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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

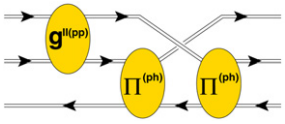

Fig. 1. Example of a Feynman diagram included in the all-order summation generated by the set of Faddeev equations. Double lines represent the dressed one-particle Green's function $g(\omega)$, which propagates quasiparticles (rightward arrows) and quasiholes (leftward arrows). The ellipses propagate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