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Role of pair-vibrational correlations in forming the odd-even mass difference

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Summary. — The Random-Phase-Approximation (RPA) amended Nilsson-Strutinskij theory, which successfully describes the pattern of binding energies of the nuclei with $N \approx Z$ and even $A = N + Z$, where N and Z are the numbers of neutrons and protons, is applied to nuclei with odd A in both the $N \approx Z$ region and the chain of Sn isotopes. The RPA correction contributes significantly to the calculated odd-even mass differences, most significantly in light nuclei.

In the Strutinskij theory [1], the nuclear binding energy B is given by

$$-B = E_{\mathrm{LD}} + \delta E_{\mathrm{i.n.}} + \delta E_{\mathrm{BCS}}. \tag{1}$$

Here, E_{LD} is the energy of a deformed liquid drop. In the subsequent terms, $\delta E_{\mathrm{i.n.}} = E_{\mathrm{i.n.}} - \tilde{E}_{\mathrm{i.n.}}$, and similarly for δE_{BCS}. The energy $E_{\mathrm{i.n.}}$ of independent nucleons is the sum of occupied single-nucleon levels in a, generally deformed, potential well and $E_{\mathrm{i.n.}} + E_{\mathrm{BCS}}$ is the total energy in the Bardeen-Cooper-Schrieffer (BCS) approximation [2] of these nucleons interacting by a pairing interaction. The "smooth" counter terms $\tilde{E}_{\mathrm{i.n.}}$ and $\tilde{E}_{\mathrm{BCS}}$ represent an average dependence of $E_{\mathrm{i.n.}}$ and E_{BCS} on the numbers of neutrons and protons and the deformation. Like $E_{\mathrm{i.n.}}$ and E_{BCS}, each of them is the sum of contributions from the neutron and the proton systems. In the smooth terms, each of these contributions is given by a closed expressions in terms of a smooth single-nucleon level density $\tilde{g}(\epsilon)$, a pair coupling constant G and the dimension of the valence space for the pairing interaction. (Conventionally, G is expressed in terms of a suitably defined smooth gap parameter $\tilde{\Delta}$.)

With Frauendorf, we extended this scheme, adding a term $\delta E_{\mathrm{RPA}} = E_{\mathrm{RPA}} - \tilde{E}_{\mathrm{RPA}}$ such that $E_{\mathrm{i.n.}} + E_{\mathrm{BCS}} + E_{\mathrm{RPA}}$ is the ground state energy in the Random Phase Approximation (RPA) [3] of the above system with an additional pairing interaction of neutrons and protons [4]. The liquid drop energy was written in the five-parameter form of Duflo and Zuker [5] with an additional dependence on deformation.

For the single-nucleon potential we chose a Nilsson potential with the parameters of ref. [6]. The deformations were taken from a previous Nilsson-Strutinskij calculation without the RPA correction [7], and a single, common pair coupling constant G was adopted for the interactions of two-neutron, two-proton and neutron-proton pairs. Because the RPA is the theory of small oscillations about a mean-field equilibrium, in this case the BCS ground state, the inclusion of the RPA correction accounts for the binding energy contribution of pair-vibrational correlations. This extended theory was found to reproduce reasonably well the pattern of binding energies of nuclei with nearly equal neutron number N and proton number Z and even $A = N + Z$, including the Wigner cusps [8], the symmetry energy coefficients, the doubly odd-doubly even mass differences for isospin $T = 0$ and the relative energies of the lowest levels with $T = 0$ and 1 in the nuclei with odd $N = Z$. One of us improved the expression for $\tilde{E}_{\mathrm{RPA}}$ [9] and applied this improved expression in revised calculations, relaxing also somewhat the strict requirement of isobaric invariance imposed on the microscopic model in ref. [4] so as to approach the conventional Nilsson-Strutinskij scheme [10]. These modifications did not alter the main conclusion of ref. [4].

In the present note we test this model for nuclei with odd $A = N+Z$. We study in particular the RPA contribution to the calculated odd-even mass differences $\Delta_{\mathrm{oe},n \text{ or } p}(N, Z)$, which we define as the mass of the nucleus (N, Z) minus the average mass of the neighbouring doubly even nuclei. The label n or p refers to the cases of odd N and odd Z, respectively. Two regions on the chart of nuclides are considered: (i) The $N \approx Z$ region, where the nuclei with even A were studied already in great detail in the work cited above. We focus here on the odd-A nuclei just "below" the $N = Z$ line, having $Z = N - 1$. The pair coupling constant G is parametrised in the form $G = G_1 A^e$ and the parameters G_1 and e fitted, as in ref. [10], to the $T = 0$ doubly odd-doubly even mass differences and the relative energies of the lowest states with $T = 0$ and 1 for odd $N = Z$. For the even-A nuclei in this region, the present calculations differ from those of ref. [10] in two respects, namely by the choice of a considerably smaller interval of interpolation of E_{RPA} across the critical G, cf. ref. [4], and by the use of N, Z and $A/2$ single-nucleon levels in the neutron, proton and neutron-proton pairing calculations. For odd A we use $(A + 1)/2$ levels in the neutron-proton calculation. (ii) The chain of Sn isotopes, where the small interpolation interval was found imperative for the reproduction of the pattern of the doubly even binding energies near $N = 50$. We also found that in order to reproduce the pattern of the doubly even binding energies near $N = 82$ as well as the neutron odd-even mass differences, the expression for G applied in the $N \approx Z$ region must be reduced by both a T-dependent factor $1 - 0.015T$ and a constant factor 0.78. We thus have two determinations of $G(^{100}\mathrm{Sn})$ differing by 22%. Being based on the most certain empirical data, the value resulting from the analysis of the chain of Sn isotopes is presumably the one that is most reliable. For a given expression for G, the liquid drop parameters are fitted to the doubly even masses of the region.

Our results are summarised in the upper left, upper right and lower left panels of fig. 1. Largely, the calculations (dark blue curves) reproduce the measured odd-even mass differences (black, dashed curves). Conspicuous deviations, where the calculated value drops to about zero, occur in the $N \approx Z$ region for N and $Z = 25$. Neither is a similar value for $N = 49$ likely to represent the reality. These rare instances of a predicted vanishing of the odd-even mass difference seem to suggest an instability of the formalism under certain circumstances, but we did not succeed in pinpointing the exact circumstances which trigger this anomaly.

The three panels display the individual contributions to the calculated odd-even mass

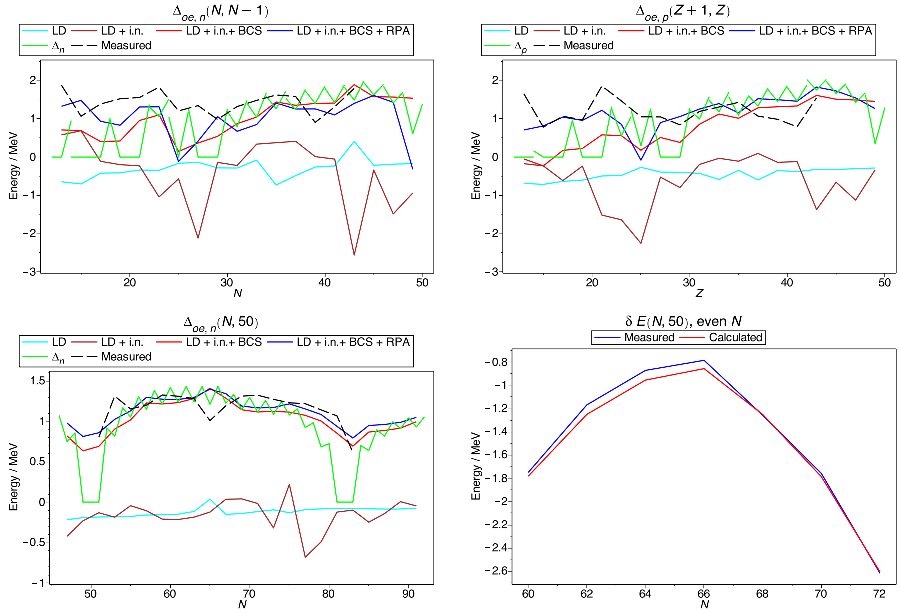

Fig. 1. – Compositions of calculated odd-even mass differences. Upper left: Odd $N = Z + 1$. Upper right: Odd $Z = N - 1$. Lower left: Odd N for $Z = 50$. Also shown are the corresponding calculated BCS gap parameters $\Delta_{n \text{ or } p}$ for both the odd-A nucleus and its doubly even neighbours and the measured odd-even mass differences. Lower right: Measured (dark blue) and calculated (red) total shell correction in a sequence of doubly even Sn isotopes.

differences. The liquid drop value is shown in cyan. Adding $\delta E_{\text{i.n.}}$ to the liquid drop energies gives the brown curves. Adding further δE_{BCS} gives the red curves and adding finally δE_{RPA} gives the dark blue curves. Also shown in green are the corresponding calculated BCS gap parameters $\Delta_{n \text{ or } p}$ for both the odd-A nucleus and its doubly even neighbours. The gap is generally lower in the odd-A nucleus than in the neighbours because in the former, the Fermi level is blocked from participation in the pair correlations. In the absence of the RPA correction, the odd-even mass differences are seen to follow quite closely the average trends of the fluctuating gaps.

In the upper *sd* shell, the RPA contribution is positive, and it makes up about half of the neutron odd-even mass difference and almost the total proton one. In fact the odd-even mass differences are small in this region in the absence of the RPA correction. For $Z = 13$ and 15 the proton odd-even mass difference is even negative. These small values are related to the fact that the pair gaps tend to vanish in these light nuclei. They render the RPA contribution very essential for the formation of the total odd-even mass differences. In the $N \approx Z$ region above ^{40}Ca, the RPA contribution is mostly small, and it can have either sign. In the Sn isotopes, it is mostly positive, and it makes up, on average, 8% of the total. It is largest near the shell closures at $N = 50$ and 82, where Δ_n vanishes.

These signs of the RPA contribution to the odd-even mass difference can be qualitatively understood from the expression for $\tilde{E}_{\text{RPA}}$ [9]. In fact, like E_{RPA}, its counter term $\tilde{E}_{\text{RPA}}$ is composed of a neutron, a proton and a neutron-proton part. Apart from a T-dependent term in the neutron-proton part, which largely matches a similar term in E_{RPA}, each part can be written $\Omega G f(a)$, where 4Ω is the valence space dimension and $a = 1/(\tilde{g}(\tilde{\lambda})G)$. Here, $\tilde{\lambda}$ is a smooth chemical potential. The function $f(a)$ is negative and has a minimum at $a \approx 2.8$. In the upper sd shell and in the Sn isotopes, a is larger than 3, so $f(a)$ has an upwards slope. The blocking of, say, the neutron Fermi level effectively dilutes the single-nucleon spectra which enter the neutron and neutron-proton parts of E_{RPA}. The resulting smaller effective level densities correspond to larger values of a and, therefore, larger values of $f(a)$. Accordingly, E_{RPA} tends to be less negative in the odd-A nucleus than in the doubly even neighbours while $\tilde{E}_{\mathrm{RPA}}$ does not exhibit this staggering. Above ^{40}Ca in the $N \approx Z$ region, a descends to values about the minimum of $f(a)$ with the result that blocking a Fermi level has little effect.

We conclude that in the model we have been studying, pair vibrational correlations play an important role in forming the odd-even mass difference, most important in light nuclei.

Finally, we convey a couple of observations unrelated to odd-even mass differences. First, as already mentioned, the RPA energy E_{RPA} is composed of contributions from each of the three parts of the pairing interaction, the two-neutron, the two-proton and the neutron-proton parts [11]. While the two first of these contributions are essentially unaffected by a neutron excess, the third one decreases numerically with an increasing surplus of neutrons because the orbits of the excess neutrons are blocked to the interaction of neutron-proton pairs. We find, however, in our calculations that even in ^{140}Sn with $T = 20$, the RPA energy is reduced to only half its value in ^{100}Sn with $T = 0$.

Second, Togashi *et al.* recently pointed out a sudden drop of the doubly even two-neutron separation energy in the Sn isotopes as a function of N at $N = 66$. They interpreted it as a second order phase transition [12]. As seen in the lower right panel of fig. 1, our model reproduces this behaviour of the two-neutron separation energy. The measured total shell correction δE shown in the figure is defined as $-B - E_{\mathrm{LD}}$, where B is the measured binding energy and E_{LD} the calculated liquid drop energy, and the calculated one as $\delta E_{\mathrm{i.n.}} + \delta E_{\mathrm{BCS}} + \delta E_{\mathrm{RPA}}$. In our calculations, the drop is related to an onset of oblate deformations with the entrance into the highly degenerate $1h_{11/2}$ shell. That oblate deformations occur in this part of the Sn isotopic chain concurs with what Togashi *et al.* find in their large scale Monte Carlo Shell Model calculations.

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