Configuration interactions constrained by energy density functionals

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Abstract. A new method for constructing a Hamiltonian for configuration interaction calculations with constraints to energies of spherical configurations obtained with energy-density-functional (EDF) methods is presented. This results in a unified model that reproduces the EDF binding-energy results in the limit of single Slater determinants, but can also be used for obtaining energy spectra and correlation energies with renormalized nucleon-nucleon interactions. The three-body and/or density-dependent terms that are necessary for good nuclear saturation properties are contained in the monopole corrections obtained from the EDF. Applications to binding energies and spectra in the region of $^{132}$Sn are given.

In nuclear structure theory the two main computational methods for heavy nuclei based upon the nucleon fermionic degrees of freedom are the Hartree-Fock or energy-density-functional (EDF) method and the configuration interaction (CI) method. The EDF method is often limited to the configuration for a single Slater determinant. The EDF has parameters that are fitted to global properties of nuclei such as binding-energies and rms charge radii [1], [2] [3].

The CI method takes into account many Slater determinants. CI often uses a Hamiltonian derived from experimental single-particle energies and a microscopic nucleon-nucleon interaction [4]. A given CI Hamiltonian is applied to a limited mass region that is related to the configurations of a few valence orbitals outside of a closed shell and the associated renormalized nucleon-nucleon interaction that is specific to that mass region [4], [5]. Spectra and binding energies (relative to the closed core) obtained from such calculations for two to four valence particles are in good agreement with experiment [4], [5]. As many valence nucleons are added the agreement with experimental spectra [6] and binding energies deteriorates (see Fig. 36 in [4]). An important part that is missing from these CI calculations is the effective two-body interaction that comes from the three-body interaction of two valence nucleons interacting with one nucleon in the core [7]. To improve agreement with experimental spectra one often adjusts some of the valence two-body matrix elements. The most important part of this adjustment can be traced to the monopole component of the two-body matrix elements that controls how the effective single-particle energies evolve as a function of proton and neutron number [7].

Fig. (1) shows Wick’s theorem applied to a closed shell for the one-body kinetic energy, the two-body interaction and the three-body interaction. The part contained in the dashed box represents the closed-shell and effective one-body parts of the Hamiltonian that might be contained in an EDF approach. Up to now this has been treated phenomenologically in the
framework of the Skyrme Hartree-Fock or relativistic Hartree methods with some parameters (typically 6-10) fitted to global experimental data. There are efforts underway to relate the parameters of these phenomenological approaches to the underlying two and three body forces between nucleons, and also to extend the functional forms to obtain improved agreement with experiment [3]. The part contained in the solid-line box is the residual interaction used for CI calculations. The remaining term is a valence three-body interaction.

In this paper we consider results for a $^{132}$Sn closed shell, but the method can be applied to other closed-shell nuclei. The single-particle energy for orbital $a$ is defined as

$$e_a = E^{(132\text{Sn} + a)} - E^{(132\text{Sn})},$$

where $E^{(132\text{Sn})}$ is the energy of the closed-shell configuration for $^{132}\text{Sn}$, and $E^{(132\text{Sn} + a)}$ is the energy of the closed-shell configuration plus one nucleon constrained to be in orbital $a$. Eq. (1) defines the one-body part of the CI calculations. Often experimental data are used for the energies in Eq. (1). In this paper we will use the results of EDF calculations for these energies.

For this paper we will use the EDF results based on the Skxxtb Skyrme interaction [1], [8]. This is the Skx interaction from [1] with the addition of a tensor part fitted to observed single-particle energies [8]. The single-particle eigenvalues of the potential obtained with Skxxtb are shown in Fig. (2). The results for the single-particle energies as defined by Eq. (1) for $^{133}\text{Sb}$ are shown in Fig. (3). The energy of the $^{133}\text{Sb}$ ground state relative to that of $^{132}\text{Sn}$ is $-9.56$ MeV with Skxxtb compared to the experimental value of $-9.68$ MeV. An important property of Skxxtb
is that the experimental single-particle energies for the low-lying single-particle states around $^{132}$Sn are reproduced with an rms deviation of about 300 keV [1], [8]. We are not aware of any other class of Skyrme interactions that can do better for the single-particle energies as defined by Eq. (1).

The major new aspect of our method is to take the monopole part of the effective two-body interaction from

$$
\bar{V}_{ab} = E^{(132}\text{Sn} + a + b) - E^{(132}\text{Sn}) - \epsilon_a - \epsilon_b,
$$

(2)

where $E^{(132}\text{Sn} + a + b)$ is the symmetry-constrained spherical EDF energy of the configuration for a closed shell plus two nucleons in orbitals $a$ and $b$. This monopole interaction contains both the two and three body terms shown by the solid-line box in Fig. (1) as well as higher-order terms to the extent that they are contained in the EDF phenomenology. We modify the monopole part of the microscopic valence interaction to reproduce the results of Eq. (2). With this modification, the CI calculations closely reproduce the EDF calculations for single-Slater determinants, even when relatively many valence nucleons are added. Thus, the CI calculations are constrained to reproduce the trends of closed-shell energies and effective single-particle energies obtained with the EDF. For our model space orbitals, Eq. (2) involves about one hundred configurations for two nucleons (proton-proton, neutron-neutron and proton-neutron), but these calculations in a spherical basis are computationally fast.

The two-body part of the CI Hamiltonian is obtained with the usual renormalization procedure [5]. For our examples, the active valence orbitals are $(0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2})$ for protons $(0h_{9/2}, 1f_{7/2}, 1f_{5/2}, 2p_{3/2}, 2p_{1/2}, 0h_{13/2})$ for neutrons. The first-order matrix elements are obtained with the $V_{\text{loc}}$ method [9] with a cut off of $\Lambda = 2.2$ fm$^{-1}$ for the N$^3$LO nucleon-nucleon interaction [10]. Core-polarization corrections are calculated in second-order up to $6h\omega$ in the excitations energy. For the harmonic-oscillator basis we use $h\omega = 7.874$ MeV, obtained from the global parametrization $h\omega = 45 A^{-2/3} - 25 A^{-1/3}$ MeV.

Two-body matrix elements $< abJ \mid V \mid abJ >$ for two protons in $a = b = 0g_{7/2}$, one proton in $a = 0g_{7/2}$ and one neutron in $b = 1f_{7/2}$, and two neutrons in $a = b = 1f_{7/2}$ are shown in Fig. (4) for the effective interaction obtained with harmonic-oscillator (black dots) and EDF (red dots) radial wavefunctions. Overall, the EDF results are close to the oscillator values, with the largest exception for some low-spin matrix elements that differ by up to about 100 keV.

For the lowest proton orbital with $a = b = (0g_{7/2})$ the renormalized N$^3$LO monopole interaction is $\bar{V}_{N^3\text{LO}} = 0.191$ MeV (it is repulsive due to the Coulomb interaction). The result obtained from Eq. (2) with Skxtb is $\bar{V}_{\text{Skxtb}} = 0.374$ MeV. Therefore, the contribution from the effective two-body interaction in the valence space due to the three-body interaction of two-valence nucleons with one nucleon in the core is $0.374 - 0.191 = 0.183$ MeV. This correction is included in CI by modifying all of the valence TBME for the $0g_{7/2}$ orbital by

$$
< abJ \mid V \mid abJ >_{\text{CI}} = < abJ \mid V \mid abJ >_{N^3\text{LO}} - \bar{V}_{N^3\text{LO}} + \bar{V}_{\text{Skxtb}}.
$$

(3)

Similar corrections are made for all other orbital pairs in our model space. The EDF corrections from Eq. (3) for the lowest orbitals are shown in Fig. (5).

The results for $^{134}$Te are shown in Fig. (6). The agreement between experiment and theory is reasonable. It can be improved (as discussed below) if the Skxtb single-particle energies were replaced by the experimental values. The purpose of this comparison is to show what can be obtained with Skxtb+N$^3$LO without any adjustment of the model parameters.

The EDF monopole corrections are on the order of 0.2 to 0.3 MeV. When many nucleons are added, the monopole contribution goes as

$$
\Delta E = n(n - 1)\bar{V}/2,
$$

(4)
Figure 3. Comparison of experiment and theory (ham) for $^{133}$Sb. Theory (ham) is based on the Skxtb EDF for the single-particle energies obtained from Eq. (1). The length of the line indicates the spin with positive parity (red) and negative parity (blue). Experimental levels that are unknown or uncertain are shown by the black dots.

Figure 4. Two-body matrix elements $<abJ|V|abJ>$ for two protons in $a = b = 0g_{7/2}$, one proton in $a = 0g_{7/2}$ and one neutron in $b = 1f_{7/2}$, and two neutrons in $a = b = 1f_{7/2}$. Comparison between results with harmonic-oscillator (solid line) and EDF (red dots) radial wavefunctions is made.

where $n$ is the number of valence nucleons. When we constrain the configuration of $^{146}$Gd ($N = 82$ and $Z = 64$) to be $(0g_{7/2})^3(1d_{5/2})^6$ for the valence protons, the CI calculation gives a binding energy increase of 97.92 MeV (relative to $^{132}$Sn). The EDF calculation (with the same assumption for the configuration) gives 98.57 MeV. These are close to each other due to our EDF monopole correction to the valence matrix elements. If the EDF monopole correction were not included in CI the results would differ by 19.3 MeV. The microscopic valence interaction on its own is too strong and gives an “over-saturation” (see Fig. 36 in [4]).

The difference 98.57 – 97.92 = 0.65 MeV for $^{146}$Gd could be considered as the contribution from the valence three-body-monopole interaction on the right-hand side of Fig. (1) together with higher-order corrections implicit in the EDF. With $\Delta E_3 = n(n-1)(n-2)V_3/6$ and $n = 14$ we obtain $V_3 = 0.0018$ MeV. Thus, valence three-body interaction is very small. But one may need to take it into account for the binding energies of nuclei with ten or more valence particles due to its $n^3$ dependence.

Next we would start to improve upon the CI+EDF calculation for $^{146}$Gd by going beyond the closed-shell configuration. Allowing for the addition of two-particle two-hole configurations we obtain a binding energy difference with $^{132}$Sn of 100.45 MeV compared to the experimental value of 101.58 MeV. The full space calculation for $^{146}$Gd should be close to experiment.

When experimental energies are known, the traditional shell-model approach is to use these for the CI calculations [4]. If we replace the single-particle energies with those that reproduce the experimental results for $^{133}$Sb as shown on the left-hand side of Fig. (3) (the $2s_1g_{7/2}$ single-particle energy is placed 328 keV below that of the $1d_{3/2}$), the results for $^{134}$Te [Fig. (7)] are in better agreement with experiment [compared to Fig. (6)] and consistent with the results obtained by Coragio et al. [4]. But for our calculations that connect directly to EDF methods, it is important to use both single-particle energies and monopole corrections from the same EDF. It is expected
Figure 5. Comparison between results with the EDF radial wavefunctions and with the addition of the EDF monopole correction (red dots).

Figure 6. Comparison of experiment and theory (ham) for $^{134}$Te. Theory (ham) is based on the Skx tb EDF for the single-particle energies and two-body monopoles, and the N$^3$LO ($V_{lowk}$) interaction in an oscillator basis renormalized to second order for the valence two-body matrix elements. The length of the line indicates the spin with positive parity (red) and negative parity (blue). Experimental levels that are unknown or uncertain are shown by the black dots.

Figure 7. Comparison of experiment and theory (hap) for $^{134}$Te. Theory (hap) is the same as (ham) in Fig. (6) except that the single-particle energies have been replaced by their experimental values. The length of the line indicates the spin with positive parity (red) and negative parity (blue). Experimental levels that are unknown or uncertain are shown by the black dots.
that the single-particle spectra from EDF will be improved with better parametrization and extended functional forms [3].

In conclusion, we have provided a new method that is able to constrain the monopole part of CI calculations to the EDF results in the limit of single-Slater determinants. This constrained CI contains all interactions implicit in EDF including the three-body and/or density dependent contribution. Results for the $^{132}\text{Sn}$ region show that the three-body contribution to the monopole interaction is generally repulsive and is similar in magnitude to the monopole part of the two-body interaction obtained from renomalized realistic interactions such as N$^3$LO. The application of the CI approach is limited to about eight valence nucleons due to matrix dimensions. But there are approximate methods that can be used to apply our new Hamiltonian to nuclei with more valence nucleons, such as Monte-Carlo methods, exact pairing (for protons or neutrons) [11], or deformed HF+GCM (within the valence model space) for protons and neutrons.

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