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A review of ^{20}Ne structure in a full microscopic self-consistent shell–model calculation with tensor correlations

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Abstract

A set of single-particle energies together with a set of two-body matrix- elements derived in a self –consistent manner from the Reid soft–core potential are used to calculate the energy levels of ^{20}Ne. We used a harmonic oscillator wave function folded with two-body correlation functions in our calculation. It is found that the calculated spectra agree very well with experiment and the best available shell-model calculations by other workers. As a result we have demonstrated that it is possible to calculate the spectroscopy of nuclei microscopically and self-consistently in such a way that both the single –particle energies and the effective two-body interactions are derived from the same procedure.

Keywords: single-particle energies, shell-model, two-body correlation functions, effective two-body interactions.

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1.0 Introduction

One of the greatest achievements of the shell model has been its ability to predict energy levels of nuclei and other unclear quantities such as electromagnetic properties. It has however, been difficult to have a single self-consistent approach in the determination of the input data to the shell-model calculations. These input data consists of a set of single-particle energies on the one hand and a set of two-body matrix elements on the other. One very popular approach in the determination of these quantities is the empirical method where the set of single-particle energies together with the set of effective two-body interactions previously determined from realistic forces are treated as free parameters. These are then adjusted until they fit the experimental spectrum. This approach has been studied extensively by Wildenthal [1] and has produced very popular effective interactions. Another approach is to insist on the original two-body effective interaction derived from realistic forces try to include those quantities missing in the theory which might hopefully improve the data. This approach pioneered by Kuo and Brown [2], Irvine and co-workers [3] etc, has been popular over the years because it gives further room for the understanding of nuclear data in terms of the effective interaction in a fundamental way. While each of these approaches has their own merits, they notoriously lack self-consistency in approach. For example, in the empirical approach once the two-body matrix elements and single-particle energies are adjusted to fit experimental data, they loose their original meaning. The two-body effective interaction and the set of single-particle energies that emerge are quite different from their original counterparts. On the other hand, most microscopic calculations would insist on retaining most of the features of the microscopic two-body effective interactions but then their single-particle energies are usually computed from experimental data [4]. It is not at all clear if this method is truly microscopic in approach since the two quantities are determined from different considerations. Some years ago, we generated a simple mass-dependent effective nucleon interaction by folding together a Hamiltonian for the rest-frame of the nucleus based on the Reid [5] soft-core potential with a simple set of two-body correlation functions [6]. We then compared this interaction with the universal *sd*-shell interaction of Wildenthal [1] and found excellent agreement. Recently [7], we used the same effective interaction to derive a set of mass- dependent single-particle energies for sd shell–model calculations. Our aim was to demonstrate that, if ^{16}O is taken as a closed shell-core for *sd* shell-model calculations as is

usually the case, then it is possible to obtain single-particle energies across the whole of the *sd* shell which are very similar to those derived at the beginning of the shell. In doing so we hope demonstrate that shell-model calculations can be done self-consistently with reasonable level of success with a suitable choice of these quantities.

The aim of this paper is to use this two-body interaction together with the set of single-particle energies of [7] to determine energy spectra of ^{20}Ne nuclei in a self-consistent manner. In doing so we hope to demonstrate that shell-model calculations can be done self consistently with a reasonable level of success with a suitable choice of these quantities. This paper is organised as follows: in Section 2 we give a summary of the method used. In section 3 we present the results of the single–particle energies, the two body effective interaction used and compare our calculated energy spectra with experiment other works on ^{20}Ne nuclei. Section 4 is devoted to the conclusion of the paper

2.0 **The shell-model effective interaction**

In this section we briefly discuss the approach developed in [6,7] for the determination of the one– and two-body effective interactions. The non- relativistic Hamiltonian for an A-nucleon system approximated as

$$H_o = \sum_i \frac{p^2}{2m} + \sum_{i>i} V_N(\vec{r}_i - \vec{r}_j). \tag{2.1}$$

where $V_N(\vec{r}_i - \vec{r}_j)$ is the NN potential and m is the nucleon mass. The NN potential of equation (2.1) as is usually the case has a large repulsive component, which makes it impossible to perform direct Hartree-Fock calculations. In the language of correlated basis functions, the Hartree-Fock trial wave function:

$$\Phi = (A!)^{-1/2} \det \phi_i(\vec{r}_j) \tag{2.2}$$

must be correlated in the form

$$\Psi = F\Phi \tag{2.3}$$

where the ϕ_i are the single-particle basis functions and *F* is a symmetric product of two-body correlation functions [8]:

$$F = S\prod_{ij} f_{ij}. \tag{2.4}$$

these correlations were designed to account for the effect of the strong repulsive component of the nucleon-nucleon interaction while *S* is the symmetrizer operator. We next require that our chosen Hamiltonian be formulated in the rest-frame of the nucleus since we are only interested in intrinsic quantities. This is achieved through a unitary transformation [3] and the transformed Hamiltonian becomes:

$$H_o \to \bar{H} = H - \frac{p^2}{2M} = \sum_{i>j}\left(\frac{p_{ij}^2}{M + V_N(\rho_i - \rho_j)}\right) \tag{2.5}$$

where $M = m_N A$ is the total mass of the nucleus, $\frac{P^2}{2M}$ is the transnational kinetic energy of the centre of mass of the nucleus, $\vec{p}_{ij} = \frac{1}{\sqrt{2}}(\rho_{ij} - \rho_j)$ is the relative momentum of the two interacting pair while $V_N(\rho_i - \rho_j)$ is taken to be the Reid [5] soft-core potential. The shell-model calculations are usually performed in a finite model space since it is impossible to determine the many-body energy operator of equation (2.5) exactly. The usual approach is to approximate it to two-body effective interactions. Using equations (2.3) and (2.4) we can define our effective two–body interaction in the form (Fiase et al., [9]):

$$H_{eff}^{(2)} = \sum_{i>j}(f_2(ij)\left(\frac{p_{ij}^2}{M + V_{ij}}\right) f_2(ij) \tag{2.6}$$

where $f_2(ij)$ are the two-body correlation operators. In those calculations it was required that the two-body correlation functions should take on the features of the chosen potential used, which in our calculation was the Reid [5] soft-core potential. Since the Reid [5] potential has the form

$$V_{ij} = \sum_{\lambda} V_{ij}^{\lambda} \tag{2.7}$$

where in the different reaction channels λ we have the central, spin-orbit and tensor components, it seems reasonable to allow the correlation operators the same degree of freedom, i.e .,

$$f_2(ij) = \sum_{\lambda} f_{ij}^{\lambda} \tag{2.8}$$

where
$$f_{ij}^{\lambda} = f_c^{\lambda}(r_{ij}) + f_{LS}^{\lambda}(r_{ij})\vec{L}.\vec{S} + f_T^{\lambda}(r_{ij})S_{ij} \tag{2.9}$$

In studies regarding nuclear matter and finite nuclei Irvine et al., [3] found three main features of the two-body correlation functions. There were (i) the 'wound induced in the two-body wave function by the repulsive core

of the N-N interaction, (ii) the tensor correlations especially in the $^3S_1$ - $^3D_1$ channel and, (iii) the meson exchange correction. It was found that the most important feature of these was the tensor correlations and Irvine et al.[3] parameterized the two-body correlation function in the form [3]:

$$\begin{aligned} f_2(ij) &= 0, \quad r_{ij} < r_c \\ f_2(ij) &= (1 - e^{-\beta(r_{ij} - r_c)^2})(1 + \alpha^{\lambda} S_{ij}), \quad r_{ij} \geq r_c \end{aligned} \tag{2.10}$$

where $r_c = 0.25fm$ and $\beta = 25fm^{-2}$ .the parameter, α^{λ} represents the strength of the tensor correlation and is non-zero only in the $^3S_1$ - $^3D_1$ channel. The two-body matrix elements of the effective Hamiltonian defined in equation (2.6) were calculated in a harmonic oscillator basis. The general expression for evaluating the two-body matrix elements:

$$< (ab) JT | H_{eff}^{(2)} | (cd) JT > AS \tag{2.11}$$

is reported in [4,7].

Furthermore one can calculate the single-particle energies from the same interaction according to the equation [9,10]:

$$\in_l = \sum_{kJT} \frac{(2T+1)(2J+1)}{2(2l+1)} < (kl) JT | H_{eff}^{(2)} | (kl) JT > AS, \tag{2.12}$$

where in this equation the sum k, is limited to the core states and *l* to the valance space orbitals. In our calculations of equations (2.8) and (2.9) there are only two free parameters. These are the oscillator size parameter and the strength of the tensor correlation, α^{λ}. We varied these to obtain the best set of the one- and two-body effective interactions to calculate the ^{20}Ne spectra.

3.0 **The Results**

The two-body effective interactions defined in equation (2.11) and the set of single-particle energies defined in equation (2.12) were calculated in a harmonic oscillator basis as reported in [6,7]. As discussed earlier we had only two free parameters, which are, the strength of the tensor correlations and the oscillator size parameter. In our calculations our 'best' set of data for calculating the two-body matrix elements of A = 20 system are $\eta\omega$ = 12*MeV* and α = 0.085. These were determined by comparing our two-body matrix elements with those of the fitting routines of Chung and Wildenthal [11] and the Wildenthal [1] universal sd-shell interaction. We used the variance, χ_F, defined by

$$\chi_F = \sum_i \frac{(ME_F(i) - ME_c(i))^2}{ME_F(i)^2} \tag{3.1}$$

where ME_F (*i*) and *MEc* (*i*) are the fitted and our calculated two-body matrix elements respectively. We found in our earlier calculations that in order to obtain a good level of agreement between the two sets of data, a constant shift, Δ_{sd} had to be applied to all the 28 diagonal matrix elements while keeping all the 35 non-diagonal matrix elements the same. Such a shift was found to vary smoothly with the variance and reaches a minimum as shown in Figure 1 where the same is plotted for the A = 20 system. For this case we obtained the minimum variance of ≈ 0.03 for the shift in energy of 1.5 *MeV* to all the diagonal matrix

elements. This shows an excellent level of agreement between the two sets of data. This procedure was repeated for other combinations of these parameters but the "best" parameters turned out to be the chosen set above. Such a shift as shown earlier will not change the spectroscopy of any isobaric states except their relative binding energies. Using similar arguments as above, the single-particle energies defined in equation (2.12) were calculated for $\alpha = 0.085 \, and \, \eta\omega = 12 MeV$ and an optimum constant shift applied to all of them to obtain their optimum values presented in Table 1. These values are not in very good agreement with experiment but if we use $\eta\omega = 13 MeV$ which is more appropriate for this region of nuclei and $\alpha = 0.085$, the optimized calculated single-particle energies turn out to be in very good agreement with experiment. These are the values later used in our calculation.

In Figure 2, we present the experimental [12] positive parity states of ^{20}Ne together with the result of a straight shell- model calculation using our interaction and the universal sd-shell (USD) effective interaction of Widenthal [1]. A state is denoted by J^{π}_{i}; T where J denotes the total angular momentum of the two-particle system while T is their corresponding isospin. From the figure we see that the first four experimental levels 0^{+}_{1}; 0, 2^{+}_{1}; 0, 4^{+}_{1};0 *and* 0^{+}_{2}; 0 at energies of 0.0, 1.63 4.25 and 6.73 *MeV* respectively are well reproduced by

our interaction, which predicts them at 0.0, 1.66, 3.82 and 5.92 *MeV* respectively. The experimental states 0^{+}_{3}; 0, 2^{+}_{3}; 0, 0^{+}_{4}; 0 *and* 2^{+}_{4}; 0 appearing at energies, 7.19, 7.83, 8.30 and 9.0 *MeV* are intruder state [13, 14, 15] and cannot be reproduced in a calculation that considers ^{16}O as a closed-shell core so we did not expect to see them in our calculation. Our calculated 6^{+}_{1}; 0 appears at an energy of 7.89 *MeV* compared to its experimental counterpart at 8.78 *MeV*. The calculated 6^{+}_{1}; 0 state in question actually reverses order with our calculated 2^{+}_{2}; 0 , which appears at an energy of 8.21 *MeV*, the order which the USD interaction has maintained with experiment. The next experimental 4^{+}_{2}; 0 state at an energy of 9.03 *MeV* is an intruder state [13.14,15]. However the next experimental 2^{+}_{5}; 0 state at an energy of 9.48 MeV and the experimental 4^{+}_{3};0 at an energy of 9.99 *MeV* are well reproduced by our calculation which puts them at 10.2 and 9.97 *MeV* respectively. It is interesting to note that the USD interaction also predicts the 4^{+}_{3};0 experiment state at an energy of 9.97 *MeV* in our calculation. Beyond the 10 *MeV* energy mark there is no one to one correspondence between our calculated energy levels and experiment. This is also the case with the USD interaction. In fact we went further to calculate the density of states above the 10 *MeV* mark and found them to be similar both with experiment and the USD interaction, although our calculated spectra is slightly more compressed compared to the USD interaction and experiment. This fact has also been observed in [4] concerning forces with strong tensor components which the Reid [5] NN forces belongs. Our calculation shows however, that we can confirm about 8 states in ^{20}Ne below 10 *MeV* mark, which are shell–model states.

4.0 **Conclusions**

We have calculated the energy spectra of ^{20}Ne with the aim to show that shell-model calculations can be performed self-consistently when both effective two-body interactions and the single-particle energies are derived microscopically in a self-consistent manner. This approach allows us to predict nuclear properties in a fundamental way. This is in contrast to the other methods like the empirical approaches which start with an assumed set of parameters and then optimize them to fit experimental data. In most microscopic shell- model calculations, the set of two-body effective interactions are derived microscopically but the set of single –particle energies are extracted from experiment [4]. The ^{20}Ne, which has been chosen as an example for our investigation, may rather be a trivial example of a shell-model calculation [16]. Indeed several successful shell-model calculations on ^{20}Ne have been performed including core breaking [14]. Here we have not engaged in detailed comparison including core breaking in our analysis. In fact our approach is designed to ask the question: Is it possible to determine nuclear properties form a completely microscopic self-consistent shell-model approach? Our modest attempt gives the answer

in affirmative and as such being a first principle approach to the shell-model calculation we do not consider the example trivial.

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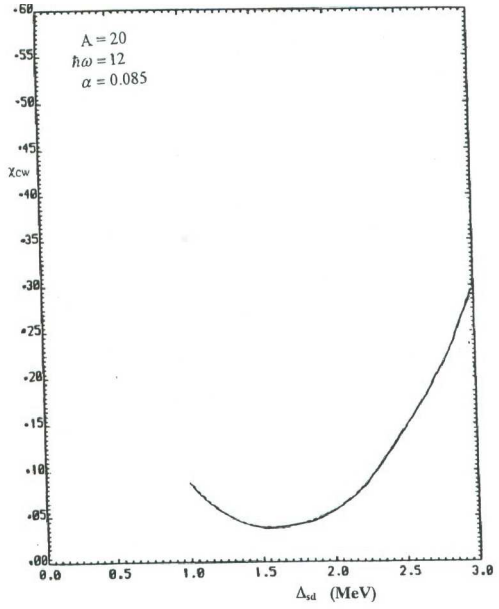
Table 1: Optimized single–particle energies for A= 20 system, for α = 0.085 and $\eta\omega$ = 12*MeV* and α = 0.085 and $\eta\omega$ = 13*MeV*.

α	$\eta\omega$	A	$\varepsilon_{1/2}$	$\varepsilon_{3/2}$	$\varepsilon_{5/2}$
0.085	2*MeV*	20	-270	0.55	-3.35
0.085	13*MeV*	20	-3.13	0.86	-4.86
		Expt.	-3.27	0.95	-4.14

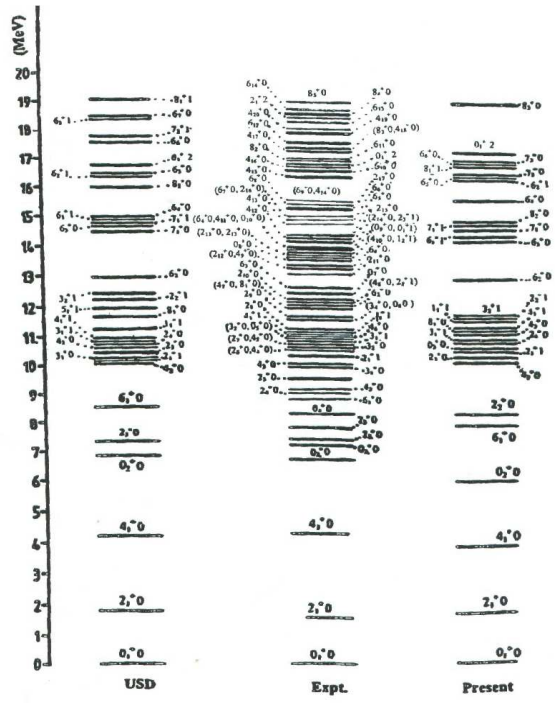
Notice the close agreement with their experimental counterparts especially for the second set of parameters.

Figure 1: Calculated variance with shift in two-body matrix elements, Δ_{sd} , for A = 20 system: α = 0.085 and $\eta\omega$ = 12*MeV*.



Notice the smooth variation of the variance with shift in energy.

Figure 2: Calculated energy spectra of ^{20}Ne nuclei compared with experiment and USD interaction of Wildenthal for α = 0.085 and $\eta\omega$ = 13*MeV*.



Single-particle energies used for the set $\alpha = 0.085$ and $\eta\omega = 13MeV$.

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