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BINDING ENERGY AND SINGLE-PARTICLE ENERGIES IN THE ^{16}O REGION

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Abstract

In this paper we present the binding energy of ^{16}O together with single-particle energies in the oxygen region by folding together a Hamiltonian in the rest-frame of the nucleus with two-body correlation functions based on the Nijmegen potential. We have found that the binding energies are very sensitive to the core radius r_c and that the effects of tensor correlations are non-negligible.Our calculated binding energy, E_B = - 127.8 MeV with r_c = 0.241 fm compares well with the experimental binding energy, E_B = - 127.6 MeV.

Keywords: Effective interactions, correlation functions, single-particle energies, binding energy.

1. Introduction

The study of nuclear properties from the fundamental nucleon – nucleon interaction has offered a formidable challenge to researchers over the years.

One example of such a challenge has been the calculation of effective interactions as input to the shell model or to the optical model. The calculation of effective interactions for the shell model starts from a suitable one- and two-body effective interactions and the approach usually is to consider all (or some) of the two-body matrix elements of the effective two-body interaction as free parameters to be adjusted empirically to fit experimental results [1]. The one-body effective interaction denoting the single-particle energies are usually chosen from the experimental spectrum e.g. of ^{17}O with respect to the core of ^{16}O.

For the calculation of these quantities no shell model calculation has so far done a satisfactory job of using quantities defined from just one procedure. In most cases, either one chooses the single- particle energies from experiment while the two-body effective interaction is chosen from theory or a combination of a semi-empirical approach where all the above theoretical quantities are adjusted to fit experimental data. Over the years, most researchers have paid more attention to the derivation of the two-body quantities while the one-body part (the single-particle energies) have usually been extracted form experiment as discussed above thereby lacking in good theoretical understanding.

It is the belief of the present authors that if one wishes to gain a complete understanding of a quantum many-body system such as the nucleus, then one should seek to understand all the above quantities from a microscopic theory before going over to other correction such as the inclusion of three- or four-body forces.

Recently, we have shown [2] that the single-particle energies could indeed be calculated quite accurately from the fundamental nucleon-nucleon force based on the

method of lowest order constrained variational (LOCV) approach. However, the two-body nucleon-nucleon interaction used in that work was the Reid [3] potential which is rather old as its derivation was based on old and erroneous phase shifts data [4]. Thus, calculations based on the Reid [3] potential should be updated to take into account more accurate phase shifts data in the various partial wave components, hence the need to update our earlier calculation reported in Ref. [2]. The present paper is divided as follows: In Section 2 we give a summary of the method of how we defined our two-body effective interaction for the shell model and then give expressions for evaluating the single-particle energies and binding energies. In Section 3 the results of the binding energy and the single-particle energies have been given. Section 4 deals with summary and conclusion of the paper.

2. Definition of the Nuclear Effective Interaction

In the formulation of the nuclear effective interactions, there are usually two steps to undertake: the first step is to write the Hamiltonian in the rest-frame of the nucleus as [5]:

$$H = \sum_i {p_i^2}/{2m} + \sum_{i>j} V_{ij} \rightarrow H' = \sum_{ij}\left({p_{ij}^2}/{M} + V_{ij} \right) \tag{1}$$

where the relative momentum of the two-particle system is defined by $\mathbf{p}_{ij} = (1/\sqrt{2})(\mathbf{p}_i - \mathbf{p}_j)$ and M = Am is the total mass of the nucleus while V_{ij} is the Nijgement potential [4]. The next step is to define an effective two-body Hamiltonian in the form [6,7]

$$H_{eff}^{(2)} = \sum_{k,i>j} f_2^{\,k}(ij)\left({p_{ij}^2}/{M} + V_{ij} \right) f_2^{\,k}(ij) \equiv h_{ij} \tag{2}$$

where the $f_2^{\,k}(ij)$ are the two-body correlation operators and k is a summation over all the reaction channels.

Previous studies regarding nuclear matter [6,7] and finite nuclei [5,8] have indicated three main features for two-body correlation functions: They can be summarised as: (a) the tensor correlations, (b) the 'wound' induced in the two-body wave function by the repulsive core of the N-N interaction, and (c) the meson-exchange corrections. It was however found that the most important of these features was the tensor correlations. Therefore our two-body correlation functions have been parameterised as [8,2]:

$$\begin{aligned} f_2^{\,k}(ij) &= 0, && r < r_c \\ &= (1 - e^{-\beta(r_{ij} - r_c)^2})(1 + \alpha^k S_{ij}), && r \geq r_c \end{aligned} \tag{3}$$

where r_c = 0.25fm and β = 25fm^{-2}. The parameter, α^k defines the strength of the tensor correlations and is non-zero only in the $^3S_1$ - $^3D_1$ channel. The S_{ij} appearing in equation (3) stands for the usual tensor operator.

Following an earlier procedure, the binding energy of a nucleus may be expressed as [9]:

$$E_c = \sum_{i \geq j} \sum_{JT} (2J+1)(2T+1)\langle (ij)JT|h|(ij)JT\rangle_{AS} \tag{4}$$

where i, j are the core state orbitals whereas the angular momentum J and isospin J are formed by the vector coupling of states i and j. The quantity, $\langle (ij)JT|h|(ij)JT\rangle_{AS}$ is obtained from the general expression for evaluating two-body matrix elements as [2,10]:

$$\langle (ab)JT|h|(cd)JT\rangle_{AS} = \frac{j_a j_b j_c j_d}{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}} \sum_{\lambda,\lambda',s} \begin{Bmatrix} l_a & l_b & \lambda \\ \frac{1}{2} & \frac{1}{2} & s \\ j_a & j_b & J \end{Bmatrix} \begin{Bmatrix} l_c & l_d & \lambda' \\ \frac{1}{2} & \frac{1}{2} & s \\ j_c & j_d & J \end{Bmatrix} X$$

$$\sum_{n\ln'l'NL} s^2 \lambda^2 \lambda'^2 (-1)^{\lambda+\lambda'+l+l'} \langle nl, NL; \lambda | n_a l_a, n_b l_b; \lambda \rangle \langle n'l', NL; \lambda' | n_c l_c, n_d l_d; \lambda' \rangle X$$

$$\{1-(-1)^{l+s+T}\} \sum_g g^2 \begin{Bmatrix} l & s & g \\ J & L & \lambda \end{Bmatrix} \begin{Bmatrix} l' & s & g \\ J & L & \lambda' \end{Bmatrix} \langle n(ls)g;T|h|n'(l's)g;T\rangle . \tag{5}$$

In equation (5) two particles in the orbits a and b with single - particle quantum numbers, $n_a(l_a \frac{1}{2})j_a$ and $n_b(l_b \frac{1}{2})j_b$, respectively couple their spins to the total angular momentum J and isospin T. The quantity λ stands for the vector coupling of l_a and l_b while g is formed by the vector coupling of the relative angular momentum l and the spin s. We here define $a = \sqrt{(2a+1)}$.

$$\begin{Bmatrix} o & p & q \\ r & s & t \\ u & v & w \end{Bmatrix}$$

denotes the usual $9j$ symbol while

$$\begin{Bmatrix} i & j & k \\ l & m & n \end{Bmatrix}$$

is a $6j$ symbol. The term, $\langle nl, NL; \lambda | n_a l_a, n_b l_b; \lambda \rangle$ stand for the usual Brody – Moshinky transformation brackets [11] which separate the relative (nl) coordinates from the centre of mass (NL) coordinates.
On the other hand, the single - particle energies were derived as [2]:

$$\varepsilon_j = \sum_{iJT} \frac{(2J+1)(2T+1)}{2(2j+1)} (2J+1)(2T+1)\langle (ij)JT|h|(ij)JT\rangle_{AS} . \tag{6}$$

The matrix elements of equations (4) and (6) were evaluated in a harmonic oscillator basis. Only two free parameters are present, (a) the oscillator size parameter, b = $\sqrt{((m\omega)/\hbar)}$ contained in the harmonic oscillator wave function and (b) the strength of the tensor correlation α^k.

3. Results of binding energy and single - particle energies

Table 1 shows our calculated binding energy for ^{16}O as a function of the core radius r_c for $\alpha^k = 0.06$ and $\hbar\omega = 14.0$ MeV suitable for the A = 16 system. By choosing the

Table 1. Calculated binding energy BE (in MeV) of ^{16}O as a function of the core radius r_c. Calculation parameters are: $\alpha^k = 0.06$, $\hbar\omega = 14.0$ MeV.

r_c (fm)	0.05	0.10	0.15	0.20	0.24	0.241	0.25	0.30
BE (MeV)	5.79	-31.1	-68.72	-103.29	-127.25	-127.80	-132.61	-155.13

0.35	0.40	0.45	0.50
-169.96	-176.79	-175.81	-167.59

various values of the core radius r_c , we found that we could only reproduce the binding of ^{16}O if r_c was equal to 0.241fm, giving us the calculated binding energy of –127.8 MeV . Higher values of r_c gave us too much binding and lower values of r_c gave us under binding. From this analysis it is clear that a suitable core radius r_c , must be found while using potentials of the Reid – type such as the Nijgemen potential [4] in LOCV calculations. In our earlier calculations with the Reid [3] potential, we had used r_c = 0.25 fm which as can be seen is very close to the value used in the present calculation.

Indeed, similar results on the binding energy of ^{16}O could be found for other values of α^k lying in the range $0.05 \leq \alpha^k \leq 0.08$ corresponding to our earlier range in previous investigations [6]. We have however chosen the above representative sample because the r_c that reproduced the binding energy of ^{16}O is similar to that used in our earlier calculations which makes it easier to compare results. We expect the choice of the optimised values of r_c and α^k to depend on the details of the nucleon – nucleon potential used and the constraints imposed on the convergence parameter, k, used in judging the convergence of the cluster expansion. For these reasons we shall await a further investigation of the above points raised which involve the inclusion of other nucleon – nucleon potentials and a study on the convergence criteria of the cluster expansion, hence we can consider the parameters used in the present study as preliminary.

Having optimised our preliminary parameters by reproducing the binding energy of ^{16}O with the above procedure, we now present the results of the single - particle energies in the oxygen region by using equation (6) following our earlier procedure found in Ref. [2]. We used the same parameters as those described above for the binding energy of ^{16}O .

It should be noted that the sum, i in equation (6) is over all the diagonal matrix elements and as observed earlier by Irvine and co-workers [12], there is an ambiguity in fitting the two-body diagonal matrix elements. This means that the calculated

single - particle energies and two-body energies could differ from their experimental counterparts only by a constant shift.
In Table 2 we apply a constant shift of -Δ (MeV) to all the single-particle energies in the form

$$\varepsilon'_j = \varepsilon_j \pm \Delta \approx \varepsilon_j^{(expt)} \quad (9)$$

Here also we find like in our earlier paper [2] that a constant shift of Δ = −17.3 MeV applied to all the single - particle energies, ε_j can bring all the calculated single - particle energies close to their experimental counterparts also listed in Table 2. This analysis confirms our earlier calculations. The determination of Δ from a theoretical approach is still an open challenge. Note that in Table 2, the d-shell spin-orbit

Table 2. Calculated single-particle energies, d-shell spin-orbit splitting, and the sd-shell splitting for ^{16}O for $\alpha^k = 0.06$, $\cong\omega = 14.0$ MeV.

	Δ (MeV)	$\varepsilon'_{0d_{3/2}}$	$\varepsilon'_{1s_{1/2}}$	$\varepsilon'_{0d_{5/2}}$	$\varepsilon_{0d_{3/2}} - \varepsilon_{0d_{5/2}}$	$\varepsilon_{1s_{1/2}} - \varepsilon_{0d_{5/2}}$
Present	-17.3	0.84	-3.17	-4.14	5.66	1.64
Expt.[13]	-	0.95	-3.27	-4.82	5.09	0.87
Ref. [13]	-	2.555	-3.017	-3.238	5.793	0.221

splitting and the sd-shell splitting were calculated directly from the calculated single – particle energies, ε_j.

It should however be noted that a shift to all the single - particle energies such as is made here will not affect the spectroscopy of nuclei under question but will only affect the relative binding energies of the different isobaric states.

4. Summary and conclusion

In this paper we have calculated the binding energy of ^{16}O by folding together a Hamiltonian in the rest – frame of the nucleus based on two-body correlation functions which take into account the short – range repulsion and the tensor component in the Nijgemen potential. By choosing $\alpha^k = 0.06$, $\cong\omega = 14.0$ MeV and $r_c = 0.241$ fm we obtained the calculated binding energy of ^{16}O as, $E_B = -127.8$ MeV which is in excellent agreement with the experimental binding energy of $E_B = -127.6$ MeV.
Having optimised our parameters with the above calculations, we next calculated the single-particle energies in the oxygen region which are shown in Table 2. The results show that our single - particle energies are in a reasonably good agreement with their experimental counterparts if we make a constant shift of – 17.3 MeV to all the single - particle energies. These results should also be compared with the theoretical attempt on single – particle energies made by Maglione and Ferreira using the G-matrix approach [13].
As remarked earlier, the choice of the parameters α^k and r_c may depend on the details of the nucleon – nucleon potential used and the constraints imposed on the convergence parameter, k, used in judging the convergence of the cluster expansion.

Thus, while still awaiting further analyses on constraints on these parameters, our present results seem very promising.
It will therefore be interesting to see the results of shell-model calculations obtained with the single-particle energies derived in this procedure together with the corresponding two-body matrix elements. In this way, structure of nuclei could be understood in a fully microscopic procedure. We hope to carry out further research in that direction.

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