The ground state binding energy of the closed shell nuclei with the density dependent $Av_{18}$ effective interaction in LOCV method

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Abstract. This work presents the calculation of the ground state binding energy of some light closed shell nuclei such as $^4$He, $^{12}$C, $^{16}$O, $^{28}$Si, $^{32}$S, $^{40}$Ca and $^{56}$Ni. We use our channel-dependent effective two-body interactions data that are produced through the lowest order constrained variational (LOCV) method for asymmetric nuclear matter with the charge-dependent $Av_{18}$ bare NN potential up to $J_{\text{max}}=2$ and $J_{\text{max}}=5$. The local density approximation approach in the harmonic oscillator basis and Brody-Moshinsky coefficients are used to produce the relative and center of mass dependent effective two-body potentials. We show that the ground state energies of the closed shell nuclei with $Av_{18}$ ($J_{\text{max}}=2$) gives more binding with respect to Reid68 bare NN potential as well as $\Delta - Reid68$. However, there is not much difference between the $Av_{18}$ ($J_{\text{max}}=5$) and Reid68 which has been defined up to $J_{\text{max}}=5$. We conclude that the contributions of higher partial waves ($J > 2$) are not very important and two-body kinetic energy in $J=1$ channel is twice as that of $J=0$ which is not the case for the two-body potential energy. Finally, our work results are compared with other theoretical approaches and experimental data.

1. Introduction

A very good progress has been made in the development of many-body techniques for the few-body nucleon systems, especially A=3-12 nuclei [1-15]. But the $A > 12$ light nuclei nucleus have been described by the variational or the cluster Monte Carlo (VMC, CMC) techniques by using the Jastrow trial variational wave-function [3-11]. The $^{16}$O and $^{40}$Ca nuclei have been also studied by the coupled-cluster method (CCM) and the no-core shell model (NCSM) [12-15] with different interactions.

The properties of closed shell nuclei were calculated by us, using the basic local density Brueckner $G$ matrix idea [16-21]. The channel-dependent effective two-body interactions (CDEI) were generated through the lowest constrained variational (LOCV) asymmetrical nuclear matter code, at different densities with the Reid type bare nucleon-nucleon interactions. Then, this dependence was converted to the local one by using the local density approximation in the harmonic oscillator basis. The result was encouraging, both with respect to the available experimental data and the different model dependent theoretical predictions [20, 21].

But a reliable many-body technique and a true nucleon-nucleon potential is needed to predict results close the empirical ones. It was demonstrated in several of our previous works, that in
the framework of the LOCV method [22, 23, 24], the many-body calculations for the nuclear matter with phenomenological potentials such as the Reid68 [25, 26, 27], give substantially too much binding and large saturation density than the empirical one. During the last three decades, situation has been the same for other techniques and potentials [16-19, 28-32]. But the inclusion of the three-body force and the Δ isobar degrees of freedom (Δ-Reid68) [16-19, 22-27] have improved the behavior of Coester line to the right direction [16-19].

In this article we intend to extend our recent works [20, 21, 33] to the operator type interactions i.e. the Au18, and calculate the properties closed shell nuclei such as the $^4$He, $^{12}$C, $^{16}$O, $^{28}$Si, $^{32}$S, $^{40}$Ca and $^{56}$Ni, in the harmonic oscillator basis by using the local density approximation. Section 2 is devoted to the evaluation of matrix elements and the binding energies of different closed shell nuclei by using the local density approximation. Finally, in section 3 we present the results and discussions.

2. The closed shell nuclei binding energy

We assume [20, 21, 33], the $[(0s_{1/2})^4]$, $[^4He+(0p_{1/2})^8]$, $[^{12}C+(0p_{1/2})^4]$, $[^{16}O+(0d_{5/2})^{12}]$, $[^{28}Si+(1s_{1/2})^4]$, $[^{32}S+(0d_{5/2})^8]$ and $[^{40}Ca+(0f_{7/2})^{16}]$ configurations for different closed shell nuclei,i.e., $^4He$, $^{12}$C, $^{16}$O, $^{28}$Si, $^{32}$S, $^{40}$Ca and $^{56}$Ni with atomic number $A$, respectively and the origin of the coordinate is fixed at the center of mass of these nuclei. Note that our formalism is exact for L-S closed shell nuclei such as $^4He$, $^{16}$O and $^{40}$Ca. The intrinsic Hamiltonian is,

$$\mathcal{H}_0 = \mathcal{H} - \frac{P^2}{2M},$$

(1)

where $P = \sum_i p_i$ and $M = Am$ are the nucleus total momentum and mass, respectively and $\sum_i r_1 = 0$. Then the expectation value of $\mathcal{H}_0$ in the harmonic oscillator basis can be written as:

$$E^{B.E.}_{Total} = < \mathcal{H}_0 > = \sum_i < i, \hbar \omega| \frac{p^2}{2m}| i, \hbar \omega > + \frac{1}{2} \sum_{ij} < ij, \hbar \omega| V(r_1, r_2)| ij, \hbar \omega > - T_{C.M.}^A,$$

(2)

where $T_{C.M.}^A = \frac{3}{4} \hbar \omega$ and the Dirac ket $|i, \hbar \omega >$ stands for $|n_i, l_i, s_i, \tau_i, m_{\tau_i}; \hbar \omega >$ i.e. the harmonic oscillator wave functions, the angular, the spin, the isospin and the isospin projection parts of the single particle states, respectively. In general, $V(r_1, r_2)$ is a non-local effective two-nucleon potential.

As we mentioned before, $\hbar \omega$ or $\gamma = \sqrt{\frac{m\omega}{\hbar}}$ is the harmonic oscillator parameter and will be fixed variationally. The matrix elements of one-body kinetic energy per nucleon (the first term) has the familiar form of,

$$T_1 = \frac{1}{2A} \sum_{i=1}^A (2n_i + l_i + \frac{3}{2}) \hbar \omega,$$

(3)

while the second term can be approximated and written as the sum of two-body kinetic and potential energies per nucleon:

$$E_2 = T_2 + V_2 = \frac{1}{2A} \sum_{ij} < ij, \hbar \omega| V(r_{12}, R_{12})| ij, \hbar \omega > =$$

$$\frac{1}{2A} \sum_{ij} < ij, \hbar \omega | - \frac{\hbar^2}{2m} [F(r_{12}, R_{12}), | \nabla^2 F(r_{12}, R_{12})]| | ij, \hbar \omega > +$$

$$\frac{1}{2A} \sum_{ij} < ij, \hbar \omega | F(r_{12}, R_{12}) V(12) F(r_{12}, R_{12})| ij, \hbar \omega >$$

(4)
In the two-body energy, we assume $\alpha = lJSTM_T$, $|j|=2j+1$ etc. and the first and the second curly brackets to be the Wigner 6-j and 9-j symbols, respectively, and $<n_1l_1,n_2l_2,\lambda |nl,NL,\lambda>$ are the familiar Brody-Moshinsky Brackets [43], i.e.,

$$E_2 = \frac{1}{2A} \sum_{1,2,k,\alpha,\alpha'} [j_1][j_2][j][\lambda][S][J] |<m_1 m_2 | T, M_T >|^2 (1 - (-1)^{j+S+T})$$

$$\left\{ \begin{array}{ccc} L & l & \lambda \\ S & j & J \end{array} \right\}^2 \left\{ \begin{array}{ccc} l_1 & \frac{3}{2} & j_1 \\ l_2 & \frac{3}{2} & j_2 \end{array} \right\}^2 \times <n_1 l_1, n_2 l_2, \lambda | nl, NL, \lambda >^2$$

$$<n\alpha, NL | V_{\alpha'}^k(\sqrt{2}r, \rho(R))\{|\alpha'><\alpha'|} | n\alpha, NL >.$$

Now, we are in a position to calculate the various closed shell nuclei binding energies per nucleon as follows:

$$E_A^{B.E.} = \frac{1}{A} E_{Total}^{B.E.} = [T_1 + T_2 + V_2 - T_{C.M.}]. \hspace{1cm} (5)$$

3. Results and Discussion

The channel break down of two-body kinetic and potential energies and one-body coulomb energy with respect to the two-nucleon channel $J$ values (as well as their variation), using the LOCV effective two-body potential with different $J_{max}$ value for $^{40}Ca$, are given in table 1. The table shows the calculations in which the CDEI's of LOCV calculation with $J_{max}$ = 5 have been used in all of the available channels (for Reid68 Day and Av18 potentials). In general, the main contribution comes from $J \leq 1$ for two-body kinetic energy and $J \leq 2$ for two-body potential energy and the other channels have a very small effect on the two-body energies of $^{40}Ca$. It is interesting that the two-body kinetic energy of $J = 1$ channel has the same size as the $J = 0$ one.

In the table 2 we have compared our calculated binding energy and RMS radius for $^4He$, $^{12}C$, $^{16}O$ and $^{40}Ca$ with different approaches, namely, the coupled cluster of Kümml [35] and Hagen [15], Green function and cluster (variational) Monte Carlo of Pieper et al. [3-11], CBF-FHNC of Fabrocini et al. [36, 37], Brueckner-Hartree-Fock of Coraggio et al. [38] with $N^3LO$ and Av$_{18}$ interactions, random phase approximation of Barbieri et al. [42] with Av$_{18}$ potential, Fermionic molecular dynamics of Roth et al. [41] and no-core shell model (NCSM) of Navrátil et al. [12, 13, 14] with $V_8$ or CD-Bonne potential. The CCM of Kümml et al. [35] (Hagen et al. [15]) calculation is with Reid68 ($V_{\text{weak} k}$) potential while the other methods have used $U_{14}$ or Av$_{18}$ plus three-nucleon interaction (TNI). We have not included neither the TNI nor the dispersion-Pauli effects in our calculation. The contribution of TNI is less than an MeV binding in light nuclei. On the other hand, in heavier nuclei we have the dispersion effect which can reduce the binding up to $2 - 3 MeV$, for example in nuclear matter. This can be estimated by comparing the results of BHF [40] on $^4He$ and $^{16}O$ and those tabulated from the experiment, i.e., for $^4He$ we have $\approx -7.08 MeV$ (experiment) and $-6.85 MeV$ (BHF) which gives $-0.23$ for TNI effect and for $^{16}O$ we have $\approx -8.55 MeV$ (experiment) and $-9.53 MeV$ (BHF) which gives $+0.98$ for dispersion effect. We should point out here that some techniques, such as BHF, have used low $k$ parts of Av$_{18}$ and obviously they should get more binding than ours. So by comparison we can conclude that in general we get reasonable result especially for $^{40}Ca$ with respect to both experimental data and others theoretical calculations. However, we have restricted our configuration space to those given in the beginning of section 2. We hope we can improve our calculations by increasing the above configuration space in the future works.
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Table 1. The channel break down (in terms of $J$) of two-body kinetic ($T_2$), potential ($V_2$) and one-body Coulomb ($V_c$) energies for $^{40}$Ca with Reid68Day and Av$_{18}$ ($J_{\text{max}} = 5$, i.e. there is no approximation for effective interaction in the $J > 2$ channels) potentials.

| $J$  | $T_2$  | $V_2$   | $V_c$   | $T_2$  | $V_2$   | $V_c$   |
|------|--------|---------|---------|--------|---------|---------|
| 0    | 5.8731 | -20.5891| 0.5776  | 4.9670 | -19.7915| 0.5776  |
| 1    | 12.1302| -19.2464| 0.3727  | 9.7487 | -16.9190| 0.3727  |
| 2    | 0.1254 | -7.3597 | 0.8705  | 0.1615 | -7.6191 | 0.8705  |
| 3    | 0.0671 | -0.3273 | 0.0708  | 0.0941 | 0.3373  | 0.0708  |
| 4-5  | 0.0012 | -1.3095 | 0.1084  | 0.0005 | -0.1635 | 0.1084  |
| 0-5  | 18.20  | -48.83  | 2.00    | 14.85  | -43.87  | 2.00    |

Table 2. The comparison of ground state binding energies per nucleon (MeV) and RMS radius (fm) of $^4He$, $^{12}C$, $^{16}O$ and $^{40}Ca$ nuclei with different models and experimental data. Note that some of the methods have included the TNI contributions (the star after the value of RMS radius means ”charge radius”).

|         | $^4He$   | $^{12}C$  | $^{16}O$  | $^{40}Ca$ |
|---------|----------|-----------|-----------|-----------|
|         | $BE$ / $A$ | $< r >$  | $BE$ / $A$ | $< r >$  | $BE$ / $A$ | $< r >$  |
| CCM – FBHF3,[35] | -5.75 | 1.63* | -5.36 | 2.57* | -5.64 | 3.17* |
| CCM,[15] | -7.3 | 2.1 | -8.8 | 1.7 | -12.5 | 1.7 |
| CMC,[3-11] | -7.6 | — | -7.7 | — | — | — |
| GFMC,[3-11] | -7.07 | — | -7.7 | — | — | — |
| CBF – FHNC,[36] | — | — | — | — | — | — |
| CBF – FHNC,[37] | — | — | — | — | — | — |
| BHF,[39] | — | — | — | — | — | — |
| BHF,[40] | -6.85 | 1.69* | -8.26 | 2.59* | -9.53 | 3.22* |
| FMD,[41] | -6.99 | 1.51* | -7.40 | 2.25* | -8.19 | 2.89* |
| HF, RPA(A) – MBPT,[42] | -8.90 | — | -9.75 | — | -10.10 | — |
| HF, RPA(B) – MBPT,[42] | -7.90 | — | -8.75 | — | -9.30 | — |
| NCSM,[12-14] | -7.18 | 1.44 | -7.5 | 2.2 | — | — |
| LOCV,[20, 21] | -4.19 | 1.77 | -2.78 | 2.41 | -5.28 | 2.46 | -7.30 | 3.04 |
| LOCV,[20, 21] | -3.21 | 1.77 | -0.44 | 2.41 | -4.49 | 2.68 | -6.97 | 2.94 |
| LOCV, [present($J_{\text{max}} = 2$)] | -4.60 | 1.75 | -3.03 | 2.41 | -5.66 | 2.46 | -7.98 | 3.39 |
| LOCV, [present($J_{\text{max}} = 5$)] | -3.53 | 1.75 | -1.6 | 2.37 | -4.19 | 2.38 | -5.84 | 2.94 |
| Experimental | -7.08 | 1.63 | -7.68 | 2.41 | -7.98 | 2.65 | -8.55 | 3.39 |