modify the HF procedure to describe the short-range correlations between the nucleons. A possible modification[4] requires a good zero-order approximation wave function which is more easily obtained via the EHF procedure here presented. Similarly in the case of p-shell nuclei, it is more convenient to describe the s-shell core nucleons by a wave function of simple analitical form.

2.- HF CALCULATIONS FOR A = 3, 4.-

We have carried out a true HF calculation on ^{3}H and $^{3,4}He$ with a central field wave function of the form

$$(1) \qquad \Psi_A = \frac{u(x_1)\,u(x_2)\ldots u(x_A)}{x_1\,x_2\ldots x_A}\,\chi_A \qquad (A = 3, 4),$$

where χ_A is the spin wave function of the A-nucleon system and the coordinates $x_1, \ldots, x_A$ are referred to an arbitrary fixed centre.

The hamiltonian of the system is

$$(2) \qquad H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V(x_{ij}) ,$$

m is the mass of the particles, x_{ij} the distance between the i-th and the j-th particle and $V(x_{ij})$ is a central (spin-dependent) potential. The hamiltonian given by eq. (2) contains a term representing the kinetic energy of the centre of mass which is

$$(3) \qquad T_{c.m.} = \frac{\left(\sum_{i=1}^{A} \underset{\sim}{p}_i\right)^2}{2Am} = \frac{1}{2Am}\left\{\sum_{i=1}^{A} p_i^2 + L\sum_{i\leq j=1}^{A} \underset{\sim}{p}_i \cdot \underset{\sim}{p}_j\right\}$$

The mean value of $\underset{\sim}{p}_i \cdot \underset{\sim}{p}_j$ with the function Ψ_A, eq. (1), is zero, therefore we can simplify $T_{c.m.}$ to

$$(4) \qquad (T_{c.m.})_{eff} = \sum_{i=1}^{A} \frac{p_i^2}{2Am}$$

and the effective hamiltonian with the motion of the centre of mass removed, is (note that the function ψ_A is symmetric in $x_1, \ldots, x_A$)

$$H_{eff} = \frac{A-1}{2m} p_1^2 + \frac{A(A-1)}{2} V(x_{12}) \tag{5}$$

The mean value of H_{eff} with the function ψ_A given by eq. (1) is

$$H_{eff} = (A-1)\frac{\hbar^2}{2m}(4\pi)^A n^{A-1} \int_0^\infty dx\, u'^2(x) + \frac{A(A-1)}{4} n^{A-2} (4\pi)^A \times$$
$$\times \int_0^\infty dx \int_0^\infty dy\; u^2(x)\, u^2(y)\, v_A(x,y) \tag{6}$$

where

$$n = \int_0^\infty dx\, u^2(x), \tag{7}$$

$$v_A(x,y) = \int_{-1}^{1'} dz\, V_A\left(\sqrt{x^2+y^2-2xyz}\right),$$

$V_A(r)$ being the mean of $V(r)$ on the spin function of the system.

The variational principle which gives the best radial function $u(x)$ may be written

$$\delta_u \langle \psi_A | H_{eff} - E | \psi_A \rangle = 0 \tag{8}$$

where δ_u denotes the functional variation with respect to $u(x)$, that is

$$\delta_u \left\{ (A-1)\frac{\hbar^2}{2m} n^{A-1} \int_0^\infty dx\, u'^2(x) + \right.$$
$$\left. + \frac{A(A-1)}{4} n^{A-2} \int_0^\infty dx \int_0^\infty dy\, u^2(x)\, u^2(y)\, v_A(x,y) - n^A E \right\} = 0. \tag{9}$$

From this equation, introducing the function

$$w(x) = \frac{u(x)}{n^{1/2}} \tag{10}$$

we obtain the following integro-differential equation

$$w''(x) + \frac{m}{\hbar^2}\left\{\frac{2A}{A-1}\,E - W_A(x)\right\} w(x) = 0\ , \tag{11}$$

where

$$W_A(x) = A\,U_A(x) + \frac{A(A-2)}{2}\int_0^\infty dy\, w^2(y)\,U_A(y) + (A-1)\frac{\hbar^2}{m}\int_0^\infty dy\, w'^2(y)\,,$$

$$U_A(x) = \int_0^\infty dy\, w^2(y)\, v_A(x,y) \tag{12}$$

For $A = 3, 4$ we have solved numerically equation (11) by iteration starting with a zero-order solution obtained by direct minimization of the mean value of the total energy with a trial function of simple analitical form. The potentials used have been the gaussian potential of Baker et al.[5] defined as

$$V(x) = V_o \exp(-\tau x^2), \qquad V_o = -51.5\ \text{MeV}, \qquad \tau = 0.390625\ \text{fm}^{-2}, \tag{13}$$

and one of the soft-core potentials of Volkov[2] defined as

$$V(x) = V_1 \exp(-\tau_1 x^2) + V_2 \exp(-\tau_2 x^2), \qquad V_1 = -83.34\ \text{MeV},$$

$$\tau_1 = 0.390625\ \text{fm}^{-2}, \qquad V_2 = 144.86\ \text{MeV}, \qquad \tau_2 = 1.48721\ \text{fm}^{-2}. \tag{14}$$

The coulomb energies for the ^{3,4}He cases have been evaluated in first order perturbation theory. The form factors and the mean-square radii have been calculated according to the formulas ($\underset{\sim}{r} = \underset{\sim}{x}_1 - (\underset{\sim}{x}_1 + \underset{\sim}{x}_2 + \ldots + \underset{\sim}{x}_A)/A$)

$$F(q^2) = \frac{f_p(q^2)}{(4\pi n)^A} \int d\underset{\sim}{r}\, \exp(i\underset{\sim}{q}\cdot\underset{\sim}{r}) \int d\underset{\sim}{x}_2 \ldots d\underset{\sim}{x}_A \left| \psi_A \right|^2 =$$

$$= \frac{f_p(q^2)}{(4\pi n)^A} \int d\underset{\sim}{x}_1 \ldots d\underset{\sim}{x}_A \left| \psi_A \right|^2 \exp\left(i\frac{A-1}{A}\underset{\sim}{q}\cdot\underset{\sim}{x}_1 - \frac{i}{A}\underset{\sim}{q}\cdot(\underset{\sim}{x}_2+\ldots+\underset{\sim}{x}_A)\right) =$$

(15)

$$= \frac{f_p(q^2)}{(4\pi n)^A} \left\{ \int d\underset{\sim}{x}_1\, u^2(x_1) \exp\left(i\frac{A-1}{A}\underset{\sim}{q}\cdot\underset{\sim}{x}_1\right) \right\} \times$$

$$\times \left\{ \int d\underset{\sim}{x}_2\, u^2(x_2) \exp\left(-\frac{i}{A}\underset{\sim}{q}\cdot\underset{\sim}{x}_2\right) \right\}^{A-1}$$

with $f_p(q^2)$ the proton charge form factor[6]

(16)
$$f_p(q^2) = \left\{ 1 + \frac{1}{12} a_p^2 q^2 \right\}^{-2}, \qquad a_p = 0.8 \text{ fm},$$

and

(17)
$$\langle R^2 \rangle^{1/2} = \frac{A-1}{A_n} \int_0^\infty dx\, x^2 u^2(x)$$

The results obtained are presented in Table I while the form factors for A = 4 are plotted in Fig. 1.

3. - EHF CALCULATIONS. -

The EHF calculations have been performed by standard minimization procedure of the mean value of the hamiltonian given by eq. (5) with a trial wave function of the form

(18)
$$\psi_A = \frac{1}{x_1 x_2 \ldots x_A} \left\{ \sum_{i=1}^{N} z_i f_i(x_1) f_i(x_2) \ldots f_i(x_A) \right\} \chi_A,$$

where the single-particle function $f_i(x)$ has been chosen as a simple gaussian

(19)
$$f_i(x) = \exp(-\alpha_i x^2)$$

TABLE I - HF calculations.

Potential	A	E (MeV)	Ec (MeV)	$\langle R^2 \rangle^{1/2}$ (fm)
Baker	3	- 7.63	0.897	1.32
Baker	4	-38.05	1.102	1.13
Volkov	3	- 6.94	0.732	1.60
Volkov	4	-28.14	0.839	1.47

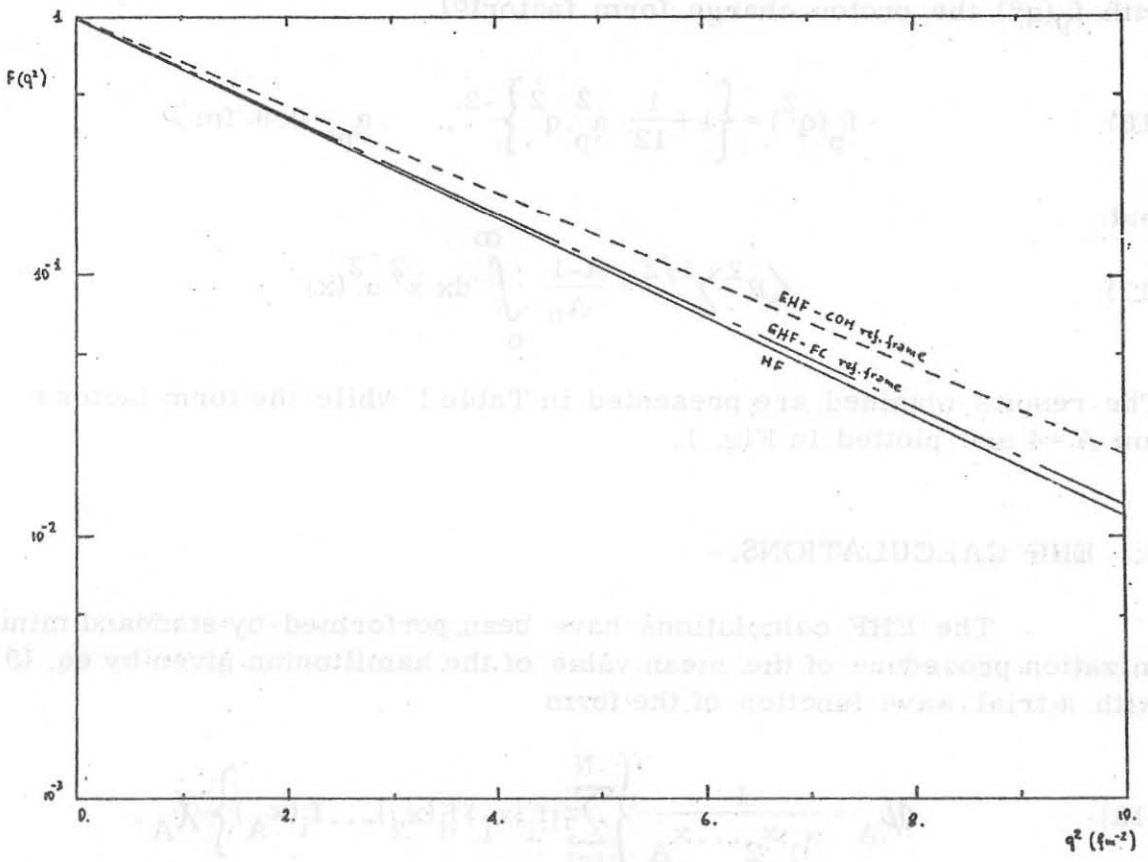

FIG. 1 - Form factors for four-body systems.

With the wave function of eq. (18) the mean value of the hamiltonian (5) results

$$(20)\quad \langle \Psi_A | H_{eff} | \Psi_A \rangle = \frac{1}{\langle 1 \rangle} \sum_{i,j=1}^{N} z_i z_j \left\{ (A-1) \frac{\hbar^2}{2m} F_{ij}^{A-1} T_{ij} + \frac{A(A-1)}{4} F_{ij}^{A-2} V_{ij}^{(A)} \right\},$$

where

$$\langle 1 \rangle = \sum_{i,j=1}^{N} z_i z_j F_{ij}^{A}, \quad F_{ij} = \int_0^\infty dx\, f_i(x) f_j(x), \quad T_{ij} = \int_0^\infty dx\, f_i'(x) f_j'(x),$$

$$(21)\quad V_{ij}^{(A)} = \int_0^\infty dx \int_0^\infty dy\, f_i(x) f_i(y) v_A(x,y) f_j(x) f_j(y),$$

$v_A(x,y)$ being given by eq. (7). As in the preceding case, the coulomb energy

$$(22)\quad E_C = \frac{1}{\langle 1 \rangle} \sum_{i,j=1}^{N} z_i z_j F_{ij}^{A-2} \int_0^\infty dx \int_0^\infty dy\, f_i(x) f_i(y) \frac{e^2}{2xy} \left[x + y - |x-y| \right] f_j(x) f_j(y),$$

has been evaluated in first order perturbation theory while the mean square radius and the form factor have been obtained from the expressions

$$(23)\quad \langle R^2 \rangle^{1/2} = \frac{1}{\langle 1 \rangle} \sum_{i,j=1}^{N} z_i z_j F_{ij}^{A-1} \int_0^\infty dx\, x^2 f_i(x) f_j(x),$$

$$(24)\quad F(q^2) = \frac{f_p(q^2)}{4 \langle 1 \rangle} \sum_{i,j=1}^{N} z_i z_j F_{ij}^{A-1} \frac{\pi^{1/2}}{(\alpha_i + \alpha_j)^{3/2}} \exp\left(- \frac{q^2}{4(\alpha_i + \alpha_j)} \right).$$

The calculations have been performed for a number $N = 1, 2, 3$ of components in the wave function (11); the energies E_1, E_2, E_3 correspondingly obtained have been extrapolated so as to estimate E_∞ which is listed in Table II together with the energy E_2 and the energy furnished by the most sophisticated computational models presently available[7,8]. The form factors for $A = 4$ practically coincide with the ones obtained in the preceding section.

TABLE II

EHF calculations. a) α_1, α_2, z_2 are the parameters of the wave function obtained for energy E_2. b) The symbols FC and COM show that the calculations have been made using a "fixed center reference frame" or the "center of mass reference frame", respectively. c) The numbers in parenthesis represent the results obtained by the most accurate models presently known.

A	potential		α_1 (fm^{-2})	α_2 (fm^{-2})	Z_2 [a]	E_2 (MeV)	E_∞ (MeV)	E_c (MeV)	$\langle R^2 \rangle^{1/2}$ (fm)
3	Baker	FC [b]	0.213	0.547	4.743	- 8.35	- 8.49 (-9.78) [c]	0.89 (0.89)	1.38 (1.49)
		COM	0.168	0.546	4.250	- 9.07	- 9.16	0.895	1.41
	Volkov	FC	0.151	0.318	2.640	- 7.14	- 7.30 (-8.46)	0.724 (0.71)	1.65 (1.72)
		COM	0.106	0.295	4.900	- 7.52	- 7.54	0.718	1.715
4	Baker	FC	0.356	0.720	4.110	-38.35	-38.64 (-40.03)	1.10 (1.10)	1.15 (1.18)
		COM	0.307	0.700	4.740	-39.08	-39.20	1.10	1.16
	Volkov	FC	0.221	0.341	2.473	-28.14	-28.34 (-30.32)	0.835 (0.83)	1.48 (1.47)
		COM	0.177	0.326	5.640	-28.31	-28.38	0.834	1.49

4. - CALCULATION IN THE CENTRE OF MASS FRAME. -

So far we have related the positions of the particles to a fixed centre and taken into account the motion of the centre of mass by subtracting its kinetic energy from the total energy of the system. We want now to describe the system in the centre of mass reference frame by the wave function

$$\Phi_A = \frac{1}{r_1 r_2 \dots r_A} \left\{ \sum_{i=1}^{N} z_i g_i(r_1) g_i(r_2) \dots g_i(r_A) \right\} \chi_A \,, \tag{25}$$

where the coordinates $\underset{\sim}{r}_1, \dots, \underset{\sim}{r}_A$ satisfy the condition

$$\underset{\sim}{r}_1 + \underset{\sim}{r}_2 \dots + \underset{\sim}{r}_A = 0 \tag{26}$$

The hamiltonian of the system is

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V(|\underset{\sim}{r}_i - \underset{\sim}{r}_j|) \tag{27}$$

$\underset{\sim}{p}_i$ being the momentum conjugated to the coordinate $\underset{\sim}{x}_i$ related to $\underset{\sim}{r}_i$ by

$$\underset{\sim}{x}_i = \underset{\sim}{r}_i + \underset{\sim}{R} \tag{28}$$

where R is the coordinate of the centre of mass and moreover $\sum_{i=1}^{A} \underset{\sim}{p}_i = 0$.

The mean value of the hamiltonian (27) with the wave function (25) results

$$\langle \Phi_A | H | \Phi_A \rangle = \int d\tau \left\{ -A \frac{\hbar^2}{2m} \Phi_A^* \Delta_{x_1} \Phi_A + \frac{A(A-1)}{2} \times \right.$$
$$\left. \times V_A(|\underset{\sim}{r}_1 - \underset{\sim}{r}_2|) |\Phi_A|^2 \right\} / \int d\tau |\Phi_A|^2 \,, \tag{29}$$

where account has been taken of the simmetry of the function Φ_A. In eq. (29) the laplacian Δ_{x_1} must be expressed in terms of the variables $\underset{\sim}{r}_i$, $d\tau = d\underset{\sim}{r}_1 \, d\underset{\sim}{r}_2 \dots d\underset{\sim}{r}_{A-1}$, and the dependence of the integrands

on $\underset{\sim}{r}_A$ is taken off by using eq. (26). If one limits the number of components of the function Φ_A to N = 1, eq. (25), and the function g(r) is a simple gaussian, then the wave function (25) and (18) give the same results (see Appendix A for the proof). The explicit form of expression (29) together with the coulomb energy, the form factor and the mean square radius are given in Appendix A. The numerical calculations have been performed with the same procedure described in the preceding section and the results are listed in Table II.

We have also investigated the effect of using a function of type (18) with single particle functions $f_i(x)$ of the more sophisticated form

$$f_i(x) = \exp(-\alpha_i x^2) + y_i \exp(-\beta_i x^2) \tag{30}$$

In the case A = 4 with Volkov potential and N = 1 the resulting energy has been E = -28.10 MeV and this value is quite close to the one obtained precedently with a two-component function and reported in Table II. For N = 2 the value E = -28.27 MeV has been obtained showing the advantage of the use of a more flexible function. However the calculations with functions as given by eq. (30) require the numerical evaluation of a number of integrals (avoided in the case of function (19)), thus increasing substantially the computing time.

We have also performed some EHF calculations using potentials with strong repulsive core or strongly velocity-dependent potentials. However the binding energy results now badly underestimated owing to the fact that with such potentials a careful description of the correlations between the particles is necessary.

5. - CONCLUSIONS. -

A survey of Tables I and II and Fig. 1 permits the following remarks.

i) The HF procedure for the nuclei with A = 3, 4 gives in general results inferior to those obtained by the EHF method and requires quite larger computing times. With the potential of Volkov the improvement is small owing to the fact that functions of type (18) or (25) do not describe accurately the interparticle correlations.

ii) The EHF procedure gives appreciably better results in the case A = 3. For non-closed shell nuclei the improvement is greater and this is promising for the extension of the calculations to p-shell nuclei.

iii) The functions determined via the EHF procedure give

without exclusions very good values for the coulomb energy and the mean square radius with both the potentials considered here (see Table II). This indicates that, in spite of the underestimation of the binding energy, the EHF functions obtained generate substantially the correct mass distribution. This feature is very useful if such a type of wave functions are to be used to describe the s-shell nucleons of a p-shell nucleus.

iv) From the computing time point of view the calculations in the centre of mass reference frame are equivalent to the ones in the fixed centre reference frame and the binding energies are in some cases considerably better.

APPENDIX A. -

We prove here that the wave functions (18) and (25), with N = 1 and a gaussian shape for the radial function, give the same binding energy. We shall limit to the case A = 3, the case A = 4 being proved in the same way. Let us write explicitly the wave function (25) for N = 1

$$\Phi_3(r_1, r_2, r_3) = \exp\left\{-\alpha(r_1^2+r_2^2+r_3^2)\right\} \tag{A1}$$

which, using the coordinates $\underset{\sim}{r} = \underset{\sim}{r}_2-\underset{\sim}{r}_1$, $\underset{\sim}{\rho} = \underset{\sim}{r}_3-\frac{1}{2}(\underset{\sim}{r}_2+\underset{\sim}{r}_1)$, $\underset{\sim}{R} = \frac{1}{3}(\underset{\sim}{r}_1 + \underset{\sim}{r}_2+\underset{\sim}{r}_3)$ can be written as

$$\Phi_3(r, \rho) = \exp(-\frac{1}{2}\alpha r^2 - \frac{3}{2}\alpha \rho^2) . \tag{A2}$$

In terms of the new coordinates the kinetic energy part of the hamiltonian (27) splits into three terms proportional to ∇_r^2, ∇_ρ^2 and ∇_R^2 respectively. The choice of the centre of mass reference frame eliminates authomatically the term ∇_R^2 and, at the same time, the product form of the function (A2) gives a mean value of hamiltonian (27) which is formally the same of the mean value of hamiltonian (5) with the wave function (18) apart from a scale factor which makes the range parameter α to be the same, at the minimum, for the wave functions (18) and (A1).

We give now the explicit form of the expression (29). In the case A = 3 we have

$$\langle \Phi_3 | \Phi_3 \rangle = \frac{\pi^3}{3^{3/2}} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^3} ,$$

$$\langle \Phi_3 | H | \Phi_3 \rangle = \frac{\pi^3}{3^{1/2}} \sum_{i,j} z_i z_j \left[\frac{2\hbar^2}{m} \frac{\alpha_i \alpha_j}{(\alpha_i+\alpha_j)^4} + \right. \tag{A3}$$

$$\left. + \frac{V_o}{(\alpha_i+\alpha_j)(\alpha_i+\alpha_j+2\tau)} \right] / \langle \Phi_3 \, \Phi_3 \rangle ,$$

$$E_C = \frac{2^{1/2}\,\pi^{5/2}\,e^2}{3^{3/2}\langle \phi_3 \, \phi_3 \rangle} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^{5/2}} ,$$

$$\langle R^2 \rangle = \frac{\pi^{3/2}}{3^{3/2}\langle \phi_3 | \phi_3 \rangle} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^4} ,$$

(A3)

$$F(q^2) = f_p(q^2) \frac{\pi^3}{3^{3/2}\langle \phi_3 | \phi_3 \rangle} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^3} \exp\left\{ - \frac{q^2}{6(\alpha_i+\alpha_j)} \right\}.$$

In the case A = 4, we have

$$\langle \phi_4 | \phi_4 \rangle = \frac{\pi^{9/2}}{8} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^{9/2}} ,$$

$$\langle \phi_4 | H | \phi_4 \rangle = \frac{3\pi^{9/2}}{8\langle \phi_4 | \phi_4 \rangle} \times$$

$$\times \sum_{i,j} z_i z_j \left[\frac{3\hbar^2}{m} \frac{\alpha_i \alpha_j}{(\alpha_i+\alpha_j)^{11/2}} + \frac{2V_o}{(\alpha_i+\alpha_j)^3 (\alpha_i+\alpha_j+2\tau)^{3/2}} \right],$$

(A4)

$$E_C = \frac{\pi^4 e^2}{2^{5/2}\langle \phi_4 | \phi_4 \rangle} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^4} ,$$

$$\langle R^2 \rangle = \frac{9\pi^{9/2}}{64\langle \phi_4 | \phi_4 \rangle} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^{11/2}} ,$$

$$F(q^2) = f_p(q^2) \frac{\pi^{9/2}}{8\langle \phi_4 | \phi_4 \rangle} \sum_{i,j} z_i z_j \frac{1}{(\alpha_i+\alpha_j)^{9/2}} \exp\left\{ - \frac{3q^2}{16(\alpha_i+\alpha_j)} \right\}$$

APPENDIX B. - Considerations on the numerical calculations. -

All the numerical calculations have been made on the IBM 7090 of the CNUCE in Pisa, with a time of cycle of 2.18 μs. The calculations described in section 2 have been performed solving numerically with a program by Lovitch and Rosati the Schroedinger equation (11). The iterative procedure involved has a fast convergence requiring 5÷8 iterations. The largest part of computing time required to examine a single case is about one minute for integrations on 100 points with a step-length of 0.1 fm. The calculations described in sections 3-5 require however a good procedure for the search of the minimum. We have begun with a simple grid program which is well adequate to the cases with a maximum number of variational parameters limited to 3. For the more complicated cases with a greater number of parameter the simple grid program becomes inefficient owing to the presence of local stationary points that the grid search along the parameters axis cannot override. We have then used the program MINUIT by James and Roos[9], and the results have been obtained after about 200÷600 calls of the function to be minimized depending on the number of parameters. The computer time required to examine a single case is 8÷12 seconds.

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