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Single particle spectra based on modern effective interactions

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Abstract

The self-consistent Green's function method is applied to ^{16}O using a G-matrix and V_{UCOM} as effective interactions, both derived from the Argonne v_{18} potential. The present calculations are performed in a larger model space than previously possible. The experimental single particle spectra obtained with the G-matrix are essentially independent of the oscillator length of the basis. The results shows that V_{UCOM} better reproduces spin–orbit splittings but tends to overestimate the gap at the Fermi energy.
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A fundamental problem in nuclear physics is how to obtain descriptions of finite nuclei starting from a microscopic nuclear Hamiltonian. Much progress has been achieved for few body systems. The Green's function Monte Carlo [1] technique is able to give exact results up to $A = 12$, while the no-core shell model [2] has been applied to even larger nuclei. A wide range of exact methods is also available for very light systems [3]. In general, it has been found that both two- and three-nucleon (2N and 3N) forces are required to reproduce the experimental observations. Other recent attempts to push the limits of ab initio methods into the medium mass region have focused on the nucleus of ^{16}O and its neighbor isotopes [4,5]. These works computed separation energies and spin orbit splittings of the orbits near the Fermi level. Coupled cluster theory appears to produce converged results for these nuclei [6]. These achievements have been possible by computing the contributions of long-range correlations (LRC) directly within very large models spaces where, however, one still needs to employ a proper effective interaction that accounts for the excluded degrees of freedom. In particular the effects due to short-range correlations (SRC) can be separated efficiently by such partitioning procedure, since they are characterized by high momenta degrees freedom [7].

Several ab initio methods employ similar partitioning techniques. Typically, two classes of microscopic approaches are possible to derive an effective interaction from a realistic nucleon–nucleon force [8]. Bloch–Horowitz theory makes use of the Feshbach projection formalism to devise an energy dependent interaction [9,10]. This gives solutions for every eigenstate with nonzero projection onto the model space, however, the energy dependence severely complicates the calculations. The G-matrix interaction [11], obtained by solving the Bethe–Goldstone equation, is also energy dependent. Alternatively, one can employ a proper unitary transformation to map a finite set of solutions of the initial Hamiltonian into states belonging to a numerically tractable space. In this case, one has the advantage to work with an energy independent interaction. Examples of such approaches are the Lee–Suzuki method [12] and the unitary correlator operator method (UCOM) [13–15]. The UCOM formalism is such that one can apply the inverse transformation to reinsert SRC into the nuclear wave function. A discussion of the similarities and differences between Lee–Suzuki and Bloch–Horowitz is given in Ref. [8]. Differently, one can derive a low momentum force, indicated as $V_{\text{low-}k}$

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[16], by using the renormalization group or the Lee–Suzuki method [8]. It should be noted that both $V_{\text{low-}k}$, and V_{UCOM} are phase shift equivalent at low energy and can be regarded as bare realistic interactions in this regime. The above methods, in principle, generate effective many-nucleon forces in addition to the 2N interactions and the intrinsic 3N ones. In practice, however, in calculating medium and large nuclei one wish to avoid as much as possible these complications, possibly by choosing interactions and model spaces that require weak overall 3N terms. It is therefore important to investigate how truncating to a 2N Hamiltonian affects the results for the different approaches outlined above.

In Ref. [17] we proposed to employ a set of Faddeev equations within the self-consistent Green's function (SCGF) approach [7] to obtain a microscopic description of LRC. This allows to couple simultaneously quasiparticles (qp) and quasiholes (qh) to both particle–hole (ph) and particle–particle/hole–hole (pp/hh) collective excitations. The latter are eventually also expressed in terms of dressed qp and qh modes. Such formalism was later applied to ^{16}O to investigate mechanisms that could possibly quench the spectroscopic factors of mean field orbits [18]. These calculations were already performed in a no-core fashion. However, the model space employed was still somewhat limited and phenomenological corrections were applied to tune the values of specific single particle (sp) energies (doing this allows studying correlations by artificially suppressing the couplings among selected excitation modes). Note that here and in the following we use the terms *sp energies* and *sp spectra* to refer to the poles of the one-body Green's function (defined below Eq. (1)). These represent the excitation energies of the $A\pm1$ neighbor nuclei, which are observable quantities. In this Letter the calculations of Ref. [18] are repeated by avoiding any phenomenology and employing a large model space. We discuss the results of 2N interactions belonging to the two types discussed above, namely a standard G-matrix and V_{UCOM}.

We consider the calculation of the sp Green's function

$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}_\alpha^n)^* \mathcal{X}_\beta^n}{\omega - \varepsilon_n^+ + i\eta} + \sum_k \frac{\mathcal{Y}_\alpha^k (\mathcal{Y}_\beta^k)^*}{\omega - \varepsilon_k^- - i\eta}, \tag{1}$$

from which both the one-hole and one-particle spectral functions, for the removal and addition of a nucleon, can be extracted. In Eq. (1), $\mathcal{X}_\alpha^n = \langle \Psi_n^{A+1} | c_\alpha^\dagger | \Psi_0^A \rangle$ ($\mathcal{Y}_\alpha^k = \langle \Psi_k^{A-1} | c_\alpha | \Psi_0^A \rangle$) are the spectroscopic amplitudes for the excited states of a system with $A+1$ ($A-1$) particles and the poles $\varepsilon_n^+ = E_n^{A+1} - E_0^A$ ($\varepsilon_k^- = E_0^A - E_k^{A-1}$) correspond to the excitation energies with respect to the A-body ground state. The one-body Green's function can be computed by solving the Dyson equation [19,20],

$$g_{\alpha\beta}(\omega) = g^0_{\alpha\beta}(\omega) + \sum_{\gamma\delta} g^0_{\alpha\gamma}(\omega) \Sigma^\star_{\gamma\delta}(\omega) g_{\delta\beta}(\omega), \tag{2}$$

where the irreducible self-energy $\Sigma^\star_{\gamma\delta}(\omega)$ acts as an effective, energy-dependent, potential that governs the single particle behavior of the system. The self-energy is expanded in a Faddeev series as in Fig. 1. This couples the exact propagator $g_{\alpha\beta}(\omega)$ (which is itself a solution of Eq. (2)) to other phonons in the

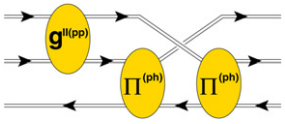

Fig. 1. Example of a Feynman diagram included in the all-order summation generated by the set of Faddeev equations. Double lines represent the dressed one-particle Green's function $g(\omega)$, which propagates quasiparticles (rightward arrows) and quasiholes (leftward arrows). The ellipses propagate collective excitations of the nucleus (Eqs. (3) and (4)).

system [17]. The relevant information regarding ph and pp/hh collective excitations is included in the polarization and the two-particle propagators. Respectively,

$$\begin{aligned} \Pi_{\alpha\beta,\gamma\delta}(\omega) = &\sum_{n\neq 0} \frac{\langle \Psi_0^A | c_\beta^\dagger c_\alpha | \Psi_n^A \rangle \langle \Psi_n^A | c_\gamma^\dagger c_\delta | \Psi_0^A \rangle}{\omega - (E_n^A - E_0^A) + i\eta} \\ &- \sum_{n\neq 0} \frac{\langle \Psi_0^A | c_\gamma^\dagger c_\delta | \Psi_n^A \rangle \langle \Psi_n^A | c_\beta^\dagger c_\alpha | \Psi_0^A \rangle}{\omega - (E_0^A - E_n^A) - i\eta} \end{aligned} \tag{3}$$

and

$$\begin{aligned} g^{\text{II}}_{\alpha\beta,\gamma\delta}(\omega) = &\sum_n \frac{\langle \Psi_0^A | c_\beta c_\alpha | \Psi_n^{A+2} \rangle \langle \Psi_n^{A+2} | c_\gamma^\dagger c_\delta^\dagger | \Psi_0^A \rangle}{\omega - (E_n^{A+2} - E_0^A) + i\eta} \\ &- \sum_k \frac{\langle \Psi_0^A | c_\gamma^\dagger c_\delta^\dagger | \Psi_k^{A-2} \rangle \langle \Psi_k^{A-2} | c_\beta c_\alpha | \Psi_0^A \rangle}{\omega - (E_0^A - E_k^{A-2}) - i\eta}, \end{aligned} \tag{4}$$

which describe the one-body response and the propagation of two-particles/two-holes. In this work, $\Pi(\omega)$ and $g^{\text{II}}(\omega)$ are obtained by solving the dressed RPA (DRPA) equations [21,22], which account for the redistribution of strength in the sp spectral function. Since this information is carried by the correlated propagator $g_{\alpha\beta}(\omega)$, Eq. (2), the SCGF formalism requires an iterative solution. It can be proven that full self-consistency guarantees to satisfy the conservation of the number of particles and other basic quantities [23].

The coupled cluster studies of Refs. [6,24] found that eight major harmonic oscillator shells can be sufficient to obtain converging results for ^{16}O with G-matrix interactions. At the same time, the experience with the calculations of Ref. [18] suggests that high partial waves do not contribute sensibly. In this work, all the orbits of the first eight shells with orbital angular momentum $l \leqslant 4$ were included. Inside this model space a G-matrix and the V_{UCOM} potential were employed as effective interactions. The former was computed using the CENS library routines [11,25]. For the latter, the UCOM matrix-elements code [26] was employed with the constraint $I_\vartheta = 0.09\ \text{fm}^3$. This choice of the UCOM correlator reproduces, in perturbation theory, the binding energies of several nuclei up to ^{208}Pb [27]. In both cases the Argonne v_{18} potential [28] was used as starting interaction. However, we chose to neglect the Coulomb and the other charge independence breaking terms in the present work. The Hartree–Fock (HF) equations (Brueckner–Hartree–Fock (BHF) for the G-matrix) were first solved for the unperturbed propagator $g^{(\text{B})\text{HF}}_{\alpha\beta}(\omega)$, which was employed in the first calculation. After that, the (dressed) solution $g_{\alpha\beta}(\omega)$ was used to generate $\Pi(\omega)$ and $g^{\text{II}}(\omega)$ in DRPA and then to solve

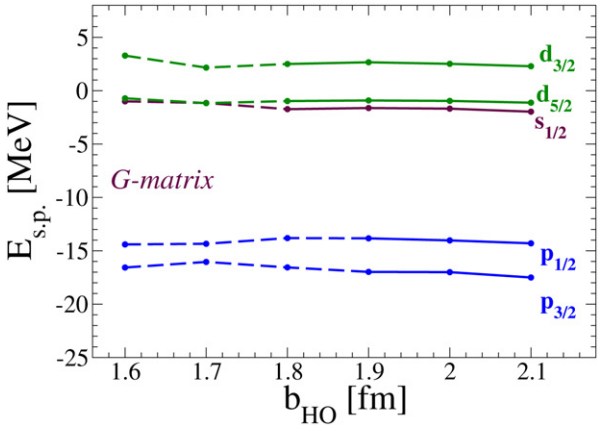

Fig. 2. Single particle spectrum obtained with the G-matrix as a function of the oscillator length. The dashed lines refer to values of b_{HO} for which the solutions are sensible to the number of sp fragments collected, at each iteration, into effective poles of $g_{\alpha\beta}(\omega)$.

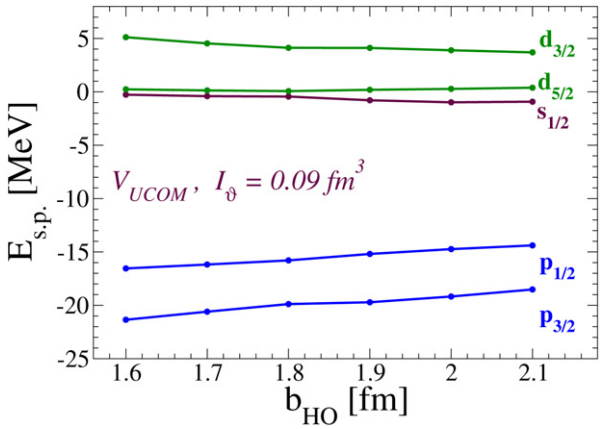

Fig. 3. Self-consistent single particle spectrum obtained with V_{UCOM} as a function of the oscillator length.

the Faddeev equations for an improved self-energy. At each iteration the two most important fragments close to the Fermi level of each partial wave were retained, both in the quasiparticle and the quasihole domains. The remaining strength was collected in few effective poles that correspond to the (B)HF orbitals. Increasing the number of poles that were iterated did not affect sensibly the sp states that will be discussed below, except in the case of the G-matrix with harmonic oscillator length $b_{\mathrm{HO}} \leqslant 1.8$ fm (as discussed below). In the present work, calculations were iterated until reaching convergence (to within 200 keV) for the sp energies nearby the Fermi level. To test the iteration procedure we computed the total number of particles obtained with V_{UCOM}. The first calculation, based on the HF propagator, gives $A = 16.4$ (a 2.5% error). At self-consistency $15.99 < A < 16.02$ (due to numerical errors), showing the adequacy of our approach. As in Ref. [18], the starting energy of the G-matrix was folded exactly in the Hartree–Fock diagram, leading to an energy dependent mean field. This is important for the present study, since a prescription to obtain an interaction independent of the starting energy can lead to an artificial gap at the Fermi surface. In solving the DRPA equations, instead, a fixed starting energy of -25 MeV was chosen. More details on the SCGF/Faddeev formalism and calculations based on it are given in Refs. [7,17,18]. As already noted, however, no phenomenological corrections were applied in the present work.

Calculations have been performed for oscillator lengths in the interval $b_{\mathrm{HO}} = 1.6$–2.1 fm. The sp spectra obtained at self-consistency are shown in Figs. 2 and 3. In the case of a G-matrix, these orbits appear independent, within numerical accuracy, of the oscillator frequency for $b_{\mathrm{HO}} \geqslant 1.9$ fm. Below this the trend is similar. However, the number of relevant poles increases for the $l = 1$ waves in the energy region of $5 \leqslant \varepsilon_p^+ \leqslant 10$ MeV. In this case, the final result becomes dependent on the number of fragments that are iterated rather than being collected in effective poles. Improved iteration algorithms that account for all the relevant low energy strength will allow resolving this issue. Those single particle levels that are not converged with respect to the number of iterated poles are shown, for completeness, by dashed lines in Fig. 2. However, they will not be considered any further in the following. No similar complications were encountered for V_{UCOM} which generates, for each shell, at most one main fragment and a smaller satellite peak near the Fermi energy. The relevant poles of Eq. (1) were therefore iterated exactly. Fig. 3 shows that the spin orbit splittings for this interaction are approximately constant, although the sp energies are not yet independent of the oscillator length. This can be understood considering that these spin orbit partners correspond to particularly simple and similar configurations (one particle or one hole on top of the correlated ground state). Conversely, separation energies are linked to the to total binging energy of neighbor isotopes. Larger model spaces will probably be required for a full convergence with V_{UCOM}.

Table 1
Spin–orbit splittings (in MeV). The experimental values refer to the spectra of ^{17}O/^{15}O [29]

b_{HO}[fm] =	1.6	1.7	1.8	1.9	2.0	2.1	exp.
G-matrix:							
$\Delta E_{p_{1/2}-p_{3/2}}$	–	–	–	3.1	3.1	3.2	6.176
$\Delta E_{d_{3/2}-d_{5/2}}$	–	–	3.5	3.6	3.5	3.4	5.084
V_{UCOM}:							
$\Delta E_{p_{1/2}-p_{3/2}}$	4.7	4.4	4.1	4.5	4.4	4.1	6.176
$\Delta E_{d_{3/2}-d_{5/2}}$	4.9	4.4	4.1	3.9	3.6	3.3	5.084

The splittings obtained from both interactions are reported in Table 1. The $0p$ results obtained with the G-matrix show little dependence of the oscillator length. These are in line with previous Green's function calculations [30] and account for about a half of the experimental value. Better solutions are obtained with the present choice of the UCOM correlator. For the $0d$ orbits the results for the two interactions are more similar to each other but not totally independent of the oscillator length.

Long-range correlations at the level of 2p1h and 2h1p were also considered in Ref. [4]. There, the effective interaction was derived in the unitary-model-operator approach and an explicit diagonalization was performed. The resulting sp ener-

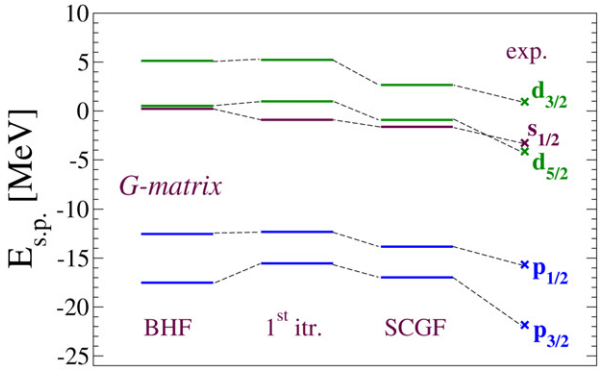

Fig. 4. Single particle spectra generated by the G-matrix in the (B)HF approximation, after the first iteration and in the full self-consistent solution. The points on the right represent the experimental values for the ^{17}O/^{15}O case [29].

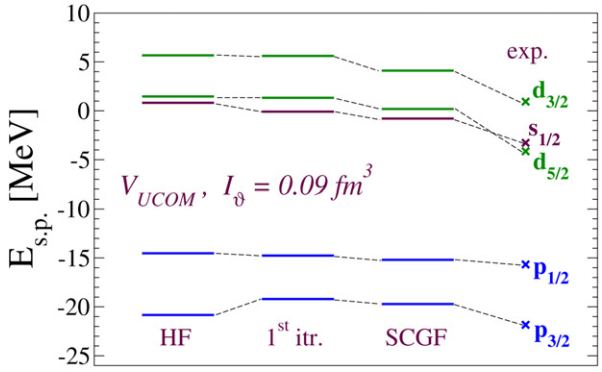

Fig. 5. Same as Fig. 4 but for the V_{UCOM} interaction.

gies showed a somewhat stronger dependence on the oscillator length than the one found in this work. The present formalism explicitly employs a basis of 2qp1qh/2qh1qp configurations. By using fully dressed quasiparticle and quasiholes additional ph excitation are included, in principle up to promoting all the nucleons above the Fermi level. The effects of self-consistency are thus twofold: additional excitations are implicitly included beyond the bare 2p1h/2h1p level and (as discussed above) these contributions are selected in such a way to preserve basic conservation laws [7,23]. The importance of these can be judged by comparing the second and third columns of Figs. 4 and 5. The spectrum obtained in Fig. 2 is nearly convergent, suggesting that the all order summation employed here and the proper accounting of the fragmentation of the sp strength allow to select most of the relevant configurations. Coupled cluster calculations are also available for ^{16}O with an analogous v_{18}/G-matrix and also including 2p1h/2h1p cluster operators [6]. These authors find convergence with respect to the model space and report splittings of the $0p$ and $0d$ orbits larger than those of Table 1 by about 1.5 and 0.5 MeV, respectively. We note that the LRC studied in this work are in the form of couplings to small amplitude excitations of the core—which can be described at the DRPA level. More complex collective modes are also present [31] and should be included for a full solution of the many-body problem. For example, the phenomenological studies of Ref. [18] suggest further contributions to the $p_{3/2}$ quasihole wave function coming from couplings to the first excited 0^+ state in oxygen. Testing this conjecture would first require being able to reproduce the correct excitation energy of this level—since it can couple effectively only when it is low enough in energy. To our knowledge this is still a challenge for the available ab initio methods.

Figs. 4 and 5 show the effects of LRC on the sp spectrum for $b_{\mathrm{HO}} = 1.9$ fm, and compare to the experimental values for the addition/removal of a neutron. For both interactions the coupling to collective phonons reduces the splitting of the $0p$ orbits, with respect to the HF approximation. Including the effects of fragmentation tends instead to compress the sd shell and to lower the whole spectrum. The self-consistent results for the energy gap between particle and hole states, $\Delta E_F = \varepsilon_{d_{5/2}} - \varepsilon_{p_{1/2}}$, are 13.0 MeV with the G-matrix and 15.4 MeV with V_{UCOM}. Both of them exceed the experimental value of 11.5 MeV. However, the differences $\varepsilon_{s_{1/2}} - \varepsilon_{p_{1/2}} = 12.2$ MeV and $\varepsilon_{d_{3/2}} - \varepsilon_{p_{1/2}} = 16.5$ MeV obtained with the G-matrix are close to the experiment (12.4 and 16.6 MeV, respectively), suggesting that the shortcomings of this interaction lie mainly in the poor description of the spin–orbit splittings. The mean square radii obtained are $r_{\mathrm{rms}} = 2.63$ fm (G-matrix) and $r_{\mathrm{rms}} = 2.45$ fm (V_{UCOM}).

Using the renormalization group with different momentum cutoffs it was shown that it is possible to shift the binding energies for $A = 3, 4$ systems along the Tjon line [32]. The same result has been obtained in the UCOM approach by modifying the correlator in the tensor-isoscalar channel [33]. Usually, tuning the binding energies to the experimental values increases the nonlocality of the interaction and leads to improved spin orbit splittings, as seen in Table 1. On the other hand, our V_{UCOM} result for ΔE_F—with 2N forces—overestimates the experiment. This behavior is seen already at the HF level for soft interactions like V_{UCOM} and $V_{\mathrm{low}\text{-}k}$ [27,34] and it is only slightly modified by the LRC considered here. We note that V_{UCOM} is obtained by applying the UCOM correlator operator to the nuclear Hamiltonian and then truncating to a two-nucleon interaction. Hence, it is not expected to generate the same results of the original interaction (Argonne v_{18} in this work). In both cases (G-matrix and V_{UCOM}), three-body forces appear necessary in order to reproduce the whole spectrum of observations. We note, however, that the UCOM method offers some advantages to reduce the contributions needed from many-body forces since it allows to treat SRC in different channels separately [15].

In conclusion, SCGF calculations have been performed for the first time in a large model space, including up to eight oscillator shells. Long-range correlations in the form of coupling sp to ph and pp/hh DRPA modes were investigated for ^{16}O. A comparison was made between the results of a G-matrix and the V_{UCOM} interactions, both derived from same realistic potential (Argonne v_{18}). The spectra of adjacent nuclei were found to be nearly convergent for the G-matrix, while they depend only weakly on the oscillator length for V_{UCOM}. In general it was found that the LRC effects considered here, tend to compress the spectra of $A \pm 1$ nuclei but do not affect sensibly the gap between quasiparticle and quasihole energies at the Fermi level.

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