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 reproduced the EDF binding-energy 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 EDF. Applications to binding-energies and spectra of nuclei in the region above ^{208}Pb are given.

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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 a configuration with a single-Slater determinant, sometimes called the single-reference (SR) EDF method. The EDF Hamiltonian has parameters that are fitted to global properties of nuclei such as binding-energies and rms charge radii [1,2]. To go beyond the SR method one can introduce a multi-reference EDF basis.

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 [3]. 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 [4,3]. 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 [4,3]. As many valence nucleons are added the agreement with experimental spectra and binding-energies deteriorates (see Fig. 36 in [3]). 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 [5]. To improve agreement
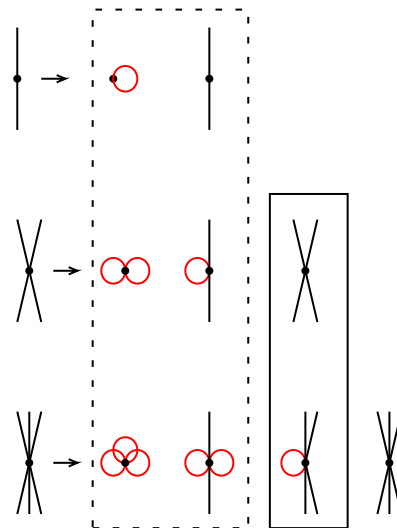

Fig. 1. Schematic diagram for the terms in the Hamiltonian obtained from Wick's theorem for a closed shell. The circles represent the summation over the orbitals in the closed shell. The black lines represent the valence particles and/or holes.

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 [5].

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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 method with some parameters (typically 6–10) fitted to global experimental data. There are efforts underway to improve the accuracy of the parameters used for EDF calculations, to extend the type of functional forms used, and to relate the parameters of these phenomenological approaches to the underlying two- and three-body forces between nucleons (see [6] and references therein). 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 Letter we discuss a new method for obtaining a Hamiltonian for valence nucleons outside of a doubly-closed shell. The specific application is made for ^{208}Pb, but it could be applied to any other doubly closed-shell system. The single-particle energy for orbital a is defined as

$$e_a = E\left(^{208}\text{Pb} + a\right) - E\left(^{208}\text{Pb}\right), \tag{1}$$

where $E(^{208}\text{Pb})$ is the energy of the closed-shell configuration for ^{208}Pb, and $E(^{208}\text{Pb} + a)$ 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 Eq. (1) when the data are known and the two states are connected by a spectroscopic factor of near unity. In this Letter we will use the results of single-reference EDF calculations restricted to spherical symmetry for these energies.

The two-body part of the CI Hamiltonian is obtained with the usual renormalization procedure [4]. For our examples, the active valence orbitals are $(0h_{9/2}, 1f_{7/2}, 0i_{13/2})$ for protons and $(0i_{11/2}, 1g_{9/2}, 0j_{15/2})$ for neutrons. For the two-body valence interaction we use the N^{3}LO nucleon–nucleon interaction [7] with two-body matrix elements obtained from the V_{lowk} method [8] with a cut-off of $\Lambda = 2.2$ fm^{-1}. Core-polarization corrections are calculated in second-order up to $6\hbar\omega$ in the excitation energy. We use harmonic-oscillator radial wavefunctions with $\hbar\omega = 6.883$ MeV.

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

$$\bar{V}_{ab} = E\left(^{208}\text{Pb} + a + b\right) - E\left(^{208}\text{Pb}\right) - e_a - e_b, \tag{2}$$

where $E(^{208}\text{Pb} + a + b)$ is the single-reference EDF energy of the configuration for a closed shell plus two nucleons constrained to be in orbitals a and b restricted to spherical symmetry. The EDF-monopole contains both terms in the solid-line box in Fig. 1, and also contains higher-order contributions implicit in the EDF functional including possible quadratic terms in the mass dependence of the single-particle energies. Whereas, the N^{3}LO monopole only contains the valence two-body interaction corrected to second order. 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 thirty configurations for two nucleons (proton–proton, neutron–neutron and proton–neutron), but these calculations in a spherical basis are computationally fast.

For this Letter we will use the EDF results based on the Skxm Skyrme interaction [1]. An important property of Skxm is that
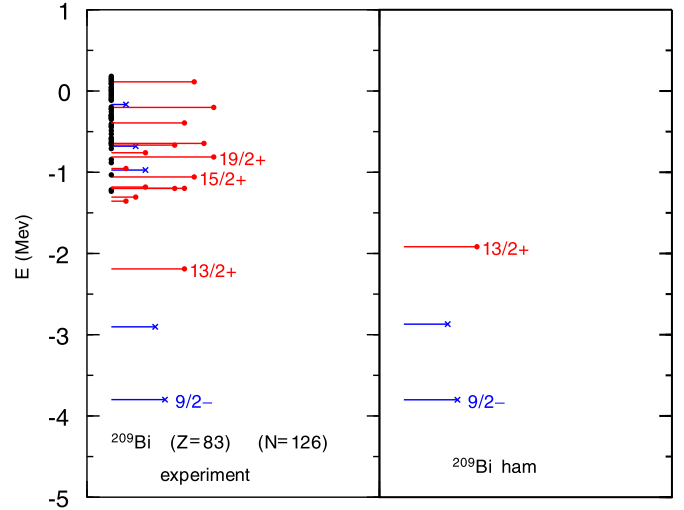

Fig. 2. Comparison of experiment and theory (ham) for ^{209}Bi. The energies are with respect to that of ^{208}Pb. The length of the lines indicate the spin with positive parity (horizontal lines ending in a circle) and negative parity (horizontal lines ending in a cross). Experimental levels that are unknown or uncertain are shown by the black dots with no horizontal line.

the experimental single-particle energies for the low-lying single-particle states around ^{208}Pb are reproduced with an rms deviation of about 300 keV. Skxm also has a reasonable value of the incompressibility (234 MeV). We are not aware of any other Skyrme interaction that can do better for the single-particle energies as defined by Eq. (1). For the lowest state for protons ($0h_{9/2}$ for ^{209}Bi) and neutrons ($1g_{9/2}$ for ^{209}Pb), the difference between experiment and theory can be reduced to on the order of 20 keV with only a small increase of $\chi^2 = 0.82$ to $\chi^2 = 0.89$ for all of the data considered in [1]. This is accomplished by using a higher weight for these two data and requires a small adjustment of the Skxm parameters. Since the precise energies of these orbitals are useful for the results presented here, we use this new Skyrme interaction called Skxmb. If we use Skxm or any other Skyrme interaction, our conclusions are the same, but the deviation with experiment is worse mainly because the single-particle energies are worse. The binding-energy of ^{208}Pb with Skxmb is 1636.46 MeV compared to the experimental value of 1636.45 MeV.

The results obtained from Skxmb for the energies of single-particle states ^{209}Bi relative to the energy of ^{208}Pb are shown in Fig. 2. The energy of the lowest state, $0h_{9/2}$, is reproduced due to the fit constraint. The next two states (related to the $1f_{7/2}$ and $0i_{13/2}$ orbitals) are also well reproduced. One observes in experiment states related to core-excitation of ^{208}Pb starting about three MeV above the ground state.

For the lowest proton orbital with $a = b = (0h_{9/2})$ the renormalized N^{3}LO monopole interaction is $\bar{V}_{\text{N}^3\text{LO}} = 0.170$ MeV (it is repulsive due to the Coulomb interaction). The result obtained from Eq. (2) with Skxmb is $\bar{V}_{\text{EDF}} = 0.288$ MeV. The difference is $\bar{V}_{\text{EDF}} - \bar{V}_{\text{N}^3\text{LO}} = 0.118$ MeV. This correction is included in CI by modifying all of the valence TBME $\langle V \rangle_J = \langle ab J | V | ab J \rangle$ for the $0h_{9/2}$ orbital by

$$\left\langle |V| \right\rangle_{J,\text{eff}} = \left\langle |V| \right\rangle_{J,\text{N}^3\text{LO}} - \bar{V}_{\text{N}^3\text{LO}} + \bar{V}_{\text{EDF}}. \tag{3}$$

Similar corrections are made for all other diagonal pairs of orbitals in the model space.

For the CI calculations we use the code NuShell [9]. The theory Hamiltonian (ham) consists of Skxmb for the single-particle energies, and two-body matrix element obtained from the renormalized N^{3}LO interaction corrected to second-order, and then fi-
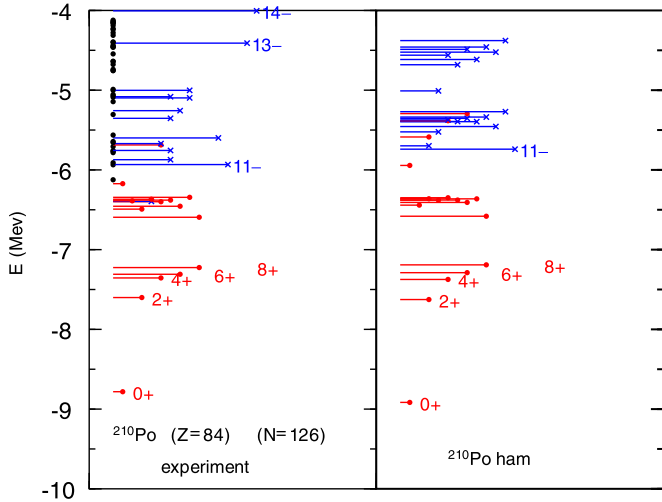
Fig. 3. Comparison of experiment and theory (ham) for ^{210}Po [see caption to Fig. 2].
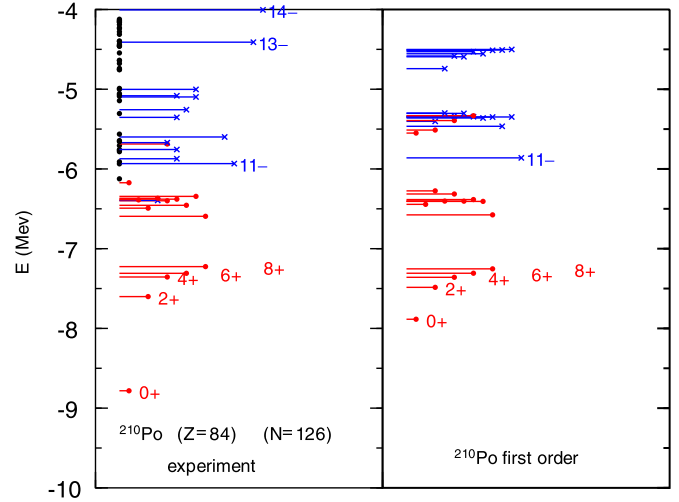

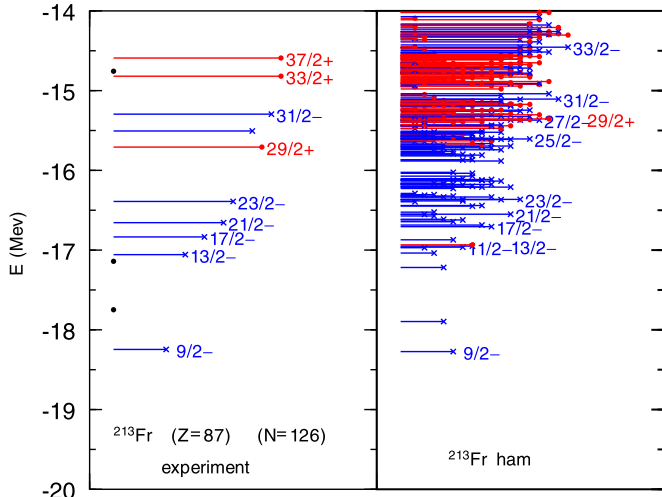**Fig. 6.** Comparison of experiment and theory (first order) for ^{210}Po [see caption to Fig. 2].
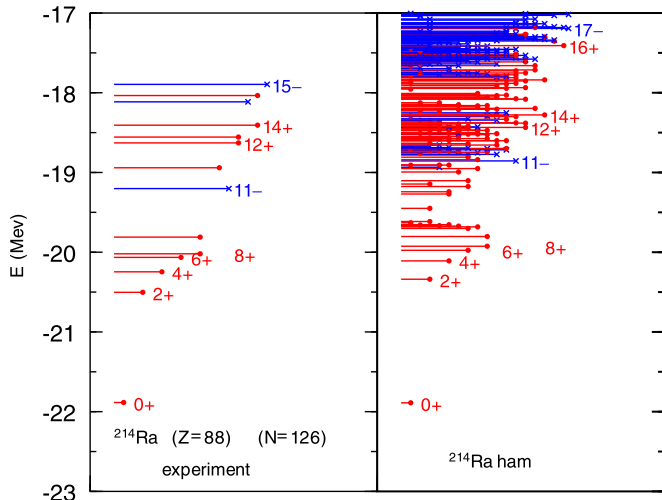

Fig. 4. Comparison of experiment and theory (ham) for ^{213}Fr [see caption to Fig. 2].

nally the two-body monopoles corrected with Skxmb with Eq. (3). The energies of ^{210}Pb, ^{213}Fr and ^{214}Rn are shown in Figs. 3–5. The agreement between experiment and theory is good for the spectra and for the absolute energy relative to ^{208}Pb. For ^{210}Po the agreement between experiment and theory is very good for levels up to three MeV above the ground state. Above three MeV the level density of experiment and theory is similar, but one expects additional levels in experiment coming from the core-excitation of ^{208}Pb. For ^{213}Fr and ^{214}Ra the theoretical level density is much higher than experiment because the experimental conditions select mainly the yrast levels. For the low-lying levels in Figs. 3–5 the agreement between the absolute energies of experiment and theory (relative to ^{208}Pb) is usually within 100 keV, but there are some exceptions with deviations up to about 300 keV (e.g. the 11– in ^{214}Ra). These deviations may be due to many factors such as lack of third-order diagrams, the use of the harmonic-oscillator basis for the renormalized N^{3}LO matrix elements, non-monopole three-body contributions, or inadequacies in the EDF Skxmb interaction.

When many nucleons are added, the monopole contribution goes as

$$\Delta E = n(n-1)\bar{V}/2, \tag{4}$$

where n is the number of valence nucleons. Thus the EDF monopole corrections become much more important as one adds many valence nucleons. When we constrain the CI to the single configuration $(0h_{9/2})^{10}$ for the valence protons, the CI calculation gives a binding-energy increase of 25.05 MeV (relative to ^{208}Pb). The EDF calculation (with the same assumption for the configuration) gives 25.24 MeV. These are close to each other due to our EDF monopole correction to the valence matrix elements. If the EDF monopole corrections were not included in CI the results would differ by $(45) \times (0.118) = 5.3$ MeV. The microscopic valance interaction on its own is too strong and gives an "over-saturation". The results for the $(1f_{7/2})^8$ configuration are 13.27 MeV for CI and 13.41 MeV for EDF. The difference between CI and EDF might be interpreted in terms of an effective valence three-body monopole interaction with strength $\Delta E_3 = 25.24 - 25.05 = 0.19$ MeV for $(0h_{9/2})^{10}$ and $\Delta E_3 = 13.41 - 13.27 = 0.14$ MeV $(1f_{7/2})^8$. With $\Delta E_3 = n(n-1)(n-2)\bar{V}_3/6$, $\bar{V}_3$ is on the order of 1–2 keV. $\bar{V}_3$ includes the three-body monopole interaction on the right-hand side of Fig. 1, but it will also include non-quadratic terms in the single-particle energies and two-body monopole energies that emerge
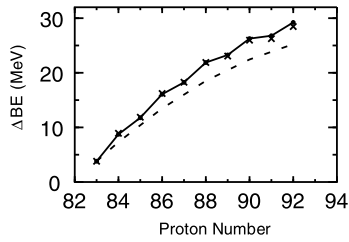

Fig. 5. Comparison of experiment and theory (ham) for ^{214}Ra [see caption to Fig. 2].

Fig. 7. Binding energies relative to ^{208}Pb. Experiment are the points connected by a line. The results of the CI(N^{3}LO + Skxmb) are shown by crosses. The results of the single-reference EDF calculation constrained to spherical symmetry are shown by the dashed line.
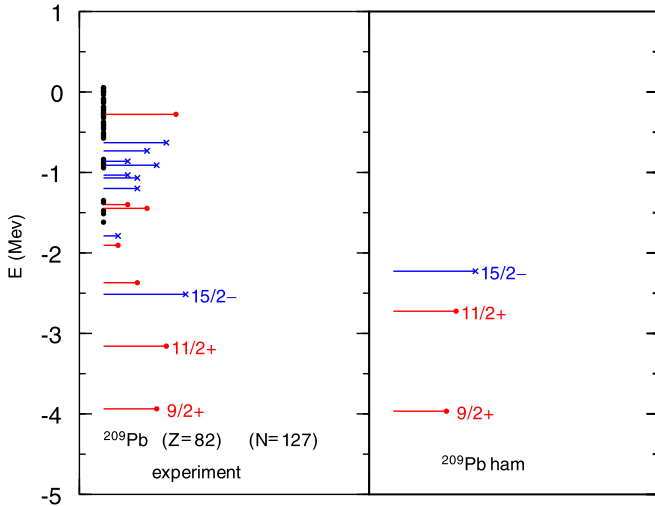

Fig. 8. Comparison of experiment and theory (ham) for ^{209}Pb [see caption to Fig. 2].

Fig. 9. Comparison of experiment and theory (ham) for ^{210}Pb [see caption to Fig. 2].

Fig. 10. Comparison of experiment and theory (ham*) for ^{210}Pb [see caption to Fig. 2]. Theory (ham*) is the same as theory (ham) except that the single-particle energies for the neutron $i_{11/2}$ and $j_{15/2}$ orbitals are taken from the experimental values in ^{209}Pb.

from the EDF solutions. ΔE_3 is small compared to other sources of error in the theory and for practical purposes it may be ignored.

The CI calculation were carried out up to ^{218}U ($Z = 92$) where the M-scheme dimension is about 1.5 million. The results for the ground state energies are compared to experiment in Fig. 7. The EDF calculation is based upon the spherical $(0h_{9/2})^n$ configuration with $n = 1$ to 10. The difference between EDF and CI can be regarded as the correlation energy in the nuclear ground state, in this case mainly due to the "pairing" interaction. The correlation results in wavefunctions that are highly mixed in the valence proton basis. For example the CI ground state of ^{218}U contains only 4.7% of the $(0h_{9/2})^{10}$ component. Up to $Z = 88$ the difference between experiment and theory for the binding energy relative to ^{208}Pb is on the order of 100 keV, and after this it gradually increases to about 700 keV for ^{218}U. One would obtain results similar to CI shown in Fig. 7 for the ground states by carrying out HFB calculations with a pairing interaction similar to that obtained from the renormalized N^{3}LO. The advantage of CI is that the entire excited-state spectrum is also obtained. The results for the spectra of the nuclei with $N = 126$, including the fact that ^{218}U is far from a proton closed-shell configuration, are similar to those obtained in [10] with the old modified Kuo–Herrling Hamiltonian [11]. For the ground state binding-energies one had to add a monopole correction in [10]. Our Hamiltonian is a modern version of Kuo–Herrling based on N^{3}LO with V_{lowk}, it is not modified, and the monopole corrections are obtained with our new method that uses information from global EDF models.

The pairing interaction also appears in Fig. 3 for ^{210}Po by the difference in energy between the ground state and the $J^\pi = 8^+$ state which is dominated (99.86%) by the $(0h_{9/2})^2$ configuration.
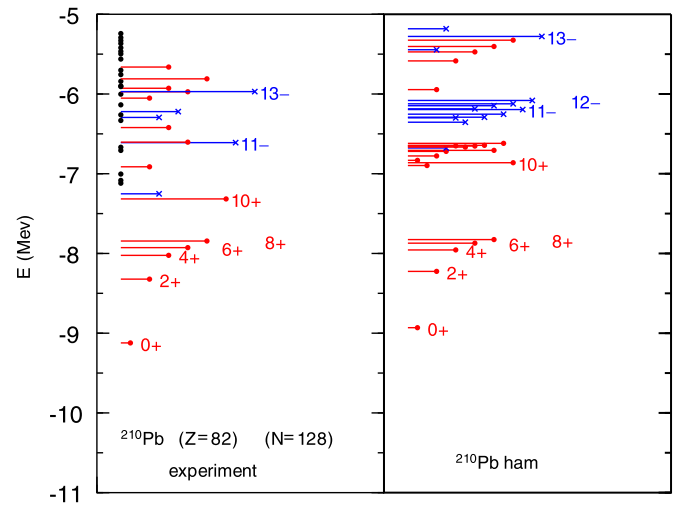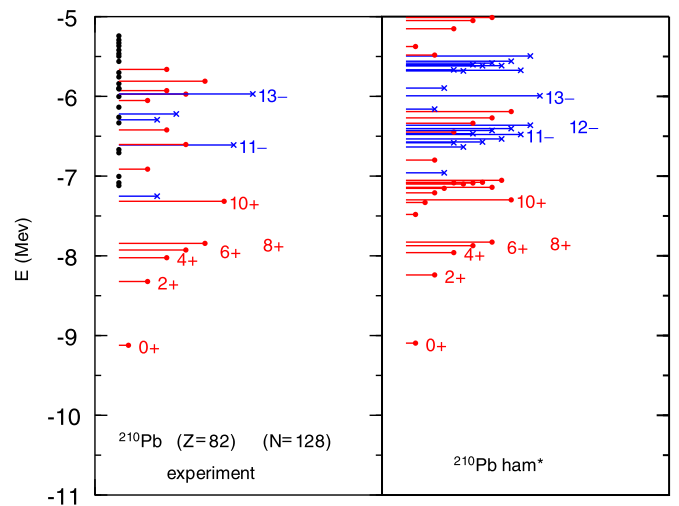
We show in Fig. 6 the spectrum for ^{210}Po obtained from the first-order N^{3}LO V_{lowk} matrix elements. Comparison with Fig. 3 (which includes second order) shows that two-thirds of the pairing comes from second-order diagrams. The tensor interaction is important for second-order pairing through the bubble-diagram which links the valence protons with the core neutrons.

Results for neutrons for the spectra of ^{209}Pb and ^{210}Pb are shown in Figs. 8 and 9, respectively. The single-particle energies of the $0i_{11/2}$ and $0j_{15/2}$ orbitals in ^{209}Pb are 200–400 keV too high with Skxmb. This is the reason why the theoretical energies of the 10^+, 11^- and 13^- states are too high in ^{210}Pb. The results for ^{210}Pb are improved when the energies of these two single-particle states are taken from experiment for ^{209}Pb (left-hand side of Fig. 8) as shown in Fig. 10. For our method to give the same results for CI and EDF in the limit of spherical single-Slater determinants, one must take both the single-particle energies and two-particle monopole energies from the EDF calculation; one cannot arbitrarily change the single-particle energies. Thus it is important to obtain EDF functionals that reproduce low-lying single-particle energies near the doubly-magic nuclei.
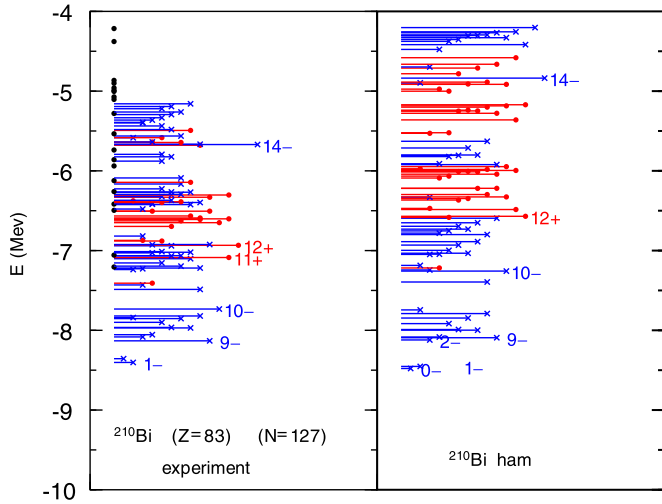
Fig. 11. Comparison of experiment and theory (ham) for ^{210}Bi [see caption to Fig. 2].
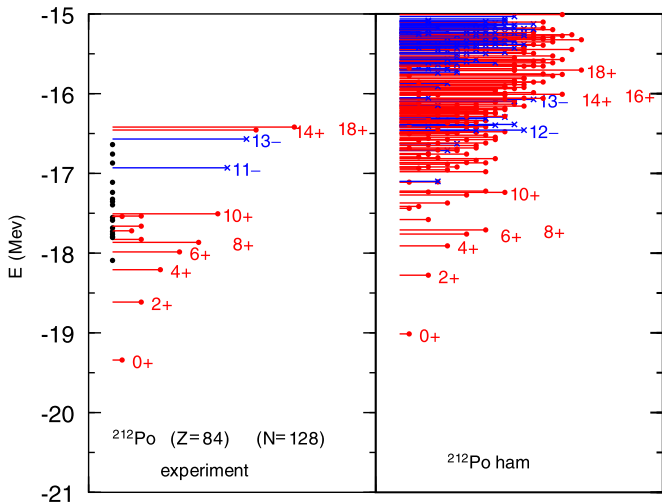

Fig. 12. Comparison of experiment and theory (ham) for ^{212}Po [see caption to Fig. 2].

Results for ^{210}Bi and ^{212}Po are shown in Figs. 11 and 12. Results for the low-lying proton–neutron spectrum of ^{210}Bi are comparable to those shown by [12]. The theoretical energies for the high-spin state would be in better agreement with experiment if the experimental single-particle energies from ^{209}Pb are used for the neutrons. But some specific disagreements remain, for example the theoretical the $J^\pi = 14^-$ state in ^{210}Bi remains about 500 keV too high compared to experiment.

The monopole interactions for the $1g_{9/2}$ neutron orbital are $\bar{V}_{\mathrm{N^3LO}} = -0.076$ MeV and $\bar{V}_{\mathrm{EDF}} = 0.017$ MeV giving a correction of $0.017 - (-0.076) = 0.093$ MeV. The monopole interactions between the $0h_{9/2}$ proton orbital and the $1g_{9/2}$ neutron orbital are $\bar{V}_{\mathrm{N^3LO}} = -0.143$ MeV and $\bar{V}_{\mathrm{EDF}} = -0.205$ MeV giving a correction of $-0.205 - (-0.143) = -0.062$ MeV. Although the EDF monopole corrections are generally positive (leading to less binding), some are negative, as in the last example. This is a result of the micro-

scopic dependence on the specific orbitals being considered and their overlaps with the central proton and neutron densities. The values depend on the isoscalar and isovector properties of the EDF functional that have parameters tuned to reproduce global properties of binding-energies.

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 calculation contains all monopole interactions implicit in EDF including three-body, density-dependent and rearrangement contributions. In the limit of spherical single-Slater determinants the CI calculations with this method reproduce the EDF results except for a very small three-body residual. The results for the $N = 126$ isotones show that this change in the monopole interaction is crucial for obtaining the correct absolute binding-energies. Second-order corrections are important for the pairing interaction. As illustrated in the case of ^{209}Pb and ^{210}Pb, the accuracy of this method based on EDF results for the monopole energies plus N^{3}LO for the renormalized residual interaction is limited by the accuracy of the EDF methods to reproduce the binding-energies for states in nuclei one nucleon removed from a closed shell [Eq. (1)]. In our examples for ^{208}Pb the Skyrme parameters were optimized for the precise ground-state energies of ^{209}Bi and ^{209}Pb leaving the rms deviation for all other nuclei about the same as shown in [1]. This method can be applied to any other doubly-closed shell system, but its accuracy will be limited by the accuracy of the EDF results for single-particle energies. Local optimizations with global constraints such as that used to obtain Skxmb may be possible for other mass regions. One can add the tensor interaction to Skyrme [13]. In the coming years we may expect improvements in EDF theory and phenomenology towards an improved universal functional. For cases where the basis dimensions are too large for exact CI methods, it would be interesting to apply our Hamiltonian to approximate methods within this model space for valence nucleons outside of ^{208}Pb.

Acknowledgements

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