Fluctuating parts of nuclear ground-state correlation energies

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(Received 10 December 2012; revised manuscript received 2 April 2013; published 3 May 2013)

Background: Heavy atomic nuclei are often described using the Hartree-Fock-Bogoliubov (HFB) method. In principle, this approach takes into account Pauli effects and pairing correlations while other correlation effects are mimicked through the use of effective density-dependent interactions.
Purpose: Investigate the influence of higher-order correlation effects on nuclear binding energies using Skyrme's effective interaction.
Methods: A cutoff in relative momenta is introduced to remove ultraviolet divergencies caused by the zero-range character of the interaction. Corrections to binding energies are then calculated using the quasiparticle-random-phase approximation and second-order many-body perturbation theory.
Result: Contributions to the correlation energies are evaluated for several isotopic chains and an attempt is made to disentangle which parts give rise to fluctuations that may be difficult to incorporate on the HFB level. The dependence of the results on the cutoff is also investigated.
Conclusions: The improved interaction allows explicit summations of perturbation series, which is useful for the description of some nuclear observables. However, refits of the interaction parameters are needed to obtain more quantitative results.

DOI: 10.1103/PhysRevC.87.054303 PACS number(s): 21.10.Dr, 21.30.Fe, 21.60.Jz

I. INTRODUCTION

The atomic nucleus is a complicated quantum-mechanical system where the probability of finding a nucleon in a certain position is a function of the positions of the other nucleons. This is generally referred to as the nucleons being correlated and makes the wave functions of heavy nuclei too complex to compute directly using *ab initio* theory. One therefore has to resort to more tractable methods that take the most important correlation effects explicitly into account, i.e., the ones that are important to describe observables, while the remaining effects are treated in an approximate way.

An often used starting point is to assume that the in-medium interaction between nucleons can be modeled using effective density-dependent internucleon potentials. Such potentials are generally employed in Hartree-Fock-Bogoliubov (HFB) calculations and their parameters are fitted to reproduce a number of experimentally known data on individual nuclei and to what is known about nuclear matter. In this way, Pauli effects and pairing type correlations are taken into account explicitly while the effects of other of correlations are described in an average way. This approach has the great advantage of being applicable to the entire nuclear chart at a reasonable computational cost. In the quest of more accurate nuclear models an important task, however, is the systematic investigation of which type of correlation effects can be modeled with the HFB method and which need a more explicit treatment.

Several studies have shown that going beyond a HFB treatment and adding corrections to binding energies resulting from shape vibrations, especially of quadrupole type, give an improved description of experiment [1–4]. These corrections are often taken into account by either using the generator-coordinate method [1] or through the use of a collective model, e.g., a Bohr Hamiltonian [2].

Alternatively, many-body perturbation theory (MBPT) offers a way to explicitly and pictorially include elementary processes that one might suspect to be responsible for correlations in different systems. For instance, within the so called random-phase approximation (RPA) one allows for an infinite number of particle-hole pairs to be excited out of the Hartree-Fock (HF) ground state and for multiple scattering between excited particles and holes. If the excitations instead are made out of the HFB ground state the same approximation is referred to as the quasiparticle-random-phase approximation (QRPA), designating the RPA for Bogoliubov quasiparticles. An even simpler step beyond HFB is the second-order many-body perturbation theory (MBPT2) starting from the HFB ground state. Clearly, the virtual excitations included in this approximation form a subset of those included in the QRPA and in the present work we show results from both levels of approximation.

Most of the effective nucleon potentials involve contact terms, i.e, interactions of zero range. This is certainly the case for interactions of the Skyrme type and such interactions give rise to divergencies when going beyond the HF level. This can be seen, e.g., by solving the two-body problem for ^2H analytically using contact interactions. Then the resulting binding energies become infinite [5,6]. The two methods used in this work for going beyond the HFB level include infinite summations of intermediate states, which inevitably leads to the same divergencies in connection with zero-range forces.

It is a major theme of the present work to eliminate such divergencies by introducing cutoffs in momenta for our chosen Skyrme-like interaction potentials [7]. This procedure

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implicitly assumes that structures in binding energies as functions of nucleon number originate in correlation effects caused by the low-momentum part of the internucleon forces. And according to the results of the present work this assumption does not appear to be that far fetched.

This paper is organized as follows. In Sec. II the regularized Skyrme interaction is introduced. In Sec. III we discuss the treatment of correlation effects using the QRPA and the MBPT2 method. In Secs. IV and V we analyze and discuss the results of our calculations.

II. LOW-MOMENTUM INTERACTION

A. Two-body interaction in the particle-hole channel

A general two-body interaction that preserves the center-of-mass coordinate of the interacting particles can be expressed as

$$\hat{V}(\boldsymbol{r}_1'\boldsymbol{r}_2'\boldsymbol{r}_1\boldsymbol{r}_2) = v(\boldsymbol{r}', \boldsymbol{r})\delta(\boldsymbol{R} - \boldsymbol{R}'),$$

where $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2)$ and $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ denote the center-of-mass and relative coordinates, respectively. The part of the potential depending on relative coordinates can be transformed to momentum space and for this part we adopt Skyrme's expansion [8] given by

$$\begin{aligned}\bar{v}(\boldsymbol{k}', \boldsymbol{k}) &= \frac{1}{(2\pi)^3}\int e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} v(\boldsymbol{r}', \boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} d\boldsymbol{r}' d\boldsymbol{r} \\ &\simeq \frac{1}{(2\pi)^3}\Bigg[t_0(1 + x_0P^\sigma) + \frac{1}{2}t_1(1 + x_1P^\sigma)(k'^2 + k^2) \\ &\quad + t_2(1 + x_2P^\sigma)\boldsymbol{k}'\cdot\boldsymbol{k} + iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\cdot\boldsymbol{k}'\times\boldsymbol{k}\Bigg].\end{aligned}$$

In this expression we have omitted the tensor potential included in Ref. [8] because it is not used in the parametrizations we employ later. This expression can be viewed as the first terms in a low-momentum expansion of the effective nuclear potential going up to second order in relative momenta (compare, e.g., Refs. [9–11] for higher-order expansions). Although this form gives a reasonable description of the low-momentum parts, the expansion becomes unrealistic for large momentum transfers. As we demonstrate later, for Hartree-Fock calculations, only the low-momentum matrix elements are important and the unphysical contributions generated by the expansion for higher momenta can be ignored.

For studies beyond the mean-field level, however, the interaction gives diverging results unless some kind of truncation is enforced, e.g., a truncation in excitation energy. Nevertheless, in some beyond-mean-field calculations, such as QRPA calculations, the results for low-lying states [12] and giant resonances [13] are in reasonable agreement with experiment, indicating that the interaction may indeed have a wider applicability beyond purely mean-field calculations.[1]

[1]Note that in the calculations of low-energy excitations the discussed divergencies did not constitute a problem. In fact, it is mainly the high-energy excitations that are modified by a momentum cutoff.

To investigate how well higher-order corrections can be described using the low-momentum part of Skyrme's interaction we follow Skyrme's original suggestion [8] and introduce a cutoff in momenta. We replace his original interaction by

$$\bar{v}^{(\Lambda)}(\boldsymbol{k}', \boldsymbol{k}) = \bar{v}(\boldsymbol{k}', \boldsymbol{k})\theta(\Lambda - k')\theta(\Lambda - k), \tag{1}$$

which vanishes at momenta above Λ $(\mathrm{fm})^{-1}$. In the limit of a large Λ one regains the results of the original untruncated interaction, but for finite values, the cutoff regularizes the interaction so that beyond-mean-field calculations converge. The introduction of the cutoff destroys the nice analytical properties of the zero-range interaction and increases the computational cost of calculating matrix elements.

B. Two-body interaction in the particle-particle channel

In the pairing channel we use the same finite-range separable-Gaussian interaction as was used in our previous studies [12,13]. Because this interaction has a finite range, no regularization is needed. We adopt an isospin invariant form, active in the $T = 1$ channel and use the same range parameter ($a = 0.66$ fm) as before. Because we only consider cases where neutrons are in open shells we tune the pairing strengths to make the lowest neutron quasiparticle energies to agree with the experimental gaps determined in Ref. [14]. The resulting isovector pairing strength becomes 560 $\mathrm{MeV(fm)}^{-1}$ when the SKX Skyrme parameters [15] are used in the particle-hole channel and becomes somewhat larger [640 $\mathrm{MeV(fm)}^{-1}$] when the SLy5 parameters [16] are used.

C. Density-dependent part of the particle-hole interaction

Skyrme's expansion of the two-body potential is often used together with a density-dependent zero-range potential that is intended to describe missing three-body and higher-order contributions as well as giving a simple representation of missing many-body effects. The density-dependent terms cause difficulties when going beyond the mean field and different recipes to define a residual interaction exist in the literature [17]. In this work we are mainly motivated by the success of the Skyrme interaction in connection with RPA type calculations and hence define the residual interaction as the so-called RPA residual interaction using the second derivative of the HF energy [18]:

$$\begin{aligned}\tilde{v}_{pmqn} &= \frac{\partial^2 E_{\mathrm{HF}}}{\partial\rho_{qp}\partial\rho_{nm}} \\ &= v_{pmqn}[\rho] + \sum_{jl}\rho_{lj}\left(\frac{\partial v_{mjnl}[\rho]}{\partial\rho_{qp}} + \frac{\partial v_{pjql}[\rho]}{\partial\rho_{nm}}\right) \\ &\quad + \frac{1}{2}\sum_{ijkl}\rho_{ki}\frac{\partial v_{ijkl}[\rho]}{\partial\rho_{nm}\partial\rho_{qp}}\rho_{lj}\Bigg|_{\rho=\rho_0}.\end{aligned}$$

The use of the RPA residual interaction in configuration interaction type calculations has been thoroughly discussed and investigated before using a non-regularized Skyrme interaction [19].

The density-dependent two-body interaction is introduced in the standard form [20]

$$\hat{V}_\rho = v_\rho^{(\Lambda)}(\boldsymbol{r}', \boldsymbol{r})[\rho(\boldsymbol{R})]^\alpha \delta(\boldsymbol{R} - \boldsymbol{R}'),$$

with a dependence on the nucleon density ρ to some power α, which take on different values for different parametrizations. The part dependent on relative coordinates is expanded to lowest order in relative momenta,

$$\bar{v}_\rho^{(\Lambda)}(\boldsymbol{k}', \boldsymbol{k}) = \frac{1}{(2\pi)^3} \int e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} v_\rho^{(\Lambda)}(\boldsymbol{r}', \boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} d\boldsymbol{r}' d\boldsymbol{r}$$
$$\simeq \frac{1}{(2\pi)^3} \frac{t_3}{6}(1 + x_3 P^\sigma)\theta(\Lambda - k')\theta(\Lambda - k),$$

and regularized with the same cutoff procedure (Λ truncation) as used for the density-independent parts.

In the practical calculations of matrix elements we start from a spherical harmonic-oscillator basis and transform the basis functions to momentum space. The Λ truncation can then be implemented using the Moshinsky transformation [21] to transform the coupled two-particle states to functions of relative and total momenta. Finally we employ the Pandya transformation [22] to obtain matrix elements in the particle-hole channel and use the Wigner-Eckart theorem to obtain angular-momentum-reduced expressions. The full implementation of this new regularized potential was done by extending the program HOSPHE (v1.02) [23].

One of the interactions employed in this work (SLy5) uses the direct part of the Coulomb interaction together with a Slater approximation for the Coulomb exchange. The Slater approximation results in a density-dependent term that mimics the HF exchange energy. To treat the HF part and the additional residual interaction consistently we have regularized the Slater term in the same way as for the other parts of the interaction.

To have a first idea about the influence of the Λ truncation we consider isospin-symmetric nuclear matter in the Hartree-Fock approximation. The corresponding zero-temperature equation of state (EOS), i.e., the energy per nucleon as a function of density is shown in Fig. 1. As seen in this figure, a Λ value of $\approx$1.5 fm^{-1} leaves the EOS unchanged up to about twice the saturation density and a value of $\approx$1.75 fm^{-1} leaves the EOS unchanged up to about three times the saturation density. Thus, when choosing a value for the regularization we consider values above 1.5 fm^{-1}, which keeps the relevant part of the EOS approximately the same.

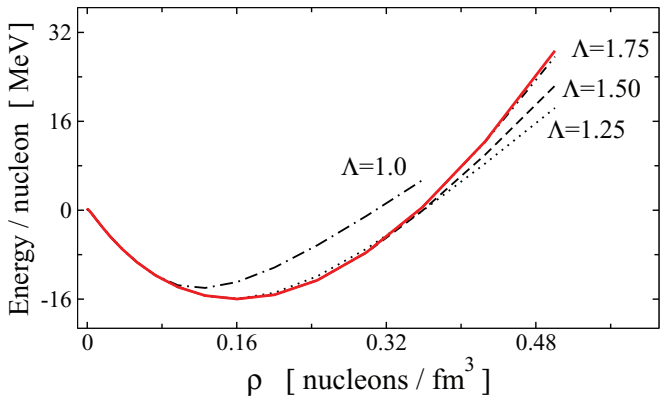

FIG. 1. (Color online) The energy per nucleon in symmetric nuclear matter (equal numbers of neutrons and protons) shown for the SLy5 [16] interaction and for different Λ fm^{-1} values in the HF approximation. The solid line illustrates the standard result for the untruncated interaction ($\Lambda = \infty$).

III. RESULTS FOR THE TOTAL CORRELATION CONTRIBUTION

An expression for the RPA correlation energy in the quasiboson approximation (QBA) is derived in Ref. [18] and using an analogous derivation one obtains a corresponding expression in the QRPA case [24]:

$$E_{\mathrm{QRPA}} = -\sum_{\nu=1}^{N} \hbar\omega_\nu \sum_{k<k'} \left|Y_{kk'}^\nu\right|^2. \tag{2}$$

To evaluate this expression we start by defining matrices containing the positive energy QRPA column vectors,

$$X = [X^1, X^2, \ldots, X^N], \quad Y = [Y^1, Y^2, \ldots, Y^N],$$

and the corresponding energies,

$$\Omega = \begin{bmatrix} \hbar\omega_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \hbar\omega_N \end{bmatrix}.$$

Then starting from the QRPA equation [22]

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} X \\ -Y \end{pmatrix} \Omega, \tag{3}$$

one can write the following pair of equations:

$$YX^{-1}A + YX^{-1}BYX^{-1} = Y\Omega X^{-1},$$
$$B^* + A^*YX^{-1} = -Y\Omega X^{-1}.$$

Summing these equations together and introducing $C = YX^{-1}$, the result is the equation

$$B^* + A^*C + CA + CBC = 0, \tag{4}$$

which is similar to the multiple scattering series derived in Ref. [25]. In terms of C, the QRPA correlation energy becomes

$$E_{\mathrm{QRPA}} = \frac{1}{2} \sum_{k<k', l<l'} B_{kk',ll'} C_{kk',ll'}. \tag{5}$$

Furthermore, by splitting the A matrix,

$$A_{kk',ll'} = (E_k + E_{k'})\,\delta_{kl}\delta_{k'l'} + \bar{A}_{kk',ll'},$$

Eq. (4) can be written

$$C_{kk',ll'} = \frac{-1}{E_k + E_{k'} + E_l + E_{l'}} (B^*_{kk',ll'} + (\bar{A}^*C)_{kk',ll'} + (C\bar{A})_{kk',ll'} + (CBC)_{kk',ll'}). \tag{6}$$

Finally, assuming that an iteration procedure for C converges, we can evaluate C order by order where the first-order

contribution

$$C^{(1)}_{kk',ll'} = \frac{-B^*_{kk',ll'}}{E_k + E_{k'} + E_l + E_{l'}}$$

is obtained by putting C equal to zero on the right-hand side of Eq. (6). Higher-order $C^{(n)}$ values are thus obtained by repeatedly inserting the previous expression $C^{(n-1)}$ on the right-hand side. By using $C^{(n)}$ in the formula for the correlation energy, Eq. (5), we obtain $E^{(n)}_{\mathrm{QRPA}}$. We have also verified numerically that the iteration converges to results consistent with Eq. (2).

An alternative approach that is less costly numerically is to evaluate the correlation contribution from second-order perturbation theory [26] starting from the HFB ground state and treating the residual part of the quasiparticle Hamiltonian as a perturbation. In this case, the only contributions that arise come from scattering to four quasiparticle states by the H^{40} part [18] of the Hamiltonian. This part of the Hamiltonian consists of the terms containing four quasiparticle creation operators and the terms containing four quasiparticle annihilation operators. The resulting energy contribution can be expressed in terms of the QRPA B matrix according to

$$E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{6}\sum_{k<k',l<l'} \frac{|B_{ll'kk'}|^2}{E_k + E_{k'} + E_{l'} + E_{l'}}. \qquad (7)$$

It is interesting to compare the QRPA and MBPT series order by order. The lowest-order QRPA term is three times larger than $E^{(2)}_{\mathrm{MBPT}}$ while the third-order $E^{(3)}_{\mathrm{MBPT}}$ is exactly obtained in the QRPA series (see Appendix). In higher orders, the two series differ as the QRPA expression only includes a subsequence of the full MBPT series.

In earlier papers by Ellis [27,28], the RPA correlation energy was investigated by starting from an unpaired ground state and summing contributions from both normal and pairing vibrations using diagrammatic techniques. In this way it was shown that in the QBA, the second-order contribution appears twice in the summation of the particle-hole ring series and once in the particle-particle series. A suggested remedy for this overcounting was to remove the second-order term from the particle-hole series and only keep it in the particle-particle series. In this work we have, however, refrained from using this approach because it is not directly applicable when starting from a HFB state where normal and pairing vibrations are generally mixed.

The corresponding correlation energies evaluated with the two methods described above are shown in Fig. 2(a). In both results, we have not included the part of the B matrix obtained in pnQRPA [22], which is associated with excitations of proton-neutron pairs. Although this contribution is certainly interesting, a first step in the direction of including these effects would involve tuning the effective interactions in the $T = 0$ pairing channel.

As seen in Fig. 2, for both methods the correlation energy amounts to a rather large part of the total binding energy. The QRPA formula predicts the largest values as the QBA overestimates the ground-state correlations [18,27–29]. Although this could possibly be corrected for, in the following we instead focus on the MBPT2 results.

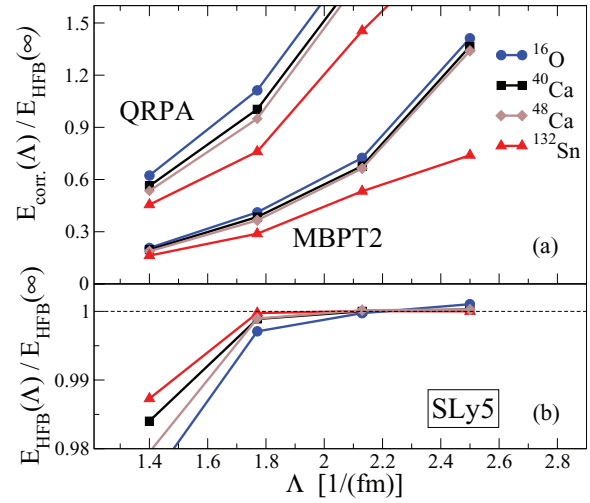

FIG. 2. (Color online) Panel (a) shows the binding energy contribution from QRPA and MBPT2 scaled with the HFB energy. Panel (b) shows the influence of the truncation on the HFB energy. Calculations were done using the SLy5 [16] parametrization for the Skyrme interaction using a basis of 14 oscillator shells.

In the case of ^{16}O, the smallest $\Lambda = 1.4$ fm^{-1} used in the figure gives a contribution from MBPT2 which is 21% of the HFB energy. This contribution gradually decreases for the heavier nuclei and becomes 16% in ^{132}Sn, indicating that the mean-field approximation becomes better in the heavier systems, as one may expect.

Figure 2(b) shows the influence the regularization has on the HFB energy. As seen in this figure, the HFB energy converges to the untruncated value as the cutoff is increased and even for rather low cutoffs of $\Lambda = 1.5$ fm^{-1} the change in total binding energy stays within a few percent. This tells us that the HFB energy is not very sensitive to higher-momentum parts of the interaction potential in the particle-hole channel.

In both the QRPA and the MBPT2, the correlation energy increases rapidly with increasing Λ; therefore we consider Λ values in the range of 1.6–1.8 fm^{-1}. These values lead to the smallest correlation energies while causing moderate changes of the HFB energies.

We solve the HFB equations in an iterative way where the nuclear densities change during iterations. Because the interaction depends on the densities, the interaction also changes in each such HFB iteration step. Recalculating the regularized density-dependent interaction in each HFB iteration is time-consuming because it involves a transformation to relative nucleon coordinates. However, because the HFB energy stays roughly the same providing Λ is large enough (see Fig. 2), it is a good approximation to neglect the regularization for the HFB part of the calculation and only regularize when generating the residual interaction. This is quite important for the method to be efficient and a strong motivation for introducing the regularization in the way done here rather than using, e.g., a Gaussian interaction. However, in this work we follow the procedure to recalculate the regularization in each HFB step to make the least amount of approximations.

Using an angular-momentum coupled notation, the correlation energy can be divided into partial contributions arising

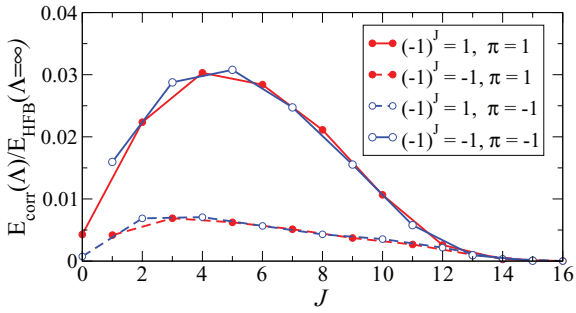

FIG. 3. (Color online) Partial contributions to the MBPT2 correlation energy for $\Lambda = 1.8$ and ^{132}Sn using SLy5.

from QRPA excitations with different total angular momentum J and parity π. Because the MBPT2 result can be seen as an approximation of the full QRPA result, we use the same division into multipole contributions also in this case. These partial contributions are shown in Fig. 3 for ^{132}Sn. As seen in this figure the largest contributions come from natural parity states with $(-1)^J = \pi$. Both positive-parity and negative-parity contributions are equally important and show maxima for $J = 4$ and $J = 5$, respectively.

IV. FLUCTUATING PARTS OF THE CORRELATION ENERGY

Both Skyrme interactions considered in this work have been fitted to reproduce binding energies and charge radii of a few magic nuclei. A difference between them is that the SKX interaction uses single-particle energies [15] in the fitting procedure, while the SLy5 interaction [16] uses properties of nuclear matter. Because these fits were done at the HF level, they effectively include the average part of the nuclear correlation energy. Going beyond the HF level by explicitly including the MBPT2 correlation energy thus requires a refit of the interaction parameters. As a first step, we refrain from performing a full refit of the interaction and instead make a simple compensation for the overbinding obtained when including this extra energy contribution.

The nuclear ground-state energy can be divided into a liquid-drop part that captures the average variations as a function of nucleon numbers and a fluctuating part that mainly depends on the shell structure. We make the same division for the correlation energy and fit a liquid-drop expression [18],

$$E_{\rm LD} = a_{\rm vol} A + a_{\rm surf} A^{2/3} + a_{\rm sym} \frac{(N-Z)^2}{A}, \qquad (8)$$

to the calculated $E^{(2)}_{\rm MBPT}$ energies. The liquid-drop part is then taken as a measure of the average part of the correlation energy. Because this part is already included in the HF fits we only keep the fluctuating part of the correlation energy $\Delta E = E^{(2)}_{\rm MBPT} - E_{\rm LD}$. Although the final goal is to obtain an effective interaction suitable for calculations beyond HF, this first approximation allows us to get an idea of the effect of including the MBPT2 correlation energy and to see whether it improves the description of nuclear ground-state energies.

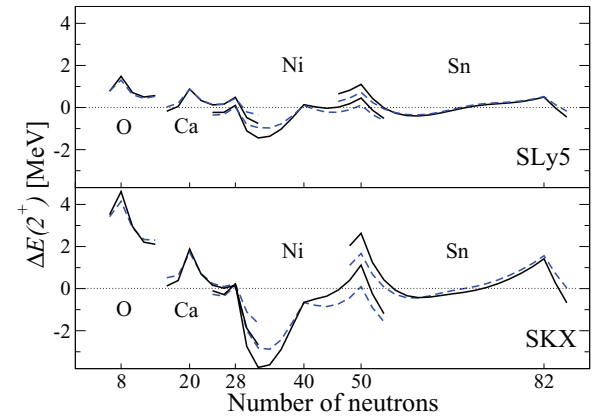

FIG. 4. (Color online) The renormalized part of the MBPT2 correlation energy associated with quadrupole shape vibrations ($J = 2^+$) shown for $\Lambda = 1.6$ (dashed curve) and $\Lambda = 1.8$ (solid curve).

In this way the renormalized correlation contributions associated with 2^+ and 3^- vibrations are extracted and shown in Figs. 4 and 5. The fluctuations show pronounced shell effects and tend to give increased binding energy contributions for the open-shell nuclei compared to the magic ones. The two different choices of Λ truncation shown in the figures give similar results, indicating that the obtained fluctuations are mainly associated with the properties of the low-momentum part of the interaction.

In the 2^+ channel, the SKX interaction gives fluctuations larger than those of the SLy5 interaction. Previous results for quadrupole correlations using the SkI3 interaction and a collective Hamiltonian [30] gave similar results with fluctuations that are somewhere in between the ones we get for the SKX and the SLy5 interactions.

Contributions from octupole vibrations are similar in magnitude to the quadrupole vibrations and show the same tendency of increasing the energies for magic nuclei as compared to their neighbors. Notable exceptions are ^{16}O and ^{40}Ca, which have Fermi levels between opposite parity shells and show the reversed trend. For such nuclei, with Fermi levels between opposite-parity shells, negative-parity excitations can be made at a lower energy cost than in the neighboring nuclei.

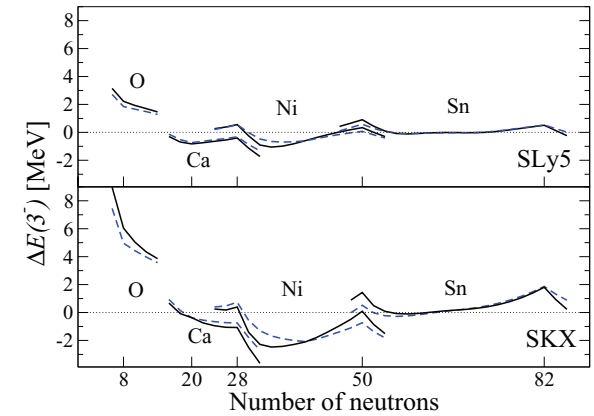

FIG. 5. (Color online) Same as Fig. 4 for octupole shape vibrations ($J = 3^-$).

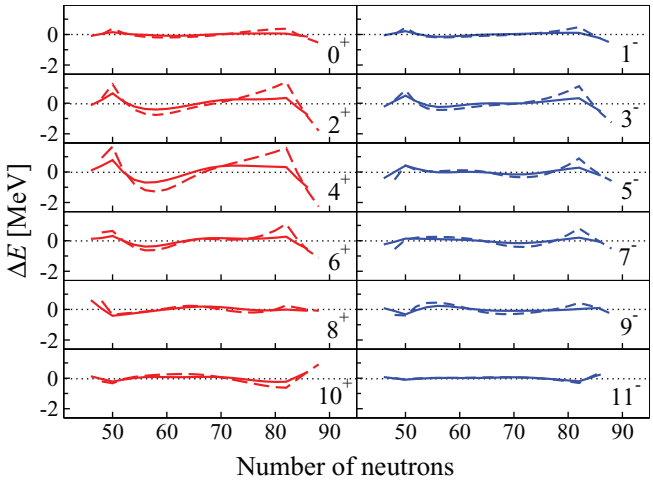

FIG. 6. (Color online) The renormalized part of the MBPT2 correlation energy separated into contributions from different multipoles for $\Lambda = 1.8$. Solid curves are for SLy5 and dashed curves for SKX. In this figure the renormalization was done by fitting Eq. (8) to Sn nuclei only.

A low energy cost then typically leads to an increase in correlation energy. The same explanation works for the magic nuclei which are generally calculated to have less correlation energy than their neighbors possibly because there is a gap in the spectra that makes excitations more expensive.

Figure 6 shows the fluctuating part of the correlation energies separated into contributions from different multipoles in the case of the Sn chain. The main fluctuations come from the $J^\pi = 2^+$, 4^+, 3^-, and 5^- channels and show the trend of making double-magic nuclei less bound relative to the semi-magic ones. Interesting exceptions are found in the 10^+ and 11^- contributions, which show the opposite trend around $N = 82$. Going even higher in multipoles, the curves tend to flatten out.

A. Comparison with experiment

When comparing with experimental ground-state energies, we restrict ourselves to contributions from the well-studied low-order multipoles $J^\pi = 0^+$, 2^+, 1^-, and 3^- where the effective interactions generally give reasonable results for low-lying collective states and giant resonances.

The differences between calculated and experimental ground-state energies using the SLy5 and the SKX [15] interactions are shown in Figs. 7 and 8. The dotted lines denote the results of the HFB treatment ($\Lambda = \infty$) using a total of 31 oscillator shells. For both interactions, the HFB results are within a few MeV of the experimental values. The SKX results differ somewhat from the ones in Ref. [15], which is due to a different treatment of the Coulomb interaction. While we calculate the Coulomb contribution directly from the proton density, in Ref. [15] some additional corrections are taken into account.

It is interesting to notice that with both interactions the HFB errors for magic nuclei with $N = 8$, 20, and 28 go up in energy compared to their neighbors, which could possibly

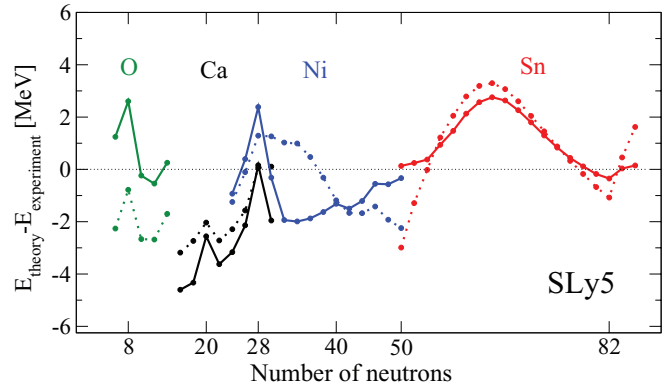

FIG. 7. (Color online) Difference between experimental [31,32] and theoretical ground-state energies in the HFB approach (dotted curves) and when adding surface vibrations corresponding to multipolarities $J^\pi = 0^+, 2^+, 1^-$, and 3^- (solid curves). The figure is drawn using the SLy5 interaction and $\Lambda = 1.8$ fm^{-1}.

be cured by making the corresponding gaps in the neutron spectra somewhat larger. With SLy5, the situation is reversed for the gaps at $N = 50$ and 82, where the errors instead dip down.

The lowest-order surface vibrations are calculated using MBPT2 and a total of 14 oscillator shells. The fluctuating part of the correlation energy is well converged using 14 oscillator shells and is extracted by fitting the liquid-drop expression to all the included nuclei. The solid lines in Figs. 7 and 8 show the results of adding these fluctuating parts to the HFB energies. As discussed previously the main effect of the surface vibrations is to push the magic nuclei up in energy as compared to the neighboring nuclei. For SLy5 this gives corrections that go in the right direction in the region of the $N = 50$ and 82 gaps, but in the opposite direction for the lighter magic nuclei. Although both interactions give rise to similar fluctuations, the larger magnitude fluctuations in combination with different HFB results obtained using the SKX parametrization compare less favorably with experiment. If a Skyrme interaction tuned at the MBPT2 level is used at the HFB level, one would expect it to predict the magic nuclei to be more bound than their neighbors to leave room for the additional correlation part.

Some of the nuclei included in the plot have the same number of neutrons and protons, which gives rise to an

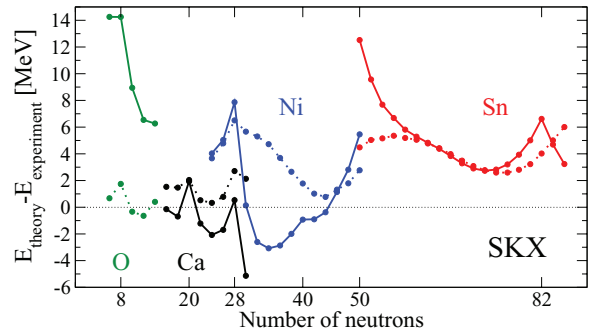

FIG. 8. (Color online) Same as 7 but for the SKX interaction.

additional contribution to the binding energy. This contribution is often modeled by adding so-called Wigner corrections (see, e.g., Ref. [33]), which give an additional binding energy contribution of roughly 2 MeV for the $N = Z$ nuclei. Such a contribution would reduce some of the remaining fluctuations but would, for example, not improve the results around ^{48}Ca. Furthermore, such a phenomenological treatment is clearly unsatisfactory and a more thorough investigation of these interesting effects is clearly called for.

In the case of $\Lambda = 1.8$ (fm)$^{-1}$ the parameters obtained from the liquid-drop fit to the SLy5 correlation energies resulting from $J = 0^+$, 2^+, 1^-, and 3^- vibrations become $\{a_{\rm vol}, a_{\rm surf}, a_{\rm sym}\} = \{0.99, -8.24, 0.77\}$ MeV, while for SKX the average contribution is roughly twice as large. A possible reason that the SKX interaction gives more correlation energy is that SKX has larger effective mass ($m*/m = 0.99$) [15] than SLy5 ($m*/m = 0.69$) [16] and thus a denser spectrum, giving smaller denominators in Eq. (7).

Typical liquid-drop parameters obtained when fitting to experimental ground-state energies are $\{a_{\rm vol}, a_{\rm surf}, a_{\rm sym}\} = \{-15.68, 18.56, 28.1\}$ MeV [18]. Thus, the main change in the average energy obtained by adding the correlations resulting from low-lying surface vibrations is to modify the surface energy. The reduction of the surface energy and the increased energy for the volume part will likely move nucleons from the bulk to the surface, leading to a more diffuse surface region. Thus, refitting the Skyrme parameters to absorb the average part of the correlations and have a model on the MBPT2 level would likely involve tuning not only the density-dependent terms but also the gradient terms, which are more sensitive to the surface region. When refitting, it is important to have as small correlation corrections as possible, so that the HFB ground state is a reasonable first approximation. In this respect the smaller average contribution obtained in the SLy5 case makes it a better starting point. Nuclear matter properties can also be used to refit, but then the nuclear matter EOS has to be calculated at the corresponding level of many-body theory (see, e.g., Ref. [34] for a description of nuclear matter at MBPT2 order).

V. SUMMARY AND CONCLUSIONS

The problem we set out to investigate was whether effective nuclear interactions can provide improved descriptions of nuclear binding energies when correlation effects beyond the HFB level are taken into account. To this end, it was essential to introduce a momentum cutoff in Skyrme's potential to obtain convergent results. The calculations show that even with a low cutoff, the average part of the correlation corrections are quite substantial (about 25% of the total binding energy with MBPT2 and $\Lambda = 1.8$ fm^{-1}). We then considered a schematic renormalization by removing the average parts of the correlation energies. The remaining fluctuations are similar for both interactions studied and not very sensitive to the exact choice of the momentum truncation. When the SLy5 Skyrme parametrization is used, the fluctuations associated with low-lying surface vibrations do lead to a reduction of the errors compared to experiment. To obtain a model that can be used with more confidence, a refit of the interaction parameters should be performed. The ideal would be to compare results of an interaction fitted on the HFB level to those of an interaction fitted on the MBPT2 level using the same set of experimental data.

Some interesting features can be learned from the obtained fluctuations. One result is that octupole vibrations are predicted to give fluctuations of magnitude similar to that of the quadrupole corrections and to contribute in a similar way. It is also interesting to see that higher multipoles such as 4^+ and 5^- gave rise to large fluctuations in the case of Sn isotopes.

Although the fluctuating parts were extracted using MBPT2, the QRPA formula is also promising because it allows for an infinite summation of diagrams. However, for it to be a practical tool, the QBA approximation must be improved and a careful study of the corrections in the quasiparticle case would be needed. Once such a formalism is in place, the correlation energy could be calculated using iterative approaches [35] similar in spirit to the ones we recently employed for the calculation of low-lying excitations [12].

In summary, we have regularized Skyrme's potential and used it to study higher-order corrections to binding energies beyond the HFB approach. Compared to other approaches, the method used here has the advantage of not relying on energy truncations to converge and that correlations resulting from many degrees of freedom (e.g., vibrational modes) can be simultaneously included. Apart from nuclear binding energies studied in this work, there are other quantities that could possibly be modeled better in a formalism that goes beyond the HFB approximation. An example is the calculation of α-decay preformation amplitudes, which show a dramatic increase as correlations between nucleons are introduced [36].

ACKNOWLEDGMENTS

B.G.C. acknowledges the Royal Physiographic Society in Lund for providing funding for the computers on which the calculations were performed. We also thank I. Ragnarsson for valuable comments on the manuscript. This work was supported in part by the Academy of Finland and the University of Jyväskylä within the FIDIPRO program.

APPENDIX: HIGHER-ORDER CORRECTIONS

Starting from the HFB ground state, denoted $|0\rangle$, and applying perturbation theory to third order gives the expression

$$E^{(3)}_{\rm MBPT} = \sum_{kk'} \frac{\langle 0|H_{\rm res}|k\rangle\langle k|H_{\rm res}|k'\rangle\langle k'|H_{\rm res}|0\rangle}{(E_0 - E_k)(E_0 - E_{k'})},$$

where the sum runs over all excited quasiparticle states and involves their excitation energies, E_k. The residual Hamiltonian can be divided into unique parts [18]

$$H_{\rm res} = H^{40} + H^{31} + H^{22}.$$

The indexes on the H^{31} term denote that it is composed of terms that are products of either a three-quasiparticle creation operator and a one-quasiparticle annihilation operator or vice verse. The other terms are defined analogously. Only certain parts of the residual quasiparticle Hamiltonian give rise to nonzero elements, which allows us to write

$$E^{(3)}_{\mathrm{MBPT}} = \sum_{kk'} \frac{\langle 0|H^{40}|k\rangle\langle k|H^{22}|k'\rangle\langle k'|H^{40}|0\rangle}{(E_0 - E_k)(E_0 - E_{k'})},$$

where one notices that the $|k\rangle$ and $|k'\rangle$ states have to be four-quasiparticle states. Rewriting the sum in terms of the QRPA matrices

$$B_{aa',bb'} = \langle bb'aa'|H^{40}|0\rangle$$

and

$$A_{aa',bb''} = [(E_b + E_{b'})\delta_{ab}\delta_{a'b'} + \bar{A}_{aa',bb'}],$$

where

$$\bar{A}_{aa',bb'} = \langle aa'|H^{22}|bb'\rangle$$

and the quasiparticle labels are ordered as $a < a'$ and $b < b'$ gives

$$E^{(3)}_{\mathrm{MBPT}} = \sum_{a<a',b<b',c<c'} \frac{B^*_{aa',cc'}\bar{A}_{cc',bb'}B_{bb',aa'}}{E_{aa'cc'}E_{bb'aa'}},$$

where we have introduced the shorthand notation $E_{abcd} = E_a + E_b + E_c + E_d$.

A term that is third order in the residual interaction can also be found from the QRPA expression by evaluating Eq. (5) to higher orders. The third-order term obtained in this way takes exactly the same form as the perturbation theory expression. Starting at fourth order, the QRPA series contains less terms than perturbation theory, for example, the H^{31} part of the quasiparticle Hamiltonian never enters in the QRPA expressions. It would be interesting to make a comparison of the QRPA energy with, for example, shell-model calculations using the same interaction to get a better idea of the accuracy of the QRPA expression and the importance of these higher-order terms in the series. A more careful treatment of particle-number fluctuations is also possible by, for example, using projected-quasiparticle perturbation theory [37].

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