Correlation energy contribution to nuclear masses

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The ground state correlation energies associated with collective surface and pairing vibrations are calculated for Pb- and Ca-isotopes. It is shown that this contribution, when added to those predicted by one of the most accurate modern nuclear mass formula (HFBCS MSk7 mass formula), reduces the associated rms error by an important factor, making mean field theory, once its time dependence is taken into account, a quantitative predictive tool for nuclear masses.

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particle-hole operators \(a_i^+a_i\) and \((a_i^+a_i)^+\) are replaced by the boson operators \(\Gamma_{ki}^+\) and \(\Gamma_{ki}\). Because collective vibration can be viewed as correlated particle-hole excitations, the corresponding boson creation operator can be written as

\[
\Gamma_{\alpha}^+(n) = \sum_{ki} (X_{ki}^\alpha(n)\Gamma_{ki}^+ + Y_{ki}^\alpha(n)\Gamma_{ki}),
\]

where \(X_{ki}^\alpha\) and \(Y_{ki}^\alpha\) are the forward-going and backward-going amplitudes fulfilling the normalization condition

\[
|\Gamma_{\alpha}(n),\Gamma_{\alpha}^+(n)| = \sum_{ki} (|X_{ki}^\alpha(n)|^2 - |Y_{ki}^\alpha(n)|^2) = 1.
\]

The equations which determine the frequencies of the vibrational modes of quantum number \(\alpha\) (with progressively high energy \(n = 1, 2, \ldots\)) are obtained from the relation

\[
[H, \Gamma_{\alpha}^+(n)] = \hbar \omega_{\alpha}(n)\Gamma_{\alpha}^+(n).
\]

In the above equation \(H\) is the total hamiltonian, sum of a single-particle and a two-body interaction term. In the present calculations we have used self-consistently the Skyrme plus pairing interaction given by the MSk7 parameter set. The RPA ground state energy is given by (cf. e.g. [11])

\[
E_{\text{RPA}} = E_{HF} - (2\lambda + 1) \sum_{\alpha, n} \hbar \omega_{\alpha}(n) \sum_k |Y_{ki}^\alpha(n)|^2,
\]

in keeping with the fact that the amplitudes \(Y_{ki}^\alpha(n)\) are directly related to the ground state correlations induced by the corresponding vibrational modes. The second term of the r.h.s. is called correlation energy.

It is well known that open shell nuclei display a finite BCS gap \(\Delta\), as a result of the pairing correlations acting between pairs of nucleons moving in time reversal states close to the Fermi energy. In closed shell nuclei, pairing correlations are not strong enough to overcome the large single-particle gap, and \(\Delta = 0\). Nevertheless, pairing plays an important role in determining the (low-lying) structure of these nuclei. In particular, it leads to pairing vibrations [9], which change in two the number of nucleons, that is vibrations which can be viewed as two correlated particles (pair addition modes) or two correlated holes (pair removal modes). An example of these modes is provided by the ground state of \(^{210}\)Pb and of \(^{206}\)Pb which can be viewed as the pair addition and the pair subtraction modes of \(^{208}\)Pb respectively. These modes are specifically probed through two particle transfer reactions [12]. The pair addition and pair subtraction modes can be written as

\[
\Gamma_{\alpha}^+(n) = \sum_k X_k^\alpha(n)\Gamma_k^+ + \sum_i Y_i^\alpha(n)\Gamma_i,
\]

and

\[
\Gamma_{\alpha}^+(n) = \sum_i X_i^\alpha(n)\Gamma_i^+ + \sum_k Y_k^\alpha(n)\Gamma_k,
\]

where \(\Gamma_{\alpha}^+ = (a_i^+a_i)^+\) creates a pair of nucleons coupled to angular momentum zero in levels with energy larger than the Fermi energy \((\varepsilon_i > \varepsilon_F)\), while \(\Gamma_{\alpha} = (a_i^+a_i)\) annihilates a pair of nucleons in occupied states \((\varepsilon_i \leq \varepsilon_F)\). Use is made of a hamiltonian \(H = H_{sp} + H_p\), sum of a single-particle term and of a pairing force with constant matrix \(H_p = -G \sum_{ij} a_i^+a_j^+a_i^{}a_j\), the commutation relation given in Eq. (3) leads to the dispersion relations

\[
\frac{1}{G} = \sum_k \frac{\Omega_k}{2\varepsilon_k - \hbar \omega_{\alpha}(n)} + \sum_i \frac{\Omega_i}{2\varepsilon_i + \hbar \omega_{\alpha}(n)},
\]

\[
\frac{1}{G} = \sum_k \frac{\Omega_k}{2\varepsilon_k + \hbar \omega_{\alpha}(n)} + \sum_i \frac{\Omega_i}{2\varepsilon_i - \hbar \omega_{\alpha}(n)},
\]

where \(\Omega = (2j + 1)/2\) is the pair degeneracy of the single-particle orbital with total angular momentum \(j\), while \(\varepsilon_j = \varepsilon_j - \varepsilon_F\). The amplitudes are

\[
X_k^\alpha(n) = \frac{\Lambda_{\alpha}(n)\sqrt{\Omega_k}}{2\varepsilon_k - \hbar \omega_{\alpha}(n)}, \quad Y_i^\alpha(n) = \frac{\Lambda_{\alpha}(n)\sqrt{\Omega_i}}{2\varepsilon_i + \hbar \omega_{\alpha}(n)},
\]

and

\[
X_i^\alpha(n) = \frac{\Lambda_{\alpha}(n)\sqrt{\Omega_k}}{2\varepsilon_i + \hbar \omega_{\alpha}(n)}, \quad Y_k^\alpha(n) = \frac{\Lambda_{\alpha}(n)\sqrt{\Omega_i}}{2\varepsilon_k - \hbar \omega_{\alpha}(n)},
\]

\(\Lambda_{\alpha}(n)\) and \(\Lambda_{\alpha}(n)\) being normalization constants determined from the relation given in Eq. (2).

In Fig. 1 we show the dispersion relations given in Eqs. (7) and (8) calculated for \(^{208}\)Pb for both protons and neutrons (cf. also Fig. 11), making use of the valence orbitals of this nucleus. The valence orbitals used in our calculations were determined with the help of a Woods-Saxon potential with standard parametrization [11] and the energies have been replaced with the experimental values whenever available. The results obtained using the standard Woods-Saxon levels coincide with those calculated making use of the experimental energies within 2%. Making use of the fact that the sum of the pairing binding energies of \(^{206}\)Pb and \(^{210}\)Pb as well as in \(^{206}\)Hg and \(^{210}\)Po are \(\approx 2\) MeV (in this last case one has to take into account the Coulomb repulsion between the two protons, cf. e.g. [13]), one obtains the values of 2.7 MeV and 2.2 MeV for the neutron pair addition and pair removal energies, the corresponding values for the proton channel being 3.5 MeV and 3.1 MeV respectively (cf. ref. [9], [12] and [11]). The associated \(Y\)'s amplitudes are displayed in Tables [10] and [11].

Inserting these results in Eq. (4), one obtains the ground state correlation energy values -0.399 MeV (neutrons) and -0.449 MeV (protons) respectively. In all calculations we have kept the contribution of the lowest \((n = 1)\) pair addition and pair subtraction modes,
in keeping with the fact that, as a rule, the \( n \neq 1 \) modes are much less collective. Pairing vibrations with multipolarity \( \lambda \neq 0 \), in particular quadrupole and hexadecapole pairing vibrations, have also been identified around closed shell nuclei (cf. \[12\], \[13\], \[14\] and refs therein). In Table III we display the contributions to the ground state energy (i.e. \( E_{RPA} \) as defined in Eq. (1)) associated with the monopole, quadrupole and hexadecapole pair addition and pair removal modes for both neutrons and protons associated with \( ^{208}\text{Pb} \), the summed contribution amounting to -1.981 MeV (\( \approx -1.196 \text{ MeV} -0.785 \text{ MeV} \)).

In Table IV we collect the corresponding contribution for a number of Pb-isotopes. Because pairing vibrations are collective modes only around closed shell nuclei, where particles and holes can be clearly distinguished, becoming non-collective two-quasiparticle modes outside closed shells (cf. e.g. ref. \[12\]) we have considered the contribution of neutron pairing vibrations only for the closed shell system (while the proton pairing vibration were taken into account for all isotopes). Also shown

\[
\begin{array}{c|c|c}
\lambda^\pi = 0^+ & \lambda^\pi = 2^+ \\
\hline
k & \lambda^\pi & \lambda^\pi \\
\hline
3d_{5/2} & 0.0618 & 0.1057 \\
2g_{7/2} & 0.0882 & 0.1512 \\
4s_{1/2} & 0.0480 & 0.0886 \\
3d_{3/2} & 0.0915 & 0.1864 \\
1h_{11/2} & 0.1542 & 0.3259 \\
1i_{11/2} & 0.1556 & 0.4172 \\
2f_{9/2} & 0.1177 & 0.8349 \\
& \lambda^\pi & \lambda^\pi \\
\hline
i & \lambda^\pi & \lambda^\pi \\
\hline
3p_{1/2} & 0.7853 & 0.0839 \\
2f_{5/2} & 0.4841 & 0.1260 \\
3p_{3/2} & 0.2870 & 0.0889 \\
1i_{13/2} & 0.3347 & 0.1402 \\
2f_{7/2} & 0.1856 & 0.0914 \\
1h_{9/2} & 0.1461 & 0.0839 \\
2f_{9/2} & 0.1177 & 0.8349
\end{array}
\]

**Table I:** RPA wavefunctions of the neutron pair addition (a) and pair removal (r) modes of \( ^{208}\text{Pb} \) with multipolarities and parity \( \lambda^\pi = 0^+, 2^+ \).
weighted sum rule were included in the calculation of $\mathcal{E}_{RPA}$. These conditions essentially select the lowest (one-two) states displaying correlated wavefunctions.

FIG. 2: Difference between the calculated and the experimental ground state energies. The curve (A) refers to the HFBCS MSk7 results of ref. [4]. The curve (B) was obtained adding $p-h$ and pairing correlations to the curve (A) and renormalizing the Skyrme parameters as indicated in the text.

Similar calculations were repeated for the calcium isotopes $^{40-48}\text{Ca}$. In this case, the contribution of the proton pairing vibrations calculated for the closed shell systems $^{40}\text{Ca}$ and $^{48}\text{Ca}$ were linearly interpolated for the other isotopes, and no hexadecapole modes were considered. In Table IV we show the corresponding results, together with the contribution of the particle-hole vibrational modes. When adding the results of Tables IV and V to the HFBCS MSk7 mass formula of Ref. [3], the parameters of the Skyrme interaction should be refitted in order to provide the best reproduction of experimental masses. This should be done on a large sample of isotopes and it is beyond the purpose of the present paper. If we restrict ourselves to Ca-isotopes (Pb-isotopes), a slight renormalization by a factor 0.9964 (0.99945) of the Skyrme parameters $t_1, W_0$ is enough to shift the calculated value of the masses upwards by $\approx 4.3$ MeV (3.5 MeV) and minimize the rms deviation, giving the results displayed in Table V and, for the Calcium isotopes, also shown in Fig. 2. Averaging the rms deviations associated with Ca- and Pb-isotopes, leads to a value of 0.505 MeV as compared to the value of 0.964 MeV obtained making use of the results of ref. [3]. Although a global readjustment of the mean field parameters should be envisaged, the fact that the locally extracted rms deviations have been reduced by a factor of $\approx 2$ can be considered meaningful.

Similarly to what was observed in assessing the role played by zero point fluctuations associated with surface and pairing vibrations in connection with the nuclear mean square radius [14, 15, 16], the alignment of rotational nuclei [17] and the pairing phase transition as a function of angular momentum [18, 19, 20], we conclude that zero point fluctuations play an important role in providing the A-dependent contributions to nuclear masses needed to make mean field theory, including its time dependence, a quantitative predictive tool.

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