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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

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COMPARISON BETWEEN
HARTREE-FOCK AND FIRST ORDER
HYPERSPHERICAL CALCULATIONS
FOR THE ALPHA PARTICLE

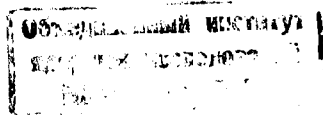
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**COMPARISON BETWEEN
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Направлено в ЯФ



For solving the many-body problem by the Hartree-Fock calculation some potentials smooth enough to be useful for this method have been proposed especially by Volkov^{/1/} and Brink and Boeker.^{/2/} These potentials have been adjusted so as to give the experimental binding energy and the size of the alpha particle for the Hartree-Fock approximation. The hyperspherical formalism^{/3,4/} gives another method of solving the many-body problem. The purpose of this paper is to give a comparison between the values obtained by the Hartree-Fock and the first order hyperspherical calculations. To this order the system of coupled differential equations of the hyperspherical formalism reduces to a single one-dimensional differential equation. The investigated two body central potentials are expressed as a superposition of Gaussian potentials with repulsive core, and do not distinguish between the singlet and triplet states. Hence, the ground state of the alpha particle contains the space completely symmetrical wave function only.

In this case the first differential equation which gives the largest contribution to the binding energy and the wave function takes the simple form

$$(T_0 + V_0(r) - E_0) \Psi_0(r) = 0, \quad (1)$$

where $T_0 = -\frac{\hbar^2}{m} \left[\frac{d^2}{dr^2} + \frac{8}{r} \frac{d}{dr} \right]$ is the kinetic energy operator acting on the first partial wave $\Psi_0(r)$ for which the total quantum number $L=0$. The potential $V_0(r)$ is obtained in putting $K=0$ and $D=9$ for the number of dimension of the space in the general expression of ref.^{5/} and is given by

$$V_0(r) = 35 \left(\frac{3}{2} \right)^2 \int_0^1 V(ur) (1-u^2)^2 u^2 du$$

for a two-body potential $V(r_{ij})$.

The problem now reduces to the one of solving a one-dimensional differential equation and extracting the binding energy and the r.m.s. radius of the $\Psi_0(r)$ wave function for the ground state to compare with the numbers obtained by Volkov and Brink and Boeker in their Hartree-Fock approach.

In Table I one gives the parameters of the Volkov and Brink and Boeker (B.B.) potentials written in the form

$$V(r_{ij}) = V_r e^{-\left(\frac{r_{ij}}{\rho}\right)^2} + V_a e^{-\left(\frac{r_{ij}}{a}\right)^2}.$$

The first term is the repulsive core of the interaction, the second is attractive. The binding energy, E_{HF} , has been obtained in neglecting the Coulomb interaction. The next column shows the binding energy E_0 given by eq. (1), and the last one the value $F(1)$ of the body form factor for a momentum transfer $k=1 \text{ fm}^{-1}$, related to the m.s. radius a^2 of ${}^4\text{He}$ by

$$a^2 \approx -6 \text{ Log } F(1).$$

On the first row are quoted the experimental data. It appears at first sight that the numbers given by the first order approximation of the hyperspherical formalism are by about 5 - 1 MeV below those given by Hartree-Fock calculations, and that the m.s. radius is generally well fitted. But it is not enough to have approximately

the same values for E_{HF} and E_0 to be sure that these values are close to the true binding energy of each particular potential.

To have an idea about the accuracy of E_0 one can try to replace the true many-body potential $\sum_{i,j>1} V(\mathbf{r}_{ij})$ by a separable potential having the same term $V_0(\mathbf{r})$ in its hyperspherical expansion. This can be done by taking the symmetrical coordinates ξ_1^{\rightarrow} defined in ref.^[6]. In this system of coordinates and with an interaction $U(\xi_1)$ one has a separable equation

$$\sum_{i=1}^3 \left[-\frac{\hbar^2}{m} \nabla_{\xi_i}^2 + U(\xi_i) - \frac{E_M}{3} \right] \Psi(\xi_1^{\rightarrow}, \xi_2^{\rightarrow}, \xi_3^{\rightarrow}) = 0 \quad (2)$$

whose completely symmetrical wave function is given by the product $\Psi(\xi_1^{\rightarrow}, \xi_2^{\rightarrow}, \xi_3^{\rightarrow}) = \prod_1^3 \psi(\xi_i)$, $\psi(\xi_i)$, being the solution of

$$\left\{ -\frac{\hbar^2}{m} \nabla_{\xi_i}^2 + U(\xi_i) - \frac{E_M}{3} \right\} \psi(\xi_i) = 0.$$

The first term of the expansion of the potential $\sum_1^3 U(\xi_i)$ into hyperspherical harmonics is equal to $V_0(\mathbf{r})$ is $U(\xi_1) = 2V(\xi_1)$. With this definition the multipoles $V_{2k}(\mathbf{r})$ of the expansion of $\sum_{i,j>1} V(\mathbf{r}_{ij})$ and of $\sum_1^3 2V(\xi_i)$ are the same but the coupling constant between the coupled equations being stronger for the last case, the ground state binding energy obtained by solving (2) will be lower than the one of the true potential.

Hence this method enables one to have a lower bound for the ground state binding energy. In Table II are quoted the numerical results obtained for E_0 and E_M for various forces including Volkov^[1], Brink and Boeker^[2], Baker et al.^[7], Eckemeier-Hackenbroich^[8] and Afnang and Tang^[9] potentials. The third row gives the average, $\frac{1}{2}(E_0 + E_M)$, which is compared to the best variational numbers set on the last line^[10]. One sees that the gap between these values do not exceed about 1 MeV even for poten-

tials having strong repulsive core like those (labelled by S₁) proposed in ref.^{/9/}.

The average energy $\frac{1}{2}(E_0 + E_M)$ gives a first and very quick^{x/} estimate of the binding energy of ⁴He. From the result of the last column one sees that the Brink and Boeker potential which has been constructed so as to fit the ⁴He binding energy by the Hartree-Fock calculation, does not give actually the expected value.

It is interesting to notice that in solving eq. (1) for the potentials of refs.^{/1,2,7/} one finds an excited state of the same symmetry than the ground state for a binding energy of about - 3 -- -4 MeV. These values will obviously be lowered in solving the complete set of the hyperspherical coupled differential equations. This excited 0⁺ state can not be reached easily by a standard method.

References

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^{x/} a few seconds of UNIVAC 1108 time.

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TABLE I

Experimental data					-28.2MeV	0.69	
Force	V_a	α	V_r	ρ	E_{HF}	E_o	$F(I)$
V_1	- 83.34	1.60	144.86	0.82	-28.01	-28.58	0.695
V_2	- 60.65	1.80	61.14	1.01	-28.88	-29.40	0.692
V_3	-106.67	1.50	106.67	1.05	-28.55	-29.26	0.724
V_4	- 76.69	1.50	408.27	0.45	-28.28	-29.15	0.728
V_5	- 70.64	1.70	75.01	1.01	-27.52	-28.09	0.696
V_6	- 73.23	1.70	81.33	1.01	-28.23	-28.75	0.694
V_7	- 54.30	1.80	74.49	0.81	-27.45	-28.03	0.693
V_8	- 53.98	1.80	100.67	0.71	-27.89	-28.45	0.692
B B	-140.6	1.4	389.5	0.7	-28.2	-29.29	0.690

V_a , V_r , E_{HF} and E_o are in MeV, α and ρ in fm.

TABLE II

Reference	(1)	(7)	(8)	(9)			(2)
Force	V_I	B	S	S_I	S_2	S_3	B B
$-E_0$ (MeV)	28,58	39,17	18,57	16,75	14,88	7,18	29,29
$-E_M$ (MeV)	32,82	42,48	37,18	44,41	45,68	44,35	46,71
$-\frac{1}{2}(E_0+E_M)$ (MeV)	30,7	40,8	27,9	30,6	30,3	25,8	38,0
$-E$ variat. ⁹	30,3	40,1	28,2	31,6	31,5	26,5	
¹⁰ (MeV)	29,9		27,7	31,1	30,2	26,5	

The variational values are taken from ref.^{9,10} after elimination of the Coulomb energy.