Revista Brasileira de Física, Volume 13, nº 1, 1983

Variationall Calculation for the Ground State of ^{12}C

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Recebido em 2 de janeiro de 1983

Abstract A variational calculation is done for the ground state of a 3a-particle system. Two simple trial wavefunctions are used and results are compared with an exact calculation done by the Hyperspherical Harmonic method. A modified Ali-Bodmer potential for the a-a interaction is considered for all calculations. We find that these simplewave functions can be very useful for phenomenological calculations.

Ttie purpose of this note is to report a variational calculation done for the ground state of the three alpha particle system. Microscopic 3α calculations have given a firm foundation of the validity of the 3α approach to C^{12} structure[1]. Therefore descriptions of C^{12} as a 3a particle system have shown relative successful results, as compared to the shell model[1-8]. A recent work has utilized a simple form of the trial wave function for the symmetric S-state of the trinucleon system to demonstrate the effect of three nucleon forces onthe nucleon charge density. The form of the wave function (without three nucleon force), utilized in ref. (9) is

$$\psi(x,y,z) = N(\alpha^3 xyz)e^{-\frac{\alpha^2}{2}(x^2+y^2+z^2)}, \qquad (1)$$

where N is a normalization constant and x, y, z the interparticle distances of che three identical particle system. Such a wave function is too restrictive, in the sense that only one parameter, viz, a controls both the short and long separation behaviours of the wave function. It would be iriteresting to examine how relatively simple wavefunctions, like the orie given by eq. (1), fare for other simple three-body systems. Another well known three-body system, whose ground state has a dominant contribution from the totally symmetric S-state is the C^{12}

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nucleus considered as a bound system of three structureless α-particles. The purpose of this calculation is not to reproduce known properties of the C^{12} nucleus, but to compare the results with an exact calculation[8], thereby sheding light on the validity of the simple forms of the trial wave functions. As we will see later (Table 1), the form of eq. (1) is too restrictive and thus gives a ground state (g.s.) binding energy (BE) of only about 1. Mev, whereas the exact calculation gives 6.6 Mev, with a simplified[8] form of the Ali-Bodmer[10] potential. We use a more generalized form of eq. (1) for our purpose

$$\psi_1(x,y,z) = N\,(\alpha^3 xyz)^{\lambda}\, e^{-\frac{\alpha^2\mu}{2}(x^2+y^2+z^2)^{\mu}}, \qquad (2)$$

where α, λ and μ are variational parameters. The factor $(a^3 xyz)$ with λ>1 will guarantee a better simulation of the impenetrability of the a-particles. On the other hand a value of μ>1 may help to cut the unphysically long tail of the wavefunction (WF1), thereby reducing the Coulomb contribution to BE and increasing tht latter. Another simple wavefunction (WF2) for C^{12} as 3α particles obtained from more microscopic basis by Perring and Skyrme[11,7] will be considered here. It is given in our coordinate system by

$$\psi_2(x,y,z) = N_2\left[p(p-x)(p-y)(p-z)\right]^2 e^{-\frac{\alpha^2}{2}(x^2+y^2+z^2)} \qquad (3)$$

where N_2 is a normalization constant, $2p = x+y+z$ and a is a variational constant to be determined.

Simple phenomenological wavefunctions like ψ and ψ_2 may be very useful in some physical calculations. Exact approaches exist like Faddeev equations[12] and the Hyperspherical Harmonics[13] (HH) where the wavefunctions are obtained naturally from the methods, but it requires much more mathematical involvement and computer time for the numerical part. The values of a, λ and μ for ψ_1 and a for ψ_2 are determined by the conditions

$$\frac{\partial}{\partial\xi}\left(\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right) = 0\ , \qquad (4)$$

($\xi = (\alpha,\lambda,\mu)$ for $\psi = \psi_1$, and $\xi = a$ for $\psi = \psi_2$),

where

$$H = T_s + 3(V_{\alpha\alpha} + V_c) \ , \tag{5}$$

and

$$T_s = -\frac{R^2}{M} \sum_{\text{cyclic}} \left[\frac{\partial^2}{\partial x^2} + \frac{2}{x}\frac{\partial}{\partial x} + \frac{y^2+z^2-x^2}{2yz} \frac{\partial^2}{\partial y \partial z} \right] \tag{6}$$

is the kinetic energy for the fully symmetric S-state. $V_{\alpha\alpha}$ and V_c are respectively the modified Ali-Bodmer potential[8,10] (it somehow reinforces Pauli principle due to the presence of the third a-particle in the α-α system and is an approximation of the nonlocality of the a-a interaction)[8] and the screened Coulomb potential, given by

$$V_{\alpha\alpha}(x) = V_r \, e^{-\mu_r^2 x^2} - V_a \, e^{-\mu_a^2 x^2} \ , \tag{7}$$

with

V_r = 360 MeV, V_a = 130 MeV,
μ_r = 0.7 fm^{-1}, μ_α = 0.475 fm^{-1}, and

Table I - Calculation of binding energy (minimum value) and rms radius

Wave-function	α	λ	μ	$\langle r^2 \rangle^{1/2}$ (fm)	- BE (MEV)
ψ_1	0.32	1.0	1.0	3.01	1.36
	0.576	3.0	1.0	2.56	5.11 (*)
ψ_2	0.570	-	-	2.51	3.81 (*)
HH	-	-	-	2.63	6.60
EXPERIMENTAL VALUE				2.37	7.27

(*) Absolute minimum of energy.

$$V_c(x) = \begin{cases} \frac{4e^2}{2r_c}\left(3 - \left(\frac{x}{r_c}\right)^2\right), & x < r_c, \\ \frac{4e^2}{x}, & x \geq r_c, \end{cases} \tag{8}$$

where $r_c \cong 1.6$ fm. We present our results in Table 1. It can be seen that for $v = \mu = 1.0$ (i.e. the form of eq. (1)) gives a BE of oniy 1.36 MeV, whereas the exact calculation[8] in the HH method gives a value 6.6 MeV. The last lines of Table 1 for ψ_1 and ψ_2 show the best calculated binding energies which compare reasonably with the exact calculation (6.6 MeV). In fig. 1 we can see the calculated chargeform factor[8], $|F(q)|^2$, obtained using the wavefunctions ψ_1(WF1), ψ_2(WF2) and the HH method. For completeness, experimental data are supplied. In general the results obtained with WFI and WF2 compare quite reasonably with the exact calculation (HH). A disagreement is worse for q>2. fm^{-1}. It suggests that one should improve both wavefunctions (ψ_1 and ψ_2) mostly for intermediate distances closer to the origin. Thus one can conclude that the simple forms of trial wavefunctions (eqs. (2), (3))

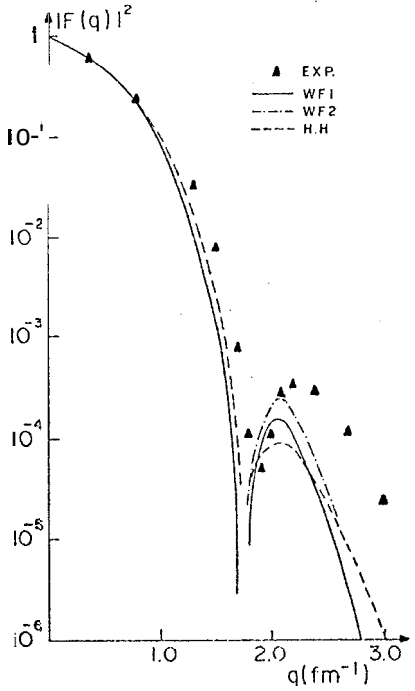

Fig. 1 - Charge form factor plots obtained by using $\psi_1$1 ψ_2(WF2) and HH method. Experimenta1 data are shown.

are not sufficient for a system of three structureless a-particles, mainly due to the Coulomb repulsion and the rather strong soft core of the Ali-Bodmer potential, representing the relative impenetrability of the a-particles. However for first physical calculations they could be useful[1,7,14]. In this work we did a systematic study of two phenomenological rravefunctions by comparing them with the results of an exact calculation where the same interaction was considered. As a conclusion, the results obtained with ψ_1 and ψ_2 are not so bad as compared with others[1,6] . In reference (6) a variational calculation is also done for C^{12} (301). However the trial wavefunction used there did not include the term which simulates the Pauli principle between the a--particles. The a-a interaction chosen and Coulomb force were not handled adequately. As a result, the calculated values were not so good.

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RESUMO

Um cálculo variacional é feito para o estado fundamental de um sistema de partículas 3a. Duas funções de ondas tentativas simples são usadas e os resultados comparados com um cálculo exato feito pelo método dos harmônicos hiperesféricos. Um potencial de Ali-Bodmer modificado para a interação a-a é considerado em todos os cálculos. A conclusão é que estas funções de ondas simples podem ser usadas em cálculos fenomenológicos.