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A Variational Calculation of ^{12}C in the a- Particle Model*

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In this paper, we discuss some physical properties of three structureless alpha particles interacting through two-body potentials and compare those properties with the wrresponding experimental observations for the ^{12}C nucleus. The wave function is expanded in terms of translationally invariant harmonic-osciilator states, the coefficients of the expansion being taken as variational parameters.

Discutem-se, neste trabalho, algumas propriedades físicas de três partículas alfas sem estrutura interagindo através de potênciais de dois corpos. Faz-se a comparação com as observações experimentais correspondentes no caso do núcleo ^{12}C. A função de onda é expandida em termos de estados de osciladores harmônicos translacionalmente invariantes. Os coeficientes da expansão são tratados como parâmetros variacionais.

1. Introduction

A representation for the interna1 structure of light doubly even nuclei with $A = 2Z$, in terms of alpha clusters, grounds mainly on the fact that the alpha particle is the most stable nuclear system. To separate a proton from this nucleus, the extremely large energy of 19.8 MeV is necessary and there is no excited state of the nucleus below this energy[1]. A number of attempts, using mainly variational methods and the Faddeev equations, have been made recently to use this model in calculating properties of the ^{12}C nucleus[2-11]. The alpha particles are assumed to be structureless rigid entities and it is postulated that inside the nucleus these particles interact with each other via a two-body potential which fits the experimental phase shifts in the alpha-alpha scattering.

The rather incomplete and contradictory results obtained up to now leave the question, whether the three-body model can account for the ground state of ^{12}C, still as an open problem.

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In this paper we address ourselves to this question using a variational method with a translationally invariant harmonic-oscillator basis. It will be possible to estimate the trend of the error by truncating the basic space in subspaces corresponding to different number of osciilator quanta in the approximation.

Some phenomenological α-α potentials with l-dependence will be taken from the literature. So, we abandon the sissumption. common to almost all previous calculations, of the negligibility of the α-α potential in the higher angular-momentum channels.

The boson character of the particles in taken into account and, with the variational function so obtained, we shall discuss the form factors of the ^{12}C nucleus. A rough estimate of the Couiomb energy is made.

2. The Trial Function

We shall try to describe the system of threí: alpha particles by a trial wave function ψ expanded in terms of translationally invariant harmonic-oscillator states φ_ν, i. e..

$$\psi = \sum a_\nu \varphi_\nu. \tag{2.1}$$

The coefficients a, are to be treated as linear variational parameters.

The function φ_ν describes the state ν of a system of three harmonic oscillators. To satisfy the conditions to be imposed. for physical reasons. on the three-alpha particie states. the three harmonic oscillators will be coupled to a zero total orbital angular momentuni (L = J = 0) and will be in a symmetric configuration state. The character of translational invariance can easily be obtained through the use of the Jacobi coordinates

$$\mathbf{x}_a = \sqrt{\frac{1}{2}}\,(\mathbf{x}_1 - \mathbf{x}_2), \tag{2.2a}$$

$$\mathbf{x}_b = \sqrt{\frac{1}{6}}\,(\mathbf{x}_1 + \mathbf{x}_2 - 2\mathbf{x}_3), \tag{2.2b}$$

$$\mathbf{x}_c = \sqrt{\frac{1}{3}}\,(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3). \tag{2.2c}$$

The construction of the functions φ_v with the mentioned required properties was discussed and carried out explicitly by Moshinsky and collaborators[12,13]. From their work. we see that the states φ_v are given by

$$|v\rangle = |n_1 n_2 l\rangle = [2/(1+\delta_{n_1 n_2})]^{1/2} \sum_{n_a n_b l_a} (-1)^{n_a + l_a}$$

$$\langle n_a\, 2l_a, n_b\, 2l_a, 0 \,|\, n_1 l, n_2 l, 0\rangle \,|\, n_a\, 2l_a, n_b\, 2l_a, 00\rangle, \tag{2.3}$$

where $|n_a\ 21,\ n_b\ 21,\ 00)$ are states of three harmonic oscillators in the coordinates (2.2) coupled to $L = 0$ and with zero quantum energy in $\mathbf{x}_c$ (the center of mass coordinate).

These states carry the irreducible representation $\mathbf{f} = \{3\}$ of the group S(3) of permutation of three objects. As the coefficients a, are parameters to be determined via a variational analysis, the function ψ preserves the mentioned characteristics of (2.3).

The number of terms summed up in (2.1) will define our approxirnation. Obviously. the function ψ should be exactly defined by (2.1) if we could take all the infinite terms of the sum.

The needed cut-off in the sum will restrict the approximation to a maximum number N of quanta. In other words. the sum will be restricted to those values of v such that

$$0 \le n_1 + n_2 + l \le \frac{1}{2} N, \tag{2.4}$$

since the total number of quanta is given by

$$N = 2n_1 + l + 2n_2 + l. \tag{2.5}$$

In the 10-quantum approximation, there are 16 values of v, i.e., 16 values for the set $(n_1 n_2 l)$ such that (2.4) is satisfied. So, in the approximation of 10 quanta, we are trying to describe the system of three alphas in a space of dimensionality 16. In our case, the dimension d of the space defined by the approximation of N quanta is given by

$$d = (q+1)(3q + r) + \frac{1}{2} \sum_{x=0}^{\bar{x}} (N_0 - 6x)(N_0 - 6x - 1), \tag{2.6}$$

where $N_0 = \frac{1}{2}$N; q and r are. respectively, the quocient and the residue of the division of $N_0 + 1$ by 6: and $\bar{x}$ is such that there is no negative contribution to the sum.

Finally, a last few words about the states *(2.3)*. The triple sum. in n_a, n_b and l_a, can be reduced to sums over only two of these indices if we take into account the "energy condition" that must be satisfied by the Moshinsky coefficients[14] $\langle n_a l_a, n_b l_b, \mathrm{L} \mid n_1 l_1, n_2 l_2, \mathrm{L}\rangle$, i. e.,

$$2n_a + l_a + 2n_b + l_b = 2n_1 + l_1 + 2n_2 + 1, \tag{2.7}$$

which, in our case. can be expressed as

$$n_a + n_b + 2l_a = n_1 + n_2 + l. \tag{2.8}$$

These states are orthonormai as can be easily seen using the sum rules for the Moshinsky coefficients derived by Aguilera-Navarro *et al*[11].

3. Matrix Elements of H

The Hamiltonian for a system of three alpha particies of mass m interacting only through two-body forces is given by

$$H = \frac{1}{2m} \sum_{s=1}^{3} p_s'^2 + \sum_{s<t}^{3} V(s, t) \tag{3.1}$$

where $V(s, t)$ may depend on the relative coordinates and momenta of particles s and t. Taking usual dimensionless coordinates $\mathbf{x}_s$ and momenta $\mathbf{p}_s$ defined by

$$\mathbf{x}_s' = \sqrt{\hbar/m\omega}\ \mathbf{x}_s, \tag{3.2a}$$

$$\mathbf{p}_s' = \sqrt{\hbar m\omega}\ \mathbf{p}_s, \quad s = 1.\ 2.\ 3 \tag{3.2b}$$

where ω is the common oscillator frequency, we can put the intrinsic Hamiltonian $\mathscr{H}$ under the form

$$\mathscr{H} \equiv H - \frac{1}{2}\hbar\omega p_c^2 = \frac{1}{2}\hbar\omega(p_a^2 + p_b^2) + \sum_{s<t}^{3} V(s, t), \tag{3.3}$$

where $\mathbf{p}_a$, $\mathbf{p}_b$ and $\mathbf{p}_c$ are momenta associated to the Jacobi coordinates defined in *(2.2)*.

In this way. the matrix elements of $\mathscr{H}$ between the states *(2.3)* are given *by*

$$\langle \nu' \mid \mathscr{H} \mid \nu\rangle = (N + 3)\hbar\omega\delta_{\nu'\nu} + 3\langle \nu' \mid U(1.2) \mid \nu\rangle, \tag{3.4}$$

where again ν stands for the set $(n_1 n_2 l)$, N is given by *(2.5)* and

$$U(1, 2) \equiv V(1, 2) - \frac{1}{3}\hbar\omega\, x_a^2. \tag{3.5}$$

Notice that we were allowed to sum over the pairs of particles. so getting our matrix elements in terms of $U(1.2)$ only. due to the definite permutational symmetry of *(2.3)*.

The matrix elements of $U(1, 2)$ are given by

$$\langle v' \mid U(1,2) \mid v \rangle = \langle n_1' n_2' l' \mid U(1,2) \mid n_1 n_2 l \rangle =$$
$$[2/(1 + \delta_{n_1' n_2'})]^{1/2} \; [2/(1 + \delta_{n_1 n_2})]^{1/2} \times$$
$$\sum_{\substack{n_a' n_a \\ n_b l_a}} (-1)^{n_a + n_a'} \langle n_a' 2l_a,\; n_b 2l_a,\; 0 \mid n_1' l' \;\; n_2' l',\; 0 \rangle \times$$
$$\langle n_a 2l_a,\; n_b 2l_a,\; 0 \mid n_1 l,\; n_2 l,\; 0 \rangle \; \langle n_a' 2l_a \parallel U(1,2) \parallel n_a 2l_a \rangle. \tag{3.6}$$

The Moshinsky coefficients were calculated with the nice closed formula derived by Trlifaj[16], and the last "reduced matrix elements are easily obtained by means of a usual[13,14] expansion in terms of Talmi integrals. i.e.

$$\langle n'l' \parallel U \parallel nl \rangle = \sum_p B(n'l', nl, p) I_p(U), \tag{3.7}$$

where p runs over the set of integer values

$$\frac{1}{2}(l' + l) \leq p \leq \frac{1}{2}(l' + l) + n' + n,$$

the Talmi integrais being defined by

$$I_p(f(r)) = \frac{2}{\Gamma(p + \frac{3}{2})} \int_0^\infty r^{2p+2} \; e^{-r_2} \; f(r) dr \tag{3.8}$$

and we give in Table 1 the relevant Talmi integrals for our present calculations. In this way, we have obtained all the matrix elements in terms of Moshinsky coefficients. Talmi integrals and the coefficients B defined by (3.7). These coefficients were calculated by means of the expression contained in Ref. *14*.

All we need now is to discuss the interaction.

$f(r)$	$I_p(f(r))$
r^λ	$\Gamma(p + \lambda/2 + 3/2) / \Gamma(p + 3/2)$
e^{-ar^2}	$(1 + a)^{-p-3/2}$

Table 1 — The relevant Talmi integrals

4. The Variational Energy

The potential $V(1,2)$ is the superposition of the nuclear *a-a* potential $V_{\alpha\alpha}$ and the Coulomb potential

$$V_c(1,2) = 4e^2/|\mathbf{x}_1' - \mathbf{x}_2'| = \sqrt{8\beta\varepsilon}\, e^2/x_a, \tag{4.1}$$

where

$$\beta = mc^2 m_0 c^2/\hbar^2 c^2, \tag{4.2}$$

$$\varepsilon = \hbar\omega/m_0 c^2, \tag{4.3}$$

and m_0c^2 is an arbitrary mass which we chose to be the electron rest mass ($m_0c^2 = 0.511\ MeV$).

While this part of the interaction is well tlefined. the same is not true for the nuclear part which will be taken from the phenomenology of *a-a* scattering.

We considered two kinds of α-α potentials. The first is due to Ali and Bodmer[17] who obtained phenomenological *a-a* potentials for $l = 0.2$ and *4* that fit the relevant phase shifts for CM energies up to 12MeV. They ured Gaussians to shape the repulsive and attractive interactions.

The other potential was obtained by Benn and Scharf[18] by means of the Gelfand-Levitan solution of the inverse problem in scattering theory. The potential is also *l*-dependent and is defined point-to-point. There are hard cores located at $r, = 1.2037$ fm. $r, = 1.4307$ fm and $r, = 1.6049$ fm where the index of r refers to the particular 1 considered. This potential reproduces exactly the experimental phase shifts.

With such potentials. we diagonalize the: Hamiltonian using the Jacobi procedure thus obtaining its eigenvalues and corresponding eigenfunctions. The diagonalization of *(3.4)*is made for different values of the oscillator parameter *(4.3)*.

In the case of the Benn-Scharf potentia,. we arbitrarily substituted the hard core by a term varying as the inverse of the relative distance between two alphas. We used this trick to avoid a more complex and sophisticated treatment due to the fact that the oscillator functions do not vanish at the core radii.

In Figures *1-4*. we show the behavior of the lowest eigenvalue when we vary the value of ε. The curves associated to N = 8 do not cross those corresponding to N = 10.

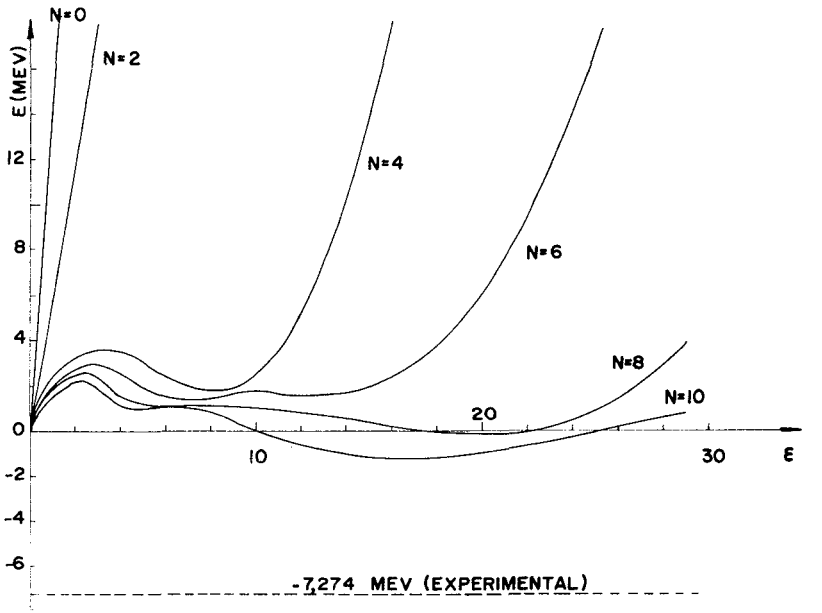

Fig. 1 - Variational energy as a function of the oscillator parameter ε for the 0.2.4.6.8 and 10-quanta approxirnation. Potential Ali-Bodmer $e_1 + e_3 + e_5$.

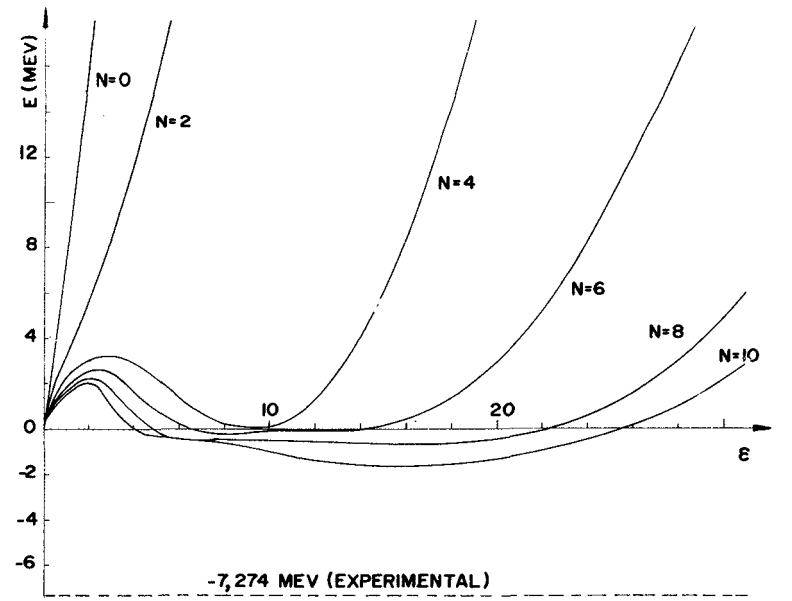

Fig. 2 - Same as Fig. 1 for Ali-Bodmer $d_0 + d_2 + d_4$.

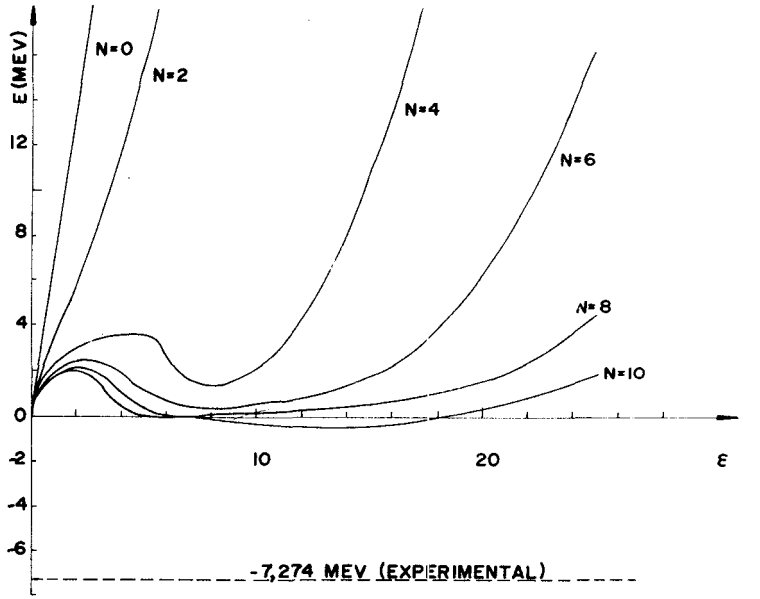

Fig. 3 - Same as Fig. 1 for Ali-Bodmer d'_0

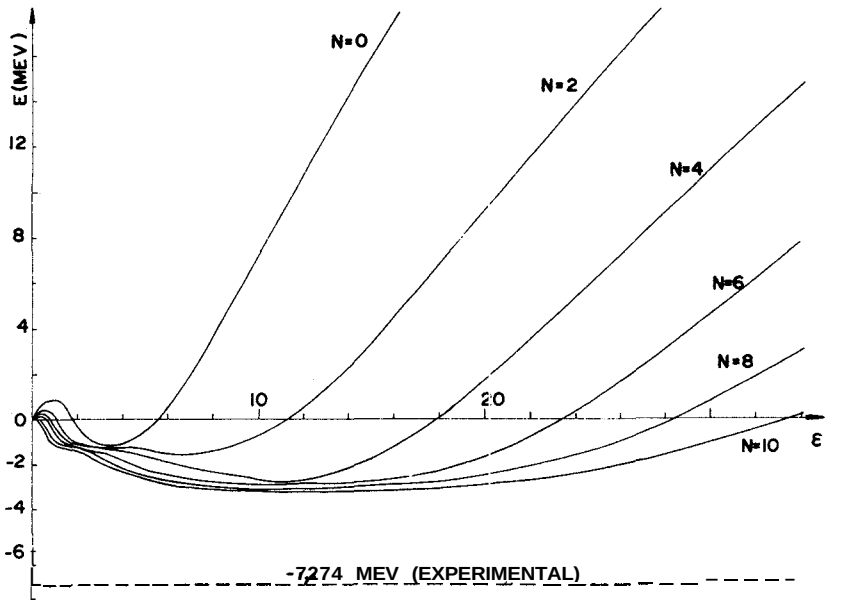

Fig. 4 - Same as Fig. 1 for the Benn-Scharf potential

In Fig. 1, we see the results for the potential e, + e, + e, of Ali-Bodmer[17]. The best energy of --1.24MeV was obtained for c = 16. Figure 2 refers to the potential $d'_0 + d'_2 + d_4$. The best result E = -1.61 MeV was for $\varepsilon = 15$. Now, using only d'_0 as a common potential for all l-states, we get an almost unbound state with E = --0.6 MeV for $\varepsilon = 13$ as shown in Fig. 3. This result is in agreement with the fact that the a-a potential is strongly l-dependent.

In Fig. 4. we have the results obtained using the Benn-Scharf[18] potential. This potential gave the best energy in the approximation of 10 quanta. For $\varepsilon = 12$. we have E = –3.19 MeV. For cornparison. we collect in Table 2 some results obtained by various authors.

Author	Ref.	E(MeV)
Daurriulat	2	+1.4
Harrington	3	7.36
Duck	4	unbound
Fulco & Wong	5	2.79
Hebach & Henneberg	6	1.48
Leung & Park	7	7.36
Abdul-Magd	8	1.0
Lim	9	1.1
Noble	10	-1.4
Visschers & Wageningen	11	2.20
Experimental	19	-7.274

Table 2 — Ground state energy of ^{12}C obtained by various authors

By taking N = 0, 2, 4, ... successively, we define spaces of increasing dimension $d = 1, 2, 4, \ldots$ (see Eq. (2.6)). The successive diagonalizations in such spaces allow us to estimate the trend of the error.

In Fig. 5. we plotted the binding energy versus the number of quanta N in the approximation. We see that the Benn-Scharf potential gives a three-alpha bound state from the very starting point, i.e, at the zero-quantum approximation, while for binding the system we need at least 4 quanta for the used Ali-Bodmer potentials. On the other hand. Fig. 5 suggests that a further approximation (N greater than 10) will favor the Ali-Bodmer potential since it seems that the Benn-Scharf potential is going to define an inconvenient plateau in the plotting.

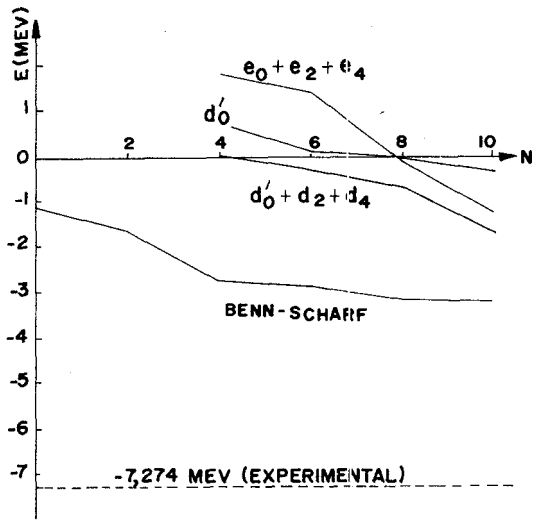

Fig. 5 - The behavior of the binding energy with increasing number of quanta for the discussed potentials.

As there are indications that the model must work better for excited states. where the particles have greater oportunity of individualization. calculations are in progress to try to describe the low lying 0^+ and 2^+ levels of ^{12}C.

5. Coulomb Energy

The Coulomb energy was calculated in the zero-quantum approximation. The best value of c in this approximation using the Benn-Scharf potential was $\varepsilon = 3$. We obtained for the Coulomb energy the value E, $= 5.28$ MeV which is in accordance with the previous value estimated by Harrington[3] of 5.44 MeV.

6. Form Factors

Although the α-model does not produce a satisfactory ground-state energy for the ^{12}C, the calculated charge form factor fits very well the experimental results[27].

The charge form factor of a system of particles of total charge Z is given by

$$F(\mathbf{q}) = \frac{1}{Z} \int \exp(i\mathbf{q} \cdot \mathbf{x})\, \rho(\mathbf{x})\, d\mathbf{x} \tag{6.1}$$

where $\hbar\mathbf{q}$ is the momentum transfer and $\rho(\mathbf{x})$ is the charge density referred to the center of mass.

If we want to get a more explicit expression for $F(\mathbf{q})$ when using the representation *(2.1)* for a system of n alphas. we start by constructing an operator which gives the probability density of finding an a-particle at some arbitrary pointz. Such operator is obviously given by

$$\hat{\Pi}_\alpha(\mathbf{z}) = \sum_{s=1}^{n} \delta(\mathbf{z} - \mathbf{x}_s) \tag{6.2}$$

where $\mathbf{x}_s$ is the position of the particle s.

As we are interested in the density referred to the center-of-mass, we write *(6.2)* in the form.

$$\hat{\Pi}_\alpha(\mathbf{Z}) = \sum_{s=1}^{n} \delta[\mathbf{x} - (\mathbf{x}_s - \mathbf{x}_{CM})] \tag{6.3}$$

with

$$n\mathbf{x}_{CM} = \sum_{s=1}^{n} \mathbf{x}_s, \tag{6.4}$$

and

$$\mathbf{x} = \mathbf{z} - \mathbf{x}_{CM}. \tag{6.5}$$

If we indicate by $\Pi_\alpha(\mathbf{x})$ the expectation value of $\hat{\Pi}_\alpha(\mathbf{x})$ with respect to the ground state. and take into account the size of the particles. we find that the charge density will be given by

$$\rho(\mathbf{x}) = \int \rho_\alpha(\mathbf{x} - \mathbf{y})\, \Pi_\alpha(\mathbf{y})\, d\mathbf{y} \tag{6.6}$$

where $\rho_\alpha(\mathbf{x})$ is the charge distribution in the a-particle. With this ρ in *(6.1)*. we have

$$F(\mathbf{q}) = F_B(\mathbf{q})\, f_\alpha(\mathbf{q}), \tag{6.7}$$

where

$$F_B(\mathbf{q}) = \frac{2}{Z} \int \exp(i\mathbf{q} \cdot \mathbf{x})\, \Pi_\alpha(\mathbf{x})\, d\mathbf{x} \tag{6.8}$$

is the body-form factor of the system and

$$f_\alpha(\mathbf{q}) = \frac{1}{2} \int \exp(i\mathbf{q} \cdot \mathbf{x})\, \rho_\alpha(\mathbf{x})\, d\mathbf{x} \tag{6.9}$$

is the charge form-factor of the α-particle.

Turning back to the three-body case and using the expansions (2.1) and (2.3). we have, after an I-expansion for the exponential. that F_B can be written as

$$F_B = \sum_{\nu'\nu} a_{\nu'} a_\nu \langle \nu' \| j_0(qy) \| \nu \rangle, \tag{6.10}$$

with

$$\mathbf{y} = \mathbf{x}_n - \mathbf{x}_{CM}.$$

The matrix elements of j_0 in the base (2.3) can be calculated in the same way as we did for the Hamiltonian in Sec. 3. The final result for F_B is then given by

$$F_B(\mathbf{q}) = F_B(q^2) = \exp(-q^2/4)\,[2/(1+\delta_{n_1 n_2})]^{1/2} \times$$

$$[2/(1+\delta_{n_1' n_2'})]^{1/2} \sum_{\nu'\nu} a_{\nu'} a_\nu \times$$

$$\sum_{\substack{n_a n_b \\ n_b' l_a}} \langle n_a 2l_a, n_b' 2l_a, 0 \,|\, n_1' l', n_2' l', 0 \rangle \langle n_a 2l_a, n_b 2l_a, 0 \,|\, n_1 l, n_2 l, 0 \rangle \times$$

$$\sum_{p=2l_a}^{2l_a+n_b'+n_b} B(n_b 2l_a, n_b' 2l_a, p)\; {}_1F_1(-p, 3/2; q^2/4), \tag{6.12}$$

where ${}_1F_1$ is a confluent hypergeometric function and q^2 is taken in units of $2\beta/3\varepsilon$.

Now we have a definite way to compute and plot the charge form factor (6.1) of the ground state of a three-α system. The coefficients a_ν are the components of the variational wavefunction (2.1) in the harmonic-oscillator basis and are determined by the diagonalization of the Hamiltonian within a certain space whose dimension is determined by the quantum number N, as discussed in Sec. 3. The correction f_α is taken from experiment[20].

In Figures 6 and 7, we present the body and charge form-factors compared to the experimental result[27]. We have taken for ε the value that gives the best energy in the 10-quantum approximation.

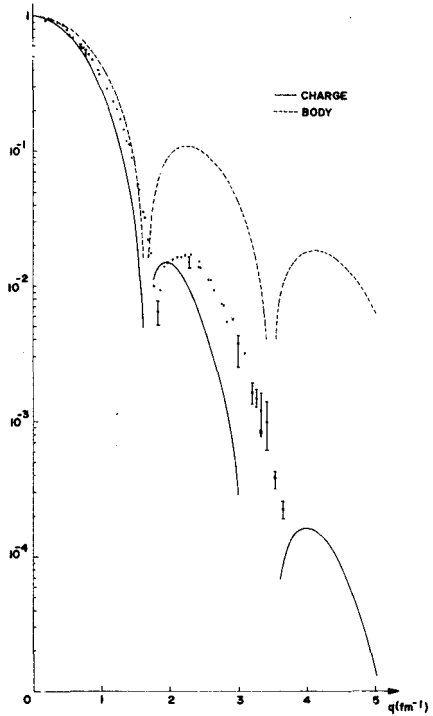

Fig 6 - Charge and body form factors of ^{12}C compared to the experiment. Ground state defined by the Ali-Bodmer potential $e_1 + e_2 + e_3$.

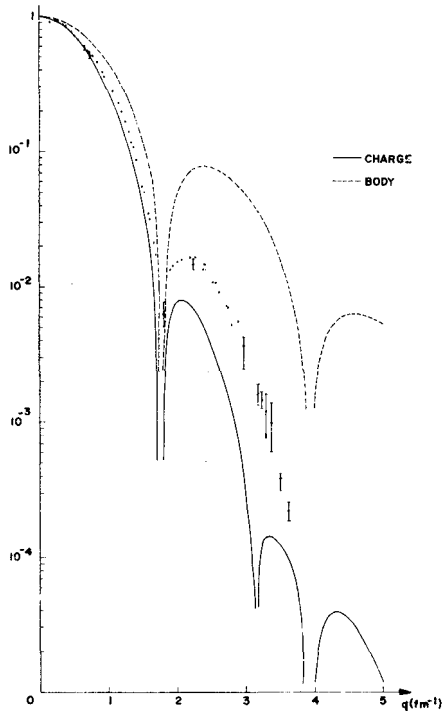

Fig. 7 - Same as Fig. 6 using the Benn-Scharf potential.

The first diffraction minimum is in a very good agreement with the experimental result, mainly in the case of the Benn-Scharf potential. The correction due to the finiteness of the a-partide produces another minimum at $q^2 \approx 10$ fm^{-2} whose experimental determination is still too hard to be carried out[21]. However, calculations that do not make use of the 3-a model also produce such minimum[22-26]. A conclusive analysis is only possible on the ground of complementary experimental data. With the help of correlated harmonic-oscillator furictions, Atti[23] obtained results that are qualitatively similar to ours with the Benn-Scharf potential.

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