Journal of Applied Mathematics and Physics, 2014, 2, 869-874
Published Online August 2014 in SciRes. http://www.scirp.org/journal/jamp
http://dx.doi.org/10.4236/jamp.2014.29098

Hartree-Fock Calculations of ^{16}O and ^{40}Ca Nuclei Using Fish-Bone Potential

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Received 24 July 2014

Abstract

Hartree-Fock calculations are carried out to describe some properties of ^{16}O and ^{40}Ca nuclei using the two forms of fish-bone potential (I and II). A computer simulation search program has been introduced to solve this problem. The Hilbert space was restricted to three dimensional variational space spanned by single spherical harmonic oscillator orbits. Binding energies, root mean square radii and form factors are found to have a good fit with experimental data.

Keywords

Nuclear Structure, Hartree-Fock Theory, Fish-Bone Potential

1. Introduction

The Hartree-Fock (HF) theory [1]-[3] and more elaborate self-consistent theories [4] [5] have been widely and successfully applied to investigate various properties of nuclear structure. Also the problem of cluster structure in nuclei has been a subject of interest since the early days of nuclear physics till now [6]. The idea is largely supported by the fact that alpha particles have exceptional stability and that they are the heaviest particles emitted in natural radioactivity. Various models have been proposed to account for possible nuclear clustering and to study its effects [7]. Later, a simple version of the model, in which the alphas are assumed to have no internal structure, is considered. The concept of clustering is very widely used in physics. The concept of alpha- clustering has found many applications to nuclear reactions and nuclear structures [8] [9].

Many such clusters are possible in principle, but the formation probability depends on the stability of the cluster, and of all possible clusters the alpha particle is the most stable due to its high symmetry and binding energy. Thus a discussion of clustering in nuclei is mainly confined to alpha-particle clustering. For the α-nuclei ^{8}Be, ^{12}C, ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, ^{32}S, the geometrical equilibrium configuration of the α-particles are generally assumed to belong to the symmetry point groups $D_{\infty h}$, D_{3h}, T_d, D_{3h}, O_h (or alternatively D_{4h}), D_{5h}, D_{6h}, respectively.

The fishbone potential [10] of composite particles simulates the Pauli effect by nonlocal terms. The α-α fish-bone potential be determined by simultaneously fitting to two-α resonance energies, experimental phase shifts,

How to cite this paper: El-Shal, A.O., Mansour, N.A., Taha, M.M., Qandil, O.S.A. (2014) Hartree-Fock Calculations of ^{16}O and ^{40}Ca Nuclei Using Fish-Bone Potential. *Journal of Applied Mathematics and Physics*, **2**, 869-874.
http://dx.doi.org/10.4236/jamp.2014.29098

and three-α binding energies. It was found that, essentially, a simple Gaussian can provide a good description of two-α and three-α experimental data without invoking three-body potentials. Many authors adopted the fishbone model because, in their opinion, this is the most elaborated phenomenological cluster-model-motivated potential. The variant of the fishbone potential has been designed to minimize and to neglect the three-body potential. Therefore, they can try to determine the interaction by a simultaneous fit to two- and three-body data [11].

2. The Theory

We consider a system of N identical bosons described by a Hamiltonian of the usual form

$$H = \hat{T} + \hat{V} = \sum_{i=1}^{N} t(i) + \sum_{i \neq j=1}^{N} v(i, j) \tag{1}$$

where $t(i)$ is the kinetic energy operator i^{th} particle and $v(i, j)$ the two-body interaction. In Hartree-Fock method, one takes for the best choice of the normalized wave function ψ the one that it minimizes the expectation value of the Hamiltonian H

$$\delta \langle \psi | H | \psi \rangle = 0 \tag{2}$$

In most Hatree-Fock calculations for light nuclei one has taken the subspace spanned by the lowest harmonic oscillator shell $l\ j>$. We assume that all the particles occupy the same orbital λ belonging to the average field. Hence the intrinsic state of the whole system would be described by the symmetric wave function

$$\psi(1, 2, ..., N) = \lambda(1)\ \lambda(2)\ \lambda(3).....\lambda(N) \tag{3}$$

In this subspace, the HF orbitals $l\ \lambda>$ are then determined by their expansion coefficients m_l^{λ}.

$$|\lambda\rangle = \sum_{j=1}^{N} m_j^{\lambda} |j\rangle \tag{4}$$

And the HF-Hamiltonian h (λ_1, λ_2, ….. λ_N) is replaced by the matrix

$$\langle i|h|j\rangle = \langle i|t|j\rangle + \sum_{\lambda} \sum_{k} \sum_{l} m_k^{*\lambda} \langle i\,k|v|j\,l\rangle_s\, m_l^{\lambda} \tag{5}$$

where

$$\langle i\,k|v|j\,l\rangle_s = \langle i\,k|v|j\,l\rangle + \langle i\,k|v|l\,j\rangle \tag{6}$$

The HF Equations are then replaced by the matrix Equation

$$\sum_{j} \langle i|h|j\rangle m_j^{\lambda} = \varepsilon\, m_i^{\lambda} \tag{7}$$

One proceeds by iteration until self-consistency is achieved.

3. Fish-Bone Potential

A fishbone potential of the α-α system was determined by Schmid E. W. [12] [13] [14]. The harmonic oscillator width parameter was fixed to a = 0.55 fm^{-2} and. The local potential was taken in the form

$$V_l(r) = v_0 \exp(-\beta r^2) + \frac{4e^2}{r} erf\left(\sqrt{\frac{2a}{3}} r\right) \tag{8}$$

where v_0 = −108.41998 MeV and β = 0.18898 fm^{-2} and called Fish-Bone I (FB-1) While this potential provides a reasonably good fit to l = 0 and l = 2 and l = 4 partial wave phase shifts, it seriously over binds the three-α system as shown in (**Table 1**). The experimental binding energy of the three-α (^{12}C) system is $E_{3\alpha}$ = −7.275 MeV.

One may conclude that there is a need for three-body potential. This was the choice Oryu and Kamada [15]. They added a phenomenological three-body potential to the fish-bone potential of Kircher and Schmid [12] [13] [14] and found that a huge three-body potential is needed to reproduce the experimental data. But, Faddeev calculations [11] reveal that the ℓ = 4 partial wave is very important to the three-α binding and, for this partial wave, the fit to experimental data is not so stellar. So Papp Z. and Moszkowski S. [11] concluded, that it may be

Table 1. L = 0 three-binding energy as a function of subsystem angular momentum l_{max} in case if fish-bone potential of Kircher and Schmid (FB-1) [12] [13] [14] and the results of Papp Z. and Moszkowski S. (FB-2) [11].

l_{max}	FB-1	FB-2
2	0.057	−0.313
4	−15.47	−7.112
6	−15.63	−7.273
8	−15.63	−7.275

possible to improve the agreement in the ℓ = 4 partial wave and achieve a better description for the three-α binding energy in the point view of the these authors.

Thus as a local potential, two Gaussians plus screened Coulomb potential are added to form Fish-Bone II (FB-2):

$$V_l(r) = v_1 \exp(-\beta_1 r^2) + v_2 \exp(-\beta_2 r^2) + \frac{4e^2}{r} erf\left(\sqrt{\frac{2a}{3}} r\right) \tag{9}$$

where v_1, β_1, v_2, β_2 and a are fitting parameters. In the fitting procedure Papp Z. and Moszkowski S. incorporated the famous ^{8}Be, l = 0 resonance state at E_{2b}^{exp} = (0.0916 − 0.000003i) MeV, the ^{12}C three-α ground state energy E_{3b}^{exp} = −7.275 MeV, and the l = 0, l = 2 and l = 4 low energy phase shifts. With parameters v_1 = −120.30683493 MeV, β_1 = 0.20206127 fm^{-2}, v_2 = 49.06187648 MeV, β_2 = 0.76601097 fm^{-2} and a = 0.64874009 fm^{-2}, they achieved a perfect fit.

For the l = 0 two-body resonance state they get E_{2b} = 0.09161 - 0.00000303i MeV, and for the three-body ground state E_{3b} = −7.27502 MeV. Notice that unlike with the Ali-Bodmer potential, they achieved this agreement by using the same potential in all partial waves. Having this new α-α fish-bone potential from the fitting procedure, they also calculated the first excited state of the three-system. This state is a resonant state, and we got $E_{3\alpha}^{res}$ = (0.54 - 0.0005i) MeV, which is again very close to the experimental value.

4. Solutions in a Three-Dimensional Space

We consider solutions in a three dimensional variational space spanned by the orthonormal states l 1>, l 2 > and l 3>. In this case, we have twenty-one different symmetrized two-body matrix elements.

A HF-orbital λ will have the general form

$$|\lambda\rangle = \sum_{j=1}^{3} m_j^{\lambda} |j\rangle \tag{10}$$

where

$$\sum_j m_j^{*\lambda} m_j^{\lambda'} = \delta_{\lambda\lambda'}, \qquad \sum_{\lambda} m_j^{*\lambda} m_{j'}^{\lambda} = \delta_{jj'} \tag{11}$$

And assume that the coefficient m_j's are real.

To investigate the HF-solutions, we have to specify the alpha-alpha potential. The specific combinations chosen as the basic states depend on the symmetry of the intrinsic structure that is expected from the molecular alpha-particle model.

Now we chose basic states which are invariant with respect to the transformation of the symmetry group T_d. Therefore, we chose our three basic states as

$$|1\rangle = |0s0\rangle \tag{12}$$

$$|2\rangle = \frac{1}{\sqrt{2}}\{|0f2\rangle - |0f-2\rangle\} \tag{13}$$

$$|3\rangle = \frac{1}{\sqrt{\eta^2+2}}\{\eta|0g0\rangle + (|0g4\rangle + |0g-4\rangle)\} \tag{14}$$

where η is a parameter determined from the T_d symmetry.

Here the oscillator shell model wave functions are given by

$$\left|\vec{r}, n\ell m\right\rangle = R_{n\ell}(r)Y_{\ell m}(\theta,\phi), \tag{15}$$

$$R_{n\ell}(r) = \left[2\Gamma(n+1)/\beta_0^3\Gamma(n+\ell+3/2)\right]^{1/2}(r/\beta_0)^{\ell} \times L_n^{\ell+1/2}(r^2/\beta_0^2)\exp(-r^2/2\beta_0^2) \tag{16}$$

$\beta_0 = (h/m_\alpha\omega)^{1/2}$ is the oscillator parameter.

5. Matrix Elements of the Kinetic and Potential Energy

Considering HF-solutions with mixed parity (where it is important in nuclear calculations), therefore, we have only twelve non-vanishing two-body matrix elements for the potential energy v_{ijkl} and three matrix elements of kinetic energy namely t_{11}, t_{22} and t_{33}. Therefore the non-vanishing HF-Hamiltonian will be

$$h_{11} = t_{11} + 1/2(N-1)\left[v_{1111}m_1^2 + v_{1212}m_2^2 + v_{1313}m_3^2\right] \tag{17}$$

$$h_{12} = h_{21} = 1/2(N-1)\left[\left(v_{1122}+v_{1221}\right)m_1m_2 + \left(v_{1223}+v_{1322}\right)m_2m_3\right] \tag{18}$$

$$h_{13} = h_{31} = 1/2(N-1)\left[v_{1232}m_2^2 + v_{1333}m_3^2 + \left(v_{1133}+v_{1331}\right)m_1m_3\right] \tag{19}$$

$$h_{23} = h_{32} = 1/2(N-1)\left[v_{2231}m_1m_2 + \left(v_{2233}+v_{2332}\right)m_2m_3\right] \tag{20}$$

$$h_{22} = t_{22} + 1/2(N-1)\left[v_{2121}m_1^2 + v_{2222}m_2^2 + v_{2323}m_3^2 + 2v_{2123}m_1m_3\right] \tag{21}$$

$$h_{33} = t_{33} + 1/2(N-1)\left[v_{3131}m_1^2 + v_{3232}m_2^2 + v_{3333}m_3^2 + 2v_{3133}m_1m_3\right] \tag{22}$$

6. Nuclear Density and Form Factor

The parity projected part of the nuclear density distribution, normalized to unity, which corresponds to a HF-solution as defined by Equations (5)-(7), is found to be

$$\rho_0(r) = (1/\beta_0^3\pi^{2/3})\left[m_1^2 + (8/105)(r^6/\beta_0^6)(m_2^2 + 2m_3^2r^2/9\beta_0^2)\right]\exp(-r^2/\beta_0^2) \tag{23}$$

The form factor corresponding to the spherical part of the density distribution (24) is

$$\begin{aligned} F_0(q) = {} & [1 - q^2\beta_0^2(3m_2^2 + 4m_3^2)/6 + q^4\beta_0^4(m_2^2 + 2m_3^2)/120 - q^6\beta_0^6(m_2^2 + 4m_3^2)/840 \\ & + q^8\beta_0^8m_3^2/15120]\exp(-q^2\beta_0^2/4) \end{aligned} \tag{24}$$

where q is the momentum transfer. The expression of $F_0(q)$ has to be multiplied by a form factor F(q) = $\exp(-q^2\beta^2{}_\alpha/4)$, which account for the α-particle distribution.

7. Discussion

By using the two types of the Fish-Bone potentials I and II and with the oscillator parameter β_0 for ^{16}O and ^{40}Ca in addition to the parameter of the alpha particle β_α, we have got the nuclear structure properties of the ^{16}O and ^{40}Ca nuclei such as binding energies, root mean square radii and form factors, and comparing the results with the experimental elastic scattering charge form factor [16] and other theoretical ones such as HF (Hrtree-Fock using Skyrme-type wave function) [17], HO + SRC (Harmonic Oscillator + Short range correlation) and HO (Harmonic Oscillator potential) [17].

Using the Fish-Bone potential I (FB-1) according to its Equation (8), the parameters used in our calculations of fishbone potential I of ^{16}O and ^{40}Ca are given in **Table 2**. The results of the binding energies and root mean square radii of ^{16}O and ^{40}Ca nuclei are given in **Table 3**.

Using the Fish-Bone potential II (FB-1) as in Equation (9), the parameters used in our calculations of fishbone potential II of ^{16}O and ^{40}Ca are given in **Table 4**. The results of the binding energies and root mean square radii of ^{16}O and ^{40}Ca nuclei using Fish-Bone Potential II are given in **Table 5**.The charge form factor of ^{16}O and ^{40}Ca nuclei using Fish-Bone Potential II are given in **Figure 1** and **Figure 2**.

In case of Fish–Bone potential I (FB-1), the binding energy of ^{16}O and ^{40}Ca nuclei and the root mean square radii are in good agreement with the experimental results as shown in **Table 3**. But we have not got form factors for both nuclei. The reason of that is obvious because the potential FB-1 have no repulsive part. Applying the repulsive part v_2 in the Fish-Bone potential II, we have got form factors for ^{16}O and ^{40}Ca nuclei as shown in

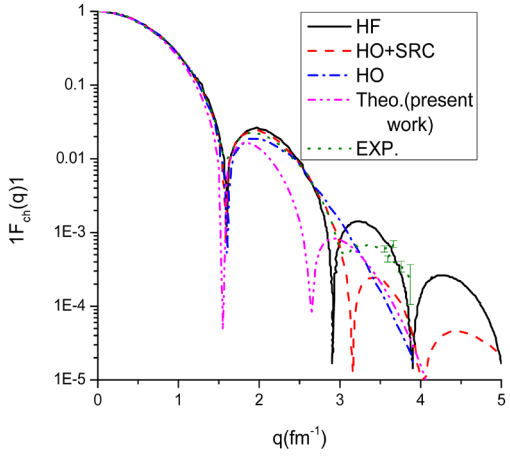

Figure 1. Charge form factors of ^{16}O nuclei using the fish-bone potential II.

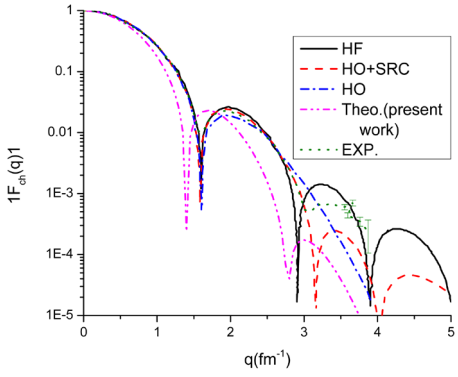

Figure 2. Charge form factors of ^{40}Ca nuclei using the fish-bone potential II.

Table 2. The parameters used in our calculations of fishbone potential I of ^{16}O and ^{40}Ca.

Nucleus	V_0 (MeV)	β_1 (fm^{-2})	a (fm^{-2})
^{16}O	−11	0.1889	0.55
^{40}Ca	−13	0.1889	0.55

Table 3. The calculated binding energies and root mean square radii of ^{16}O and ^{40}Ca using the fish-bone potential I.

Nucleus	Theor. B. E. (MeV)	Exp. B. E.(MeV)	Theor. rms (fm)	Exp. Rms (fm)
^{16}O	−14.55	−14.40	2.55	2.7
^{40}Ca	−63.74	−62.047	3.24	3.49

Table 4. The parameters used in our calculations of fish-bone potential II of ^{16}O and ^{40}Ca.

Nucleus	V_1 (MeV)	V_2 (MeV)	β_1 (fm^{-2})	β_2 (fm^{-2})	a (fm^{-2})
^{16}O	−51	135	0.2021	0.7660	0.6487
^{40}Ca	−60	180	0.2021	0.7660	0.6487

Table 5. The calculated binding energies and root mean square radii of ^{16}O and ^{40}Ca using the fish-bone potential II.

Nucleus	Theor. B.E. (MeV)	Exp.B.E. (MeV)	Theor. rms (fm)	Exp. Rms (fm)
^{16}O	−13.9207	−14.40	2.7991	2.71
^{40}Ca	−62.7059	−62.047	3.24	3.49

Figure 1 and **Figure 2**, which are in acceptable agreement with the experimental points in addition to other theoretical ones. **Table 4** shows the parameters of the (FB-2) potential which gives us the binding energies and the root mean square radii of ^{16}O and ^{40}Ca, and we found that these values are in good agreement with the experimental data (**Table 5**).

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