Fluctuating parts of nuclear ground state correlation energies

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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 cut-off in relative momenta is introduced in order to remove ultraviolet divergences caused by the zero-range character of the interaction. Corrections to binding energies are then calculated using the quasiparticle-random-phase approximation (QRPA) and second order many-body perturbation theory (MBPT2).

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 cut-off 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.

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I. INTRODUCTION

The atomic nucleus is a complicated quantum mechanical system where the probability to find 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 nuclear matter too complex to compute directly using ab initio theory. One therefore has to resort to more tractable methods which take the most important correlation effects explicitly into account, i.e. the ones that are important in order to describe observables, while the remaining effects are treated in an approximate way.

An often used starting point is to assume that the 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 (GCM) [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 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 QRPA designating RPA for Bogoliubov quasi-particles. 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 is 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 divergences 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 divergences in connection with zero-range forces.

It is a major theme of the present work to eliminate such divergences by introducing cut-offs in momenta for our chosen Skyrme-like interaction potentials\[3\]. This procedure 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 Quasiparticle-random-phase approximation (QRPA) and the MBPT2 method. In sects. 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

\[
\tilde{V}(r_1', r_2') = v(r', r) \delta (R - R'),
\]

where \( R = \frac{1}{2} (r_1 + r_2) \) and \( r = r_1 - r_2 \) denotes 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\[3\] given by

\[
\tilde{v}(k', k) = \frac{1}{(2\pi)^3} \int e^{-ik'r'} v(r', r) e^{ikr} dr'dr
\]

\[\simeq \frac{1}{(2\pi)^3} \left[ t_0 (1 + x_0 P^2) + \frac{1}{2} t_1 (1 + x_1 P^2) (k'^2 + k_0) + t_2 (1 + x_2 P^2) k' \cdot k + i W_0 (\sigma_1 + \sigma_2) \cdot k' \times k \right].\]

In this expression we have omitted the tensor potential included in Ref.\[3\] since it is not used in the parametrizations we will employ later. This expression can be viewed as the first members in a low-momentum expansion of the effective nuclear potential going up to second order in relative momenta (compare e.g.\[3,4\] 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 will 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\[1\].

In order 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\[3\] and introduce a cut-off in momenta. We replace his original interaction by

\[\tilde{v}^{(\Lambda)}(k', k) = \tilde{v}(k', k) \theta(\Lambda - k') \theta(\Lambda - k),\]

which vanishes at momenta above \( \Lambda (\text{fm})^{-1} \). In the limit of a large \( \Lambda \) one regains the results of the original untruncated interaction, but for finite values, the cut-off regularizes the interaction so that beyond-mean field calculations converge. The introduction of the cut-off 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\[12\, 13\]. Since 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 (\( a = 0.66 \text{ fm} \)) as before. Since we will only consider cases where neutrons are in open shells we tune the pairing strengths to make the lowest neutron quasi-particle energies to agree with the experimental gaps determined in\[14\]. The resulting isovector pairing strength becomes 560 MeV(fm)^{-1} when the SKX Skyrme parameters\[15\] are used in the particle-hole channel and somewhat larger (540 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 which is intended to describe missing three-body and

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1 Note that in the calculations of low-energy excitations the discussed divergences did not constitute a problem. In fact, it is mainly the high-energy excitations which are modified by a momentum cut-off.
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 \cite{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 \cite{18}.

\[
\tilde{v}_{\rho} = \frac{\partial^2 E_{HF}}{\partial \rho_{q} \partial \rho_{n}} = \rho v_{\rho_{mqn}} \rho + \sum_{j} \rho_{j} \left( \frac{\partial v_{mjnl}[\rho]}{\partial \rho_{q}} + \frac{\partial v_{pjnl}[\rho]}{\partial \rho_{nm}} \right) + \frac{1}{2} \sum_{ijkl} \rho_{i} \rho_{j} \left( \frac{\partial v_{ijkl}[\rho]}{\partial \rho_{nm}} \right) \bigg|_{\rho = \rho_{0}}.
\]

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 \cite{19}.

The density-dependent two-body interaction is introduced in the standard form \cite{20}

\[
\tilde{V}_{\rho} = \rho^{(A)}(r', r) \rho^{(A)}(R) \delta(R - R'),
\]

with a dependence on the nucleon density \( \rho \) to some power \( \alpha \) which take on different values for different parameterizations. The part dependent on relative coordinates is expanded to lowest order in relative momenta

\[
\tilde{v}_{\rho}^{(A)}(k', k) = \frac{1}{(2\pi)^{3}} \int e^{-ik' \cdot r'} \rho^{(A)}(r', r) e^{ik \cdot r} d^{3}r' d^{3}r
\]

\[
\simeq \frac{1}{(2\pi)^{3}} t_{3} \frac{1}{6} \left( 1 + x_{3} P_{3} \right) \theta(\Lambda - k') \theta(\Lambda - k),
\]

and regularized with the same cut-off procedure (\( \Lambda \)-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 \( \Lambda \)-truncation can then be implemented using the Moshinsky transformation \cite{21} to transform the coupled two-particle states to functions of relative and total momenta. Finally we employ the Pandya transformation \cite{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 HOSPHIE (v1.02) \cite{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 which mimics the HF exchange energy. In order 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.

In order to have a first idea about the influence of the \( \Lambda \)-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 \( \Lambda \)-value of \( \approx 1.5 \text{ (fm)}^{-1} \) leaves the EOS unchanged up to about twice the saturation density and a value of \( \approx 1.75 \text{ (fm)}^{-1} \) leaves the EOS unchanged up to about three times the saturation density. Thus, when choosing a value for the regularization we will consider values above \( 1.5 \text{ (fm)}^{-1} \) which keeps the relevant part of the EOS approximately the same.

### III. RESULTS FOR THE TOTAL CORRELATION CONTRIBUTION

An expression for the RPA correlation energy in the quasi-boson approximation (QBA) was derived in \cite{18} and using an analogous derivation one obtains a corresponding expression in the QRPA case \cite{24}

\[
E_{QRPA} = - \sum_{\nu} \hbar \omega_{\nu} \sum_{k < k'} |Y_{kk'}^{\nu}|^2.
\]

In order to evaluate this expression we start by defining matrices containing the positive energy QRPA vectors

\[
X = [X^1, X^2, ..., X^N], \quad Y = [Y^1, Y^2, ..., Y^N]
\]
and corresponding energies
\[
\Omega = \begin{bmatrix} h\omega_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & h\omega_N \end{bmatrix}.
\]

Then starting from the QRPA equation \[22\]
\[
\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} X \\ -Y \end{pmatrix} \Omega
\]
(3)
one can write the 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
\[
B^* + A^*C + CA + CBC = 0 \]
(4)
which is similar to the multiple scattering series derived in Ref. \[25\]. In terms of \(C\), the QRPA correlation energy becomes
\[
E_{\text{QRPA}} = \frac{1}{2} \sum_{k<k',l<l'} B_{kk',ll'} C_{kk',ll'}.
\]
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
\[
C_{kk',ll'} = \frac{-1}{E_k + E_{k'} + E_l + E_{l'}} \times \left( B_{kk',ll'}^* + (A^C)_{kk',ll'} + (C\bar{A})_{kk',ll'} 
+ (CBC)_{kk',ll'} \right).
\]
(6)

Finally, assuming that an iteration procedure for \(C\) converges, we can evaluate \(C\) order by order where the first order contribution
\[
C_{kk',ll'}^{(1)} = \frac{-B_{kk',ll'}^*}{E_k + E_{k'} + E_l + E_{l'}}
\]
is obtained by putting \(C\) equal to zero on the right hand side of Eq. 6. Higher orders \(C^{(n)}\) 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. 3, we obtain \(E_{\text{QRPA}}^{(n)}\). Numerically we have also verified that the iteration converges to results consistent with Eq. 2.

An alternative approach which is less costly numerically is to evaluate the correlation contribution from second order perturbation theory \[20\] starting from the HFB ground state and treating the residual part of the quasi-particle Hamiltonian as a perturbation. In this case, the only contributions that arise come from scattering to four particle Hamiltonian as a perturbation. In this case, the only contributions that arise come from scattering to four quasi-particle states via the \(H_4^{(0)}\) part \[18\] of the Hamiltonian. This contribution can be expressed in terms of the QRPA \(B\) matrix according to
\[
E_{\text{MBPT}}^{(2)} = \frac{1}{6} \sum_{k<k',l<l'} \frac{|B_{ll'kk'}^*|^2}{E_k + E_{k'} + E_l + E_{l'}}.
\]
(7)

It is interesting to compare the QRPA and MBPT series order by order. The lowest order QRPA term is three times larger than \(E_{\text{MBPT}}^{(2)}\) while the third order \(E_{\text{MBPT}}^{(3)}\) is exactly obtained in the QRPA series. 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 since 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 panel (a)
of Fig. 2. 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 as the QBA overestimates the ground state correlations [18, 27–29].

In the case of $^{16}\text{O}$, the smallest $\Lambda = 1.4 \text{ (fm)}^{-1}$ 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 $^{132}\text{Sn}$.

Panel (b) of Fig. 2 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 cut-off is increased and even for rather low cutoffs of $\Lambda = 1.5 \text{ (fm)}^{-1}$ 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 potential in the particle-hole channel.

In both the QRPA and in MBPT2, the correlation energy increases rapidly with increasing $\Lambda$ and in the following we will consider $\Lambda$ 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.

Since the HFB energy stays roughly the same, 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 in order for the method to be practical since otherwise one would have to recalculate the regularized density-dependent interaction in each HFB iteration. This is a strong motivation for introducing the regularization in the way done here rather than using for example a Gaussian interaction. For the purpose of making the least amount of approximations, we have however used the time-consuming strategy to recalculate the regularization in each HFB step.

Using an angular-momentum coupled notation, the correlation energy can be divided into partial contributions arising from QRPA excitations with different total angular momentum $J$ and parity $\pi$. Since the MBPT2 result can be seen as an approximation to the full QRPA results we use the same division into multipole contributions also in this case. These partial contribution are shown in Fig. 3 for $^{132}\text{Sn}$. 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.

The internucleon potentials we employ have parameters which are fitted in order to give reasonable nuclear properties at the HFB level. Therefore the average part of the correlation energies is already effectively included through the fitting of the model parameters. The total 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. Rather than performing a full refit of the interaction to have a model on the MBPT2 level, in this first study we will make a simple compensation for this overbinding. We compensate by fitting a liquid-drop expression [18]

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

to the correlation energy $E_{MBPT}^{(2)}$ which is then subtracted to give the fluctuating part of the correlation energy $\Delta E = E_{MBPT}^{(2)} - E_{LD}$. The main goal is to get an idea what kind of fluctuations one obtains and to see if these are correlated with errors obtained in the description of ground-state energies.

In this way the renormalized correlation contributions associated with $2^+$ and $3^-$ vibrations are extracted and shown in Figs. 11 and 15. 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 $\Lambda$-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 larger fluctuations than the SLy5 interaction. Previous results for quadrupole correlations using the SkI3 interaction and a collective Hamiltonian 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.

Fig. 6 shows the fluctuating part of the correlation energies 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.

![Figure 4](image1.png)

Figure 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 $\Lambda = 1.8$ (full curve).

![Figure 5](image2.png)

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

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 difference between calculated and experimental ground-state energies using the SLy5 and the SKX 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 [15] which is due to a different treatment of the Coulomb...
interaction. While we calculate the direct Coulomb contribution directly from the proton density, in some interaction. It is interesting to notice that with both interactions the errors for magic nuclei with \( N = 8, 20 \) and 28 go up in energy compared to their neighbors which could possibly 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, compares less favorable with experiment. If a Skyrme interaction tuned at the MBPT2 level is used on the HFB level, one would expect it to predict the magic nuclei to be more bound than their neighbors in order 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 additional contribution to the binding energy. This contribution is often modeled by adding so called Wigner corrections (see e.g. \(^3\)) which gives 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 not improve the results around \(^{48}\)Ca for example. 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 \( \{a_{\text{col}}, a_{\text{surf}}, a_{\text{sym}}\} = \{0.99, -8.24, 0.77\} \) 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 \( (m_s / m = 0.99) \) \(^9\) than SLy5 \( (m_s / m = 0.69) \) \(^{10}\) and thus a denser spectrum, giving smaller denominators in Eq. 7.

Typical liquid-drop parameters obtained when fitting to experimental ground-state energies are \( \{a_{\text{col}}, a_{\text{surf}}, a_{\text{sym}}\} = \{-15.68, 18.56, 28.1\} \) MeV \(^{11}\). 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 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. \(^{34}\) 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 cut-off in Skyrme’s potential in order to obtain convergent results. The calculations show that even with a low cut-off, 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 so sensitive to the exact choice of the momentum truncation. When the SLy5 Skyrme parametrization is used, the fluctuations associated with low-lying surface vibrations does lead to a reduction of the errors compared to experiment. In order 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 HFB level to those of an interaction fitted on the MBPT2 level using the same set of experimental data.

Some interesting features can anyway be learned from the obtained fluctuations. One result is that octupole vibrations are predicted to give fluctuations of similar magnitude as 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.

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

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 in order 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 alpha-decay preformation amplitudes which shows a dramatic increase as correlations between nucleons are introduced.

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