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

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What are pair-vibrational correlations?

Pairing Hamiltonian

$$H = \sum_i \epsilon_i a_i^\dagger a_i - G\, P^\dagger P, \qquad P = \frac{1}{2} \sum_i a_{\bar{\imath}} a_i .$$

Often treated in the BCS approximation. Exact solution exists.
Example: Bang, Krumlinde, Nucl. Phys. A 141, 18 (1970):

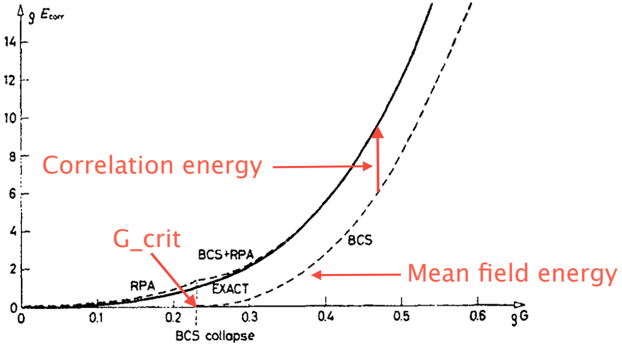


Fig. 1. Ground-state correlation energy (see text) as a function of G for a model of 32 equidistant levels with 32 particles (uniform model). ρ is the density of levels.

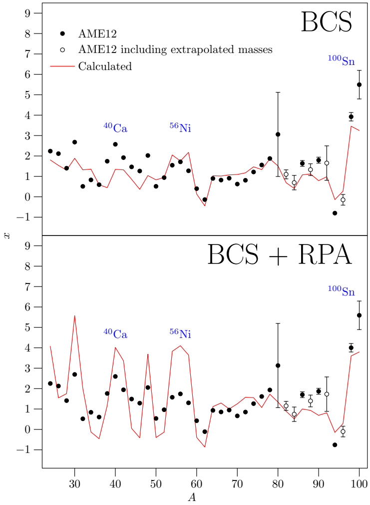
Empirical evidence?

- Scarce because phenomenological parametrisations of the total energy mostly allow neglecting the vibrational correlations.
- Evidence from systematics of "Wigner x"?
- Definition of x: For given A,

$$-B = E_0 + \frac{T(T+x)}{2\theta} + E_{\text{Coul}},$$

$$T = \begin{cases} 0,2,4, & A \equiv 0 \mod 2, \\ 1,3,5, & A \equiv 2 \mod 2, \end{cases}$$

B = binding energy.
E_{Coul} = Coulomb energy
T = isospin, here $= (N-Z)/2$.
E_0, θ, x constants.



Model (1)

(Bentley, Neergård, Frauendorf, Phys. Rev. C 89, 034302 (2014); Neergård, Nucl. Theor. 36, 195 (2017).)

- $-B = E_{\text{LD}} + \delta E, \quad \delta E = \delta E_{\text{i.n.}} + \delta E_{\text{BCS}} + \delta E_{\text{RPA}}$.
- E_{LD} = energy of deformed liquid drop. 5 parameters, symmetry terms $\propto T(T+1)$ (Duflo, Zuker, Phys. Rev. C 52, 23 (1995)).
- Deformations from previous Nilsson-Strutinskij calculation without δE_{RPA} (Bentley, thesis (2010)).
- $\delta E_{\text{i.n.}} = E_{\text{i.n.}} - \tilde{E}_{\text{i.n.}}$ *etc.*
- $E_{\text{i.n.}} + E_{\text{BCS}} + E_{\text{RPA}}$ = minimum of the Hamiltonian

  $$H = \sum_{n,p} \sum_i \epsilon_i a_i^\dagger a_i - G \sum_{n,p,np} P^\dagger P, \quad P_{np} = \sqrt{\tfrac{1}{2}} \sum_i a_{\bar{\imath}p} a_{in} \,,$$

  split into successive contributions of the first term (i.n. = independent nucleons) and the BCS and RPA approximations to the interaction energy. To escape the singularity of the RPA contribution at $G = G_{\text{crit}}$, it is interpolated in a narrow interval round this G (narrower here than in our published work).
- Nilsson single-nucleon levels ϵ_i. Labelled in increasing order by index i. Parameters of Bengtsson, Ragnarsson, Nucl. Phys. A 436, 14 (1985).

Model (2)

- N and Z Cramers degenerate levels are included in the n and p BCS and RPA calculations, $\lceil A/2 \rceil$ level of each kind in the np RPA calculation. For odd N or Z the Fermi level is blocked.
- $\tilde{E}_{\text{i.n.}}$, $\tilde{E}_{\text{BCS}}$, $\tilde{E}_{\text{RPA}}$ are "smooth" counter terms. They are given by closed expressions in terms of smooth level densities $\tilde{g}_{n,\ p \text{ or } np}(\epsilon)$, the pair coupling constant G and the numbers of participating single-nucleon levels. $\tilde{g}_{np}(\epsilon)$ is calculated from average levels.
- For odd $N = Z$, what is described so far models the lowest state with isospin $T = 0$. The binding energy B^* of the lowest state with $T = 1$ is calculated from that of the $N + 1, Z - 1$ ground state with the liquid drop Coulomb displacement energy.
- $G = G_1 A^e$, where G_1, e minimise the total rms deviation from

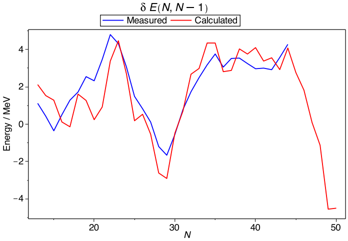
  $\frac{1}{2}((B(N-1, N-1) + B(N+1, N+1)) - B(N, N),$

  $B(N, N) - B^*(N, N), \quad \text{odd } N \geq 13 \ .$

  (Arguments N, Z throughout.) For given G_1, e the liquid drop parameters are determined by minimisation of the rms deviation from the doubly even binding energies measured for $0 \leq N - Z \leq 10$. Above, when δE_{RPA} was omitted, G_1, e were optimised separately for this situation.

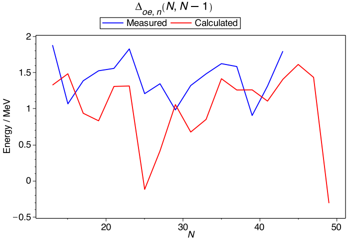
Odd A

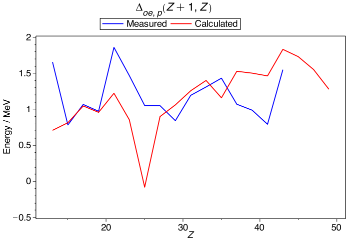
- This model describes reasonably well the pattern of even-A binding energies near $N = Z$ as well as the excitation energies $B(N,N) - B^*(N,N)$. The Wigner x shown earlier is an example.
- We now apply it to the nuclei with $Z = N - 1$ (odd A).
- δE(measured) $= -B$(measured) $- E_{\text{LD}}$.
- The model reproduces these binding energies as well as those for even A.
- No new parameters were introduced.



Odd-even mass difference

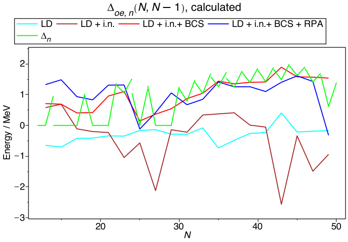
- $\Delta_{\mathrm{oe},n}(N,Z) = \frac{1}{2}(B(N-1,Z) + B(N+1,Z)) - B(N,Z), \quad \text{odd } N.$ Similarly for protons.
- The model reproduces trends in their measured variations albeit crudely.
- The origin of very low calculated values for $N, Z = 25$ at variance with the data and for $N = 49$ remains to by fully analysed.

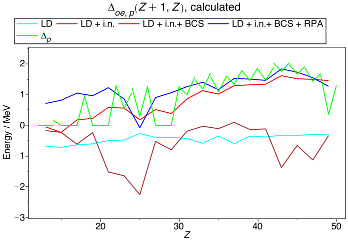




Composition of the calculated $\Delta_{\text{oe},n \text{ or } p}$

- The RPA contribution to $\Delta_{\text{oe},n}$ is positive for $N < 24$. For $N > 24$ it is mostly numerically small and takes both signs. In the upper *sd* shell it equals on average 0.6 MeV, which is about half of the total.
- The RPA contribution to $\Delta_{\text{oe},p}$ is predominantly positive. In the upper *sd* shell it equals on average 0.9 MeV, which is about the total.
- The figures show the gap parameter $\Delta_{n \text{ or } p}$ for both the odd nuclei and their doubly even neighbours.





Composition of the calculated $\Delta_{\mathrm{oe},n \text{ or } p}$ (continued)

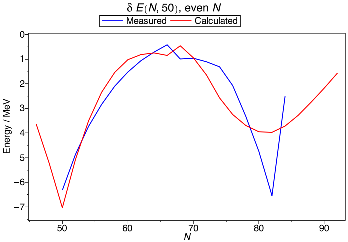
- Quite generally, the blocking of the odd orbit reduces $\Delta_{n \text{ or } p}$ in the odd nucleus relative to its neighbours. An average of the fluctuating $\Delta_{n \text{ or } p}$ values very roughly gives $\Delta_{\mathrm{oe},n \text{ or } p}$ in the absence of the RPA correction.
- The signs of the RPA contributions to $\Delta_{\mathrm{oe},n \text{ or } p}$ can be qualitatively understood from the expression for $\tilde{E}_{\mathrm{RPA},n,\ p \text{ or } np}$ (which I have not shown). Apart from a T-dependent term in $\tilde{E}_{\mathrm{RPA},np}$, which largely matches a similar term in $E_{\mathrm{RPA},np}$, it 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 $a \approx 2.8$. Blocking a Fermi level tends to increase the effective a. In the upper *sd* shell, a is larger than 3.5, so $f(a)$ has an upwards slope, which makes E_{RPA} sensitive to this blocking. Above ^{40}Ca it descends to values about the minimum of $f(a)$.

Sn isotopes, first attempt

- Turning now to the chain of Sn isotopes, we fit for given G_1, e the liquid drop parameters to the binding energies measured for even N.
- However, 5 parameters are too many for a single isotopic chain. Therefore, in the volume and surface energy coefficients, we fix the ratios of the coefficient of $T(T+1)$ and the constant terms at their values in a global fit, Mendoza-Temis, Hirsch, Zuker, Nucl. Phys. A 843, 14 (2010). This leaves 3 parameters.
- In a first attempt, G_1, e are inherited from the analysis of the $N \approx Z$ region:

$$G = 5.583A^{-0.6908} \text{ MeV}$$

- The empirical minimum of δE at the $N = 82$ shell closure is badly described.

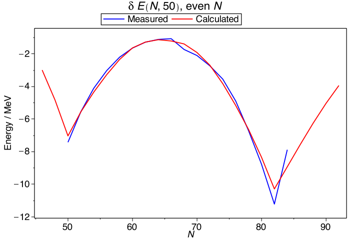


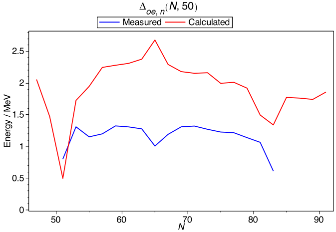
Sn isotopes, second attempt

- A T-dependent attenuation which preserves $G(^{100}\text{Sn})$ is added:

$$G = 5.583A^{-0.6908}\ \text{MeV} \times (1 - 0.015T)$$

- δE is now described equally well for even N at both shell closures.
- $\Delta_{\text{oe},n}$ is vastly overestimated.



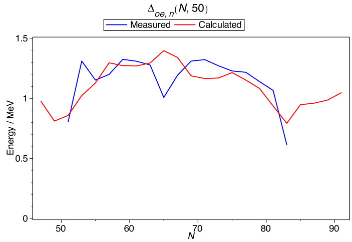


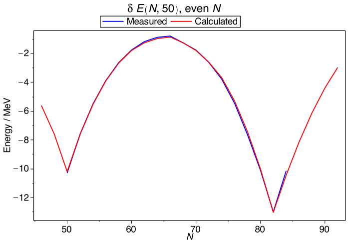
Sn isotopes, third attempt

- A general attenuation is added:

$$G = 5.583A^{-0.6908}\ \text{MeV}$$
$$\times (1 - 0.015T) \times 0.78$$

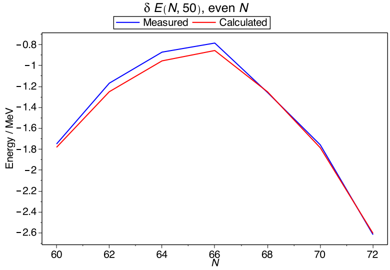
- This brings $\Delta_{\text{oe},n}$ in place.
- The empirical δE is almost perfectly reproduced for even N.
- We now have two determinations of $G(^{100}\text{Sn})$ differing by 22%, from $N = Z$ nuclei and from Sn isotopes. Most probably the first, which is influenced by an interpretation of incomplete spectra of doubly odd nuclei with $A \approx 90$, is too high.





Second order phase transition

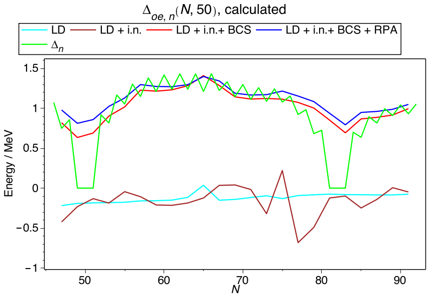
- Our theory reproduces a "second order phase transition" at $N = 66$ discussed by Togashi *et al.*, Phys. Rev. Lett. 121, 062501 (2018).
- The kink in the plot of δE is related in the calculations to the onset of oblate deformations with the entrance into the $1h_{11/2}$ shell.



- Otherwise the calculated shapes are spherical. These findings qualitatively agree with those of Togashi *et al.*
- The empirical kink is badly described in our two first attempts. Thus pairing is essential for its formation in the calculations.

Composition of the calculated $\Delta_{\mathrm{oe},n}$

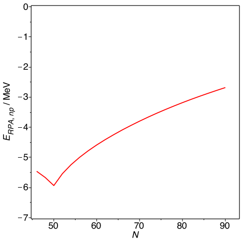
- The RPA contribution to $\Delta_{\mathrm{oe},n}$ is positive except for one very small negative value for $N = 65$. This reflects values of a larger than 3.
- On average, it is 8% of the total.
- It is largest near the shell closures, where Δ_n vanishes.



- Δ_n vanishes in the two closed shell nuclei and their odd neighbours. Inside shells, an average of its fluctuating value again gives very roughly $\Delta_{\mathrm{oe},n}$ in the absence of the RPA correction.
- Note that the BCS contribution does not vanish in the closed shell ± 1 nuclei only because the closed shell ± 2 nuclei have non-vanishing Δ_n.

$E_{\mathrm{RPA},np}$

The neutron-proton pair-vibrational correlation energy $E_{\mathrm{RPA},np}$ is expected to decrease numerically with increasing neutron excess because the orbits of the excess neutrons are blocked to the formation of neutron-proton pairs. Yet, in ^{140}Sn with $T = 20$ it is only reduced to half its value in ^{100}Sn with $T = 0$.



Conclusions

- A model was considered which is derived by Strutinskij renormalisation from the Hamiltonian of nucleons in a Nilsson potential well interacting by a pairing force that renders the Hamiltonian isobarically invariant in the limit of equal spectra of single neutrons and protons.
- In this model, pair-vibrational correlations contribute mostly positively to the odd-even mass difference $\Delta_{\mathrm{oe},n \text{ or } p}$.
- In $Z = N - 1$ nuclei in the upper *sd* shell, this contribution is about half of $\Delta_{\mathrm{oe},n}$ and about all of $\Delta_{\mathrm{oe},p}$.
- It decreases for $Z = N - 1$ with increasing A.
- In almost all the odd-N Sn isotopes, it is positive and it amounts, on average, to 8% of the total. It is largest near the shell closures due to a reduction of the gap parameters $\Delta_{n \text{ or } p}$.
- In ^{140}Sn with $T = 20$, the neutron-proton pair-vibrational correlation energy remains half as large as in ^{100}Sn with $T = 0$.