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

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Reference

Phys. Rev. C 99, 054315 (2019).

What are pair-vibrational correlations?

Pairing Hamiltonian

$$H = \sum_k \epsilon_k a_k^\dagger a_k - G\, P^\dagger P, \qquad P = \tfrac{1}{2} \sum_k a_{\bar{k}} a_k .$$

Often treated in the BCS approximation. Exact solution exists.

Example of such a calculation: Bang, Krumlinde, Nucl. Phys. A 141, 18 (1970).

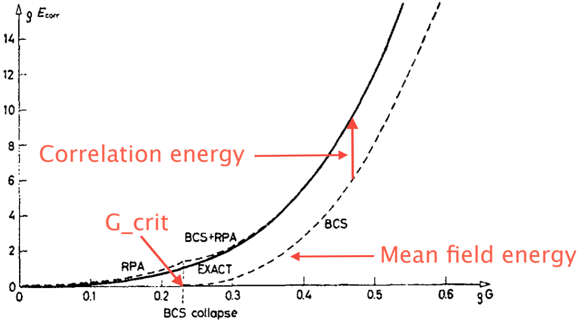


Fig. 1. Ground-state correlation energy (see text) as a function of G for a model of 32 equidistant levels with 32 particles (uniform model). ρ is the density of levels.

(Authors' $E_{\text{corr}} = \langle H \rangle_0 - \langle H \rangle$, where $|0\rangle$ is the $G = 0$ ground state.)

Model ("RPA-amended Nilsson-Strutinskij")

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

Total energy

$$E(N,Z) = E_{\mathrm{LD}} + \sum_{\tau=n,p} (\delta E_{\mathrm{i.n.},\tau} + \delta E_{\mathrm{BCS},\tau}) + \sum_{\tau=n,p,np} \delta E_{\mathrm{RPA},\tau}.$$

("i.n." = "independent nucleons".)

$$\delta E_x = E_x - \tilde{E}_x.$$

The "smooth" counter terms $\tilde{E}_x$ absorb the average parameter dependence of E_x.

The "microscopic" energy

$$E_{\mathrm{mic}} = \sum_{\tau=n,p} (E_{\mathrm{i.n.},\tau} + E_{\mathrm{BCS},\tau}) + \sum_{\tau=n,p,np} E_{\mathrm{RPA},\tau}$$

approximates the minimum for given N and Z of

$$H = \sum_{\tau=n,p} \sum_{k=1}^{2\Omega_\tau} \epsilon_{k\tau} a_{k\tau}^\dagger a_{k\tau} - \sum_{\tau=n,p,np} G_\tau P_\tau^\dagger P_\tau$$

$$P_\tau = \frac{1}{2} \sum_{k=1}^{2\Omega_\tau} a_{\bar{k}\tau} a_{k\tau}, \quad \tau = n, p, \quad P_{np} = 2^{-\frac{3}{2}} \sum_{k=1}^{2\Omega_{np}} (a_{\bar{k}p} a_{kn} + a_{\bar{k}n} a_{kp}).$$

$$\Omega_\tau = N_\tau, \quad \tau = n, p, \quad \Omega_{np} = \lceil A/2 \rceil, \quad N_n = N, \quad N_p = Z.$$

Single-nucleon energies. Parametrisation of the pair coupling constants

The states $|k\tau\rangle$ are egenstates (eigenvalues $\epsilon_{k\tau}$) of a Nilsson Hamiltonian h_τ (next slide).

The pair coupling constants G_τ are determined by three parameters $\bar{G}, \zeta, \alpha$:

$$G_\tau = \bar{G} A^\zeta (1 - \alpha M_T M'_T),$$
$$M_T = (N - Z)/2, \quad M'_T = 1, -1, 0, \quad \tau = n, p, np.$$

"Limit of isobaric invariance":

1. $h_n = h_p$.
2. $\alpha = 0$.
3. All Ω_τ are equal.

The index k labels the energies $\epsilon_{k\tau}$ is non-decreasing order such that

1. $|k+1,\tau\rangle = |\bar{k}\tau\rangle, \quad$ odd k,
2. $|kp\rangle = t_-|kn\rangle$ in the limit of isobaric invariance.

Nilsson Hamiltonian

$$h_\tau = \frac{\mathbf{p}^2}{2M_\tau} + \frac{1}{2}\left(M_\tau \sum_{q=1}^{3} (\omega_q x_q)^2 + 2\epsilon_4 \omega_0 \rho^2 P_4(\cos\theta_\mathrm{t}) \right)$$
$$-\kappa_{N_\mathrm{sh},\tau} \mathring{\omega} \left(2\mathbf{l}_\mathrm{t} \cdot \mathbf{s} + \mu_{N_\mathrm{sh},\tau} (\mathbf{l}_\mathrm{t}^2 - \langle \mathbf{l}_\mathrm{t}^2 \rangle_{N_\mathrm{sh}}) \right),$$
$$\omega_q \propto 1 - \tfrac{2}{3}\epsilon_2 \cos(\gamma + q\tfrac{2\pi}{3}), \quad \prod_{q=1}^{3} \omega_q = \mathring{\omega}^3, \quad \mathring{\omega} = 41A^{-1/3}\ \mathrm{MeV}.$$

"Streched" spherical coordinates $(\rho, \theta_\mathrm{t}, \phi_\mathrm{t}) \equiv$ Cartesian $\xi_{q\tau} = x_q \sqrt{M_\tau \omega_q}$.

Parameters $\kappa_{N_\mathrm{sh},\tau}, \mu_{N_\mathrm{sh},\tau}$ of Bengtsson, Ragnarsson, Nucl. Phys. A 436, 14 (1985).

The three deformation parameters $\epsilon_2, \gamma, \epsilon_4$ are generated for each nucleus by an conventional Nilsson-Strutinskij calculation without the RPA correction (Bentley, thesis, University of Notre Dame 2010).

The term in red is the "spatial" potential (for later reference).

Independent nucleons + BCS, even N_τ

$$E_{\mathrm{i.n.},\tau} + E_{\mathrm{BCS},\tau} = \sum_{k=1}^{2\Omega_\tau} v_{k\tau}^2 \epsilon_{k\tau} - \frac{\Delta_\tau^2}{G_\tau}$$

$$\left.\begin{matrix} u_{k\tau} \\ v_{k\tau} \end{matrix}\right\} = \sqrt{\tfrac{1}{2}\left(1 \pm \frac{\epsilon_{k\tau} - \lambda_\tau}{E_{k\tau}}\right)}, \quad E_{k\tau} = \sqrt{(\epsilon_{k\tau} - \lambda_\tau)^2 + \Delta_\tau^2}.$$

$\lambda_\tau, \Delta_\tau$ obey

$$\sum_{k=1}^{2\Omega_\tau} v_{k\tau}^2 = N_\tau, \quad G_\tau \sum_{k=1}^{2\Omega_\tau} u_{k\tau} v_{k\tau} = 2\Delta_\tau.$$

Always solution with $\Delta_\tau = 0$.
Solution with $\Delta_\tau > 0$ and lower energy only when $G_\tau > G_{\mathrm{cr},\tau}$, where

$$\frac{4}{G_{\mathrm{cr},\tau}} = \min_{\epsilon_{N_\tau \tau} < \lambda_\tau < \epsilon_{(N_\tau+2)\tau}} \sum_{k=1}^{2\Omega_\tau} \frac{1}{|\epsilon_{k\tau} - \lambda_\tau|}.$$

$G_{\mathrm{cr},\tau} = 0$ if $\epsilon_{(N_\tau+2)\tau} = \epsilon_{N_\tau \tau}$.
This occurs when the nucleus is spherical and has an open subshell of nucleons of the kind τ.

Independent nucleons + BCS, odd N_τ

For odd N_τ the BCS ground state is assumed contain a quasinucleon annihilated by $\alpha_{N_\tau\tau}$, where

$$\alpha_{k\tau} = u_{k\tau} a_{k\tau} - v_{k\tau} a^\dagger_{\bar{k}\tau}.$$

Then $|N_\tau\tau\rangle$ is fully occupied and $|(N_\tau + 1)\tau\rangle$ is fully empty.

The odd nucleon contributes $\epsilon_{N_\tau\tau}$ and the rest of $E_{\text{i.n.},\tau} + E_{\text{BCS},\tau}$ is calculated as if $N_\tau - 1$ nucleons of type τ inhabited the remaining orbits.

The odd nucleon is said to block the Fermi level.

RPA, even N and Z

The calculation of $E_{\text{RPA},\tau}$ for even N and Z is based on Neergård, Phys. Rev. C 80, 044313 (2009).

Labels $\tau\tau' = nn, pp, np$ alternative to and synonymous with $\tau = n, p, np$.

The RPA involves linear relations in the space spanned by the operators $a_{\bar{k}\tau'} a_{k\tau} + a_{\bar{k}\tau} a_{k\tau'}$.

A linearly independent set of these operators is labelled by odd k.

Matrices and vectors are indexed by these k:

$$\mathrm{E}_{\tau\tau'} : \ E_{\tau\tau',kl} = \delta_{kl}(E_{k\tau} + E_{k\tau'})$$

$$\mathrm{U}_{\tau\tau'} : \ U_{\tau\tau',k} = u_{k\tau} u_{k\tau'}, \quad \mathrm{V}_{\tau\tau'} : \ V_{\tau\tau',k} = -v_{k\tau} v_{k\tau'},$$

$$\mathrm{A}_{\tau\tau'} = \mathrm{E}_{\tau\tau'} - G_{\tau\tau'} \left(\mathrm{U}_{\tau\tau'} \mathrm{U}_{\tau\tau'}^T + \mathrm{V}_{\tau\tau'} \mathrm{V}_{\tau\tau'}^T \right),$$

$$\mathrm{B}_{\tau\tau'} = -G_{\tau\tau'} \left(\mathrm{U}_{\tau\tau'} \mathrm{V}_{\tau\tau'}^T + \mathrm{V}_{\tau\tau'} \mathrm{U}_{\tau\tau'}^T \right).$$

Then $E_{\text{RPA},\tau\tau'} = \frac{1}{2} \left(\sum_k \sqrt{z_{\tau\tau',k}} - \operatorname{tr} \mathrm{E}_{\tau\tau'} \right)$,
where $z_{\tau\tau',k}$ are the eigenvalues of $(\mathrm{A}_{\tau\tau'} + \mathrm{B}_{\tau\tau'})(\mathrm{A}_{\tau\tau'} - \mathrm{B}_{\tau\tau'})$.

The terms $\sqrt{z_{\tau\tau',k}}$ are the RPA frequencies

The expression for $E_{\text{RPA},\tau\tau'}$ can be interpreted as a difference of zero point energies of harmonic oscillators.

RPA, odd N_τ

Odd N: Because the field $\alpha^\dagger_{Nn}\alpha^\dagger_{(N+1)n}$ kills the BCS ground state, the index $k = N$ must be omitted in the calculation of $E_{\mathrm{RPA},n}$.

P_{np} and $P^\dagger_{np}$ have terms proportional to $\alpha^\dagger_{Np}\alpha_{Nn}$ and $\alpha^\dagger_{Np}\alpha^\dagger_{(N+1)n}$, which act on the BCS ground state for odd N, but the first of these terms carries an energy near 0, which would cause numeric instability.

We therefore omit $k = N$ in the calculation of $E_{\mathrm{RPA},np}$, as well.

In physical terms, the unpaired nucleon is thus assumed to act, like in the BCS approximation, as a spectator to interactions among the remaining nucleons inhabiting a valence space which excludes the half filled single-nucleon level.

For odd $N = Z$, and in the limit of isobaric invariance, ignoring the aforesaid excitations of the BCS ground state is solidly justified because they havde zero matrix elements provided the two-quasinucleon state has $T = 0$.

Odd Z analogous.

Interpolation

For $\tau = \tau'$ and $G_\tau > G_{\mathrm{cr},\tau}$ the RPA has a Goldstone mode from number conservation.

The emergence of this mode gives rise to the singularity of E_{RPA} at $G = G_{\mathrm{cr}}$ observed in the plot of Bang and Krumlinde (Bentley, Neergård, Frauendorf, *op. cit.*).

For $\tau\tau' = np$ and $N = Z$, and in the limit of isobaric invariance, a similar Goldstone mode results from isospin conservation.

To circumvent the associated singularities, we interpolate $E_{\mathrm{RPA},\tau\tau'}$ across $G_\tau = G_{\mathrm{cr},\tau}$ in such cases where they occur.

Details at the end of my talk if time permits.

$\tilde{E}_{\mathrm{i.n.},\tau}$ and $\tilde{E}_{\mathrm{BCS},\tau}$

(Strutinsky, Nucl. Phys. A 95, 420 (1967).)

$$\tilde{E}_{\mathrm{i.n.},\tau} = 2\int_{-\infty}^{\tilde{\lambda}_\tau} \epsilon \tilde{g}_\tau(\epsilon) d\epsilon, \quad 2\int_{-\infty}^{\tilde{\lambda}_\tau} \tilde{g}_\tau(\epsilon) d\epsilon = N_\tau,$$

$$\tilde{g}_\tau(\epsilon) = \frac{1}{2\gamma_{\mathrm{Str}}\sqrt{\pi}} \sum_k L\left(m_{\mathrm{Str}}, \tfrac{1}{2}, \left(\frac{\epsilon - \epsilon_{k\tau}}{\gamma_{\mathrm{Str}}}\right)^2\right) \exp\left(-\left(\frac{\epsilon - \epsilon_{k\tau}}{\gamma_{\mathrm{Str}}}\right)^2\right),$$

$$\gamma_{\mathrm{Str}} = \overset{\circ}{\omega}, \quad m_{\mathrm{Str}} = 3.$$

The sum in the expression for $\tilde{g}_\tau(\epsilon)$ includes all such k that $\epsilon_{k\tau} < 47.5$ MeV $+ 5\,\gamma_{\mathrm{Str}}$ and $N_{\mathrm{sh}} \leq 9$.

$$\tilde{E}_{\mathrm{BCS},\tau} = -\tfrac{1}{2}\Omega_\tau \tilde{\Delta}_\tau \exp(-\chi_\tau),$$

$$\tilde{\Delta}_\tau = \frac{\Omega_\tau}{2\tilde{g}_\tau \sinh \chi_\tau}, \quad \chi_\tau = \frac{1}{\tilde{g}_\tau G_\tau}, \quad \tilde{g}_\tau = \tilde{g}_\tau(\tilde{\lambda}_\tau).$$

The expression for $\tilde{E}_{\mathrm{BCS},\tau}$ is obtained by considering equidistant levels spaced by $1/\tilde{g}_\tau$ and replacing sums by integrals.

$\tilde{E}_{\mathrm{RPA},\tau\tau'}$

(Neergård, Phys. Rev. C 94, 054328 (2016).)

$$\tilde{E}_{\mathrm{RPA},\tau\tau'} = \frac{2\tilde{\Delta}_{\tau\tau'}}{\pi} \int_0^\infty \ln \left(\frac{1}{\chi_{\tau\tau'}} \tanh^{-1} \left((\tanh \chi_{\tau\tau'}) \sqrt{\frac{x^2 + l_{\tau\tau'}^2}{x^2 + l_{\tau\tau'}^2 + 1}} \right) \right) dx,$$

$$\tilde{\Delta}_{\tau\tau'} = \frac{\Omega_{\tau\tau'}}{2\tilde{g}_{\tau\tau'} \sinh \chi_{\tau\tau'}} \sqrt{1 - \left(\frac{\tilde{g}_{\tau\tau'}(\tilde{\lambda}_{\tau\tau'}(N_\tau) - \tilde{\lambda}_{\tau\tau'}(N_{\tau'})) \tanh \chi_{\tau\tau'}}{\Omega_{\tau\tau'}} \right)^2},$$

$$l_{\tau\tau'} = \frac{\tilde{\lambda}_{\tau\tau'}(N_\tau) - \tilde{\lambda}_{\tau\tau'}(N_{\tau'})}{2\tilde{\Delta}_{\tau\tau'}}$$

$$\chi_{\tau\tau'} = \frac{1}{\tilde{g}_{\tau\tau'} G_{\tau\tau'}}, \quad \tilde{g}_{\tau\tau'} = \tilde{g}_{\tau\tau'} \left(\tilde{\lambda}_{\tau\tau'} \left(\frac{N_\tau + N_{\tau'}}{2} \right) \right), \quad 2 \int_{-\infty}^{\tilde{\lambda}_{\tau\tau'}(x)} \tilde{g}_{\tau\tau'}(\epsilon) d\epsilon = x.$$

$\tilde{g}_{\tau\tau'}(\epsilon)$ is given by the previous expression for $\tilde{g}_\tau(\epsilon)$ with $\epsilon_{k\tau}$ replaced by $(\epsilon_{k\tau} + \epsilon_{k\tau'})/2$. Notice $\tilde{\lambda}_{\tau\tau}(N_\tau) = \tilde{\lambda}_\tau$, $\tilde{\Delta}_{\tau\tau} = \tilde{\Delta}_\tau$, $\chi_{\tau\tau} = \chi_\tau$.

The derivation of the expression for $\tilde{E}_{\mathrm{RPA},\tau\tau'}$ is based on the same principles as Strutinskij's derivation of his expression for $\tilde{E}_{\mathrm{BCS},\tau}$.

Liquid drop energy

$$E_{\mathrm{LD}} = -\left(a_v - a_{vt}\frac{|M_T|(|M_T|+1)}{A^2}\right)A + \left(a_s - a_{st}\frac{|M_T|(|M_T|+1)}{A^2}\right)A^{2/3}B_s + a_c\frac{Z(Z-1)}{A^{1/3}}B_c.$$

For given paring parameters $\bar{G}, \zeta, \alpha$, the five parameters a_x are fitted with the full expression for $E(N,Z)$ to measured doubly even binding energies in the region of the nuclear chart considered.

The table shows the values which result for the optimal pairing parameters. Unit MeV. The rms deviation from the data is given in the last column. The fit for the ^{102}Zr region only includes 9 nuclei.

	a_v	a_{vt}	a_s	a_{st}	a_c	rms
$N \approx Z$	15.23	112.5	16.52	148.9	0.6601	1.018
Around Sn	15.37	115.2	16.97	157.5	0.6737	0.515
Around ^{102}Zr	14.78	151.2	16.07	355.5	0.5774	0.043

Calculation of B_s and B_c, step 1

The equipotential surfaces of the spatial single-nucleon potential are expanded on spherical harmonics,

$$r \propto 1 + \sum_{|m| \le l > 0} (-)^m \alpha_{lm} \sqrt{\frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta) \exp(-im\phi).$$

The non-zero coefficients with $l \le 4$ to 2nd order in $\epsilon_{2,4}$ are

$$\alpha_{20} = \tfrac{2}{3}\epsilon_{20} + \tfrac{5}{63}\epsilon_{20}^2 - \tfrac{2}{21}\epsilon_{20}\epsilon_4 - \tfrac{10}{63}\epsilon_{22}^2 + \tfrac{50}{231}\epsilon_4^2,$$

$$\alpha_{22} = \alpha_{2(-2)} = \tfrac{2}{3}\epsilon_{22} - \tfrac{10}{63}\epsilon_{20}\epsilon_{22} - \tfrac{1}{63}\epsilon_{22}\epsilon_4,$$

$$\alpha_{40} = -\epsilon_4 + \tfrac{12}{35}\epsilon_{20}^2 - \tfrac{30}{77}\epsilon_{20}\epsilon_4 + \tfrac{4}{35}\epsilon_{22}^2 + \tfrac{243}{1001}\epsilon_4^2,$$

$$\alpha_{42} = \alpha_{4(-2)} = \sqrt{\tfrac{48}{245}}\epsilon_{20}\epsilon_{22} + \sqrt{\tfrac{1215}{5929}}\epsilon_{22}\epsilon_4,$$

$$\alpha_{44} = \alpha_{4(-4)} = \sqrt{\tfrac{8}{35}}\epsilon_{22}^2,$$

$$\epsilon_{20} = \epsilon_2 \cos\gamma, \quad \epsilon_{22} = -\sqrt{\tfrac{1}{2}}\,\epsilon_2 \sin\gamma.$$

(Obtained by computer algebra. Some coefficents for $\gamma = 0$ deviate from Seeger, Howard, Nucl. Phys. A 238, 491 (1975).)

Calculation of B_s and B_c, step 2

The parameters α_{lm} are inserted into the expressions of Swiatecki, Phys. Rev. 104, 993 (1956). They were derived for $\gamma = 0$ but the terms of total rank ≤ 8 can be continued unambiguously to $\gamma \neq 0$ by the requirement that they are scalar polynomials in α_{lm}. To this order,

$$B_s = 1 + \tfrac{2}{5} p_{20} - \tfrac{4}{105} p_{30} - \tfrac{66}{175} p_{40} - \tfrac{4}{35} p_{21} + p_{02},$$

$$B_c = 1 - \tfrac{1}{5} p_{20} - \tfrac{4}{105} p_{30} + \tfrac{51}{245} p_{40} - \tfrac{6}{35} p_{21} - \tfrac{5}{27} p_{02},$$

$$p_{20} = \alpha_{20}^2 + 2\alpha_{22}^2, \quad p_{30} = \alpha_{20}(\alpha_{20}^2 - 6\alpha_{22}^2), \quad p_{40} = p_{20}^2,$$

$$p_{21} = (\alpha_{20}^2 + \tfrac{1}{3}\alpha_{22}^2)\alpha_{40} + \sqrt{\tfrac{20}{3}}\alpha_{20}\alpha_{22}\alpha_{42} + \sqrt{\tfrac{70}{9}}\alpha_{22}^2\alpha_{44},$$

$$p_{02} = \alpha_{40}^2 + 2\alpha_{42}^2 + 2\alpha_{44}^2.$$

$$\text{Notice:} \quad p_{20} = \alpha_2^2, \quad p_{30} = \alpha_2^3 \cos 3\gamma', \quad p_{40} = \alpha_2^4,$$

$$\alpha_{20} = \alpha_2 \cos\gamma', \quad \alpha_{22} = \sqrt{\tfrac{1}{2}}\, \alpha_2 \sin\gamma'.$$

Isobaric analogues

The scheme described so far is designed to model, for given N and Z, the lowest energy for $T \approx M_T$.

In most nuclei, this is the ground state energy, but for odd $N = Z$ the ground state may have $T \approx 1$.

The lowest states with $T \approx 1$ is for odd $N = Z$ the isobaric analogue of the ground state for neutron and proton numbers $(N', Z') = (N + 1, Z - 1)$.

We therefore calculate its energy $E^*(N, Z)$ by

$$E^*(N, Z) = E(N', Z') + a_c \frac{Z(Z-1) - Z'(Z'-1)}{A^{1/3}} B_c$$

with B_c evaluated at the deformation of the doubly even nucleus.

Pairing parameters for $N \approx Z$. Odd-even mass difference

Sample for determination of liquid drop parameters:

Measured doubly even masses for $24 \leq A \leq 100,\ 0 \leq N - Z \leq 10$.

Pairing parameter α set to 0.

$\bar{G}, \zeta$ fitted to the known empirical value of the following quantities for odd N between 13 and 49:

$$E(N,N) - \frac{E(N-1,N-1) + E(N+1,N+1)}{2}, \quad E^*(N,N) - E(N,N).$$

(Remember that for odd N the energy $E(N,N)$ is the lowest $T \approx 0$ energy and $E^*(N,N)$ is the lowest $T \approx 1$ energy.)

Result:

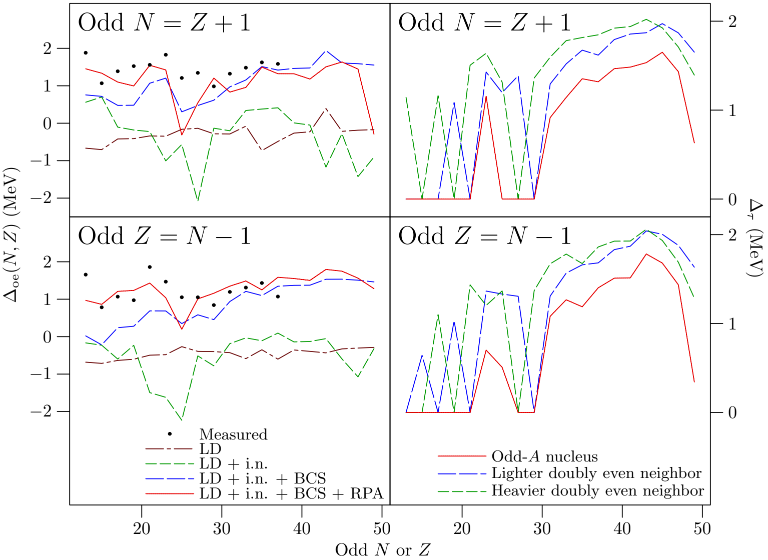
$$G_\tau = 7.196 A^{-0.7461} \text{ MeV} \quad \text{(independently of } \tau\text{)}.$$

Odd-even mass difference:

$$\text{Odd } N, \text{ even } Z: \quad \Delta_{\text{oe}}(N,Z) = E(N,Z) - \frac{E(N-1,Z) + E(N+1,Z)}{2}.$$

Odd Z, even N analogous.

Results for $Z = N - 1$



Why is the RPA contribution to $\Delta_{\rm oe}(N, Z)$ different in light an heavy nuclei?

Because $\tilde{E}_{\rm RPA,\tau}$ is a smooth function of N and Z, the contribution of $\delta E_{\rm RPA,\tau}$ to $\Delta_{\rm oe}(N, Z)$ stems mainly from $E_{\rm RPA,\tau}$.

The impact on $E_{\rm RPA,\tau}$ of the presence of an unpaired nucleon may be qualitative understood to result from the effective dilution of the single-nucleon spectrum by the blocking of the Fermi level.

On may see the effect of such a dilution by considering the expression for $\tilde{E}_{\rm RPA,\tau}$, which describes an average parameter dependence of $E_{\rm RPA,\tau}$.

In a good approximation, the dependence of $\tilde{E}_{{\rm RPA},np}$ on I_{np} is linear in $|N - Z|$ (Neergård, *op. cit.* 2016).

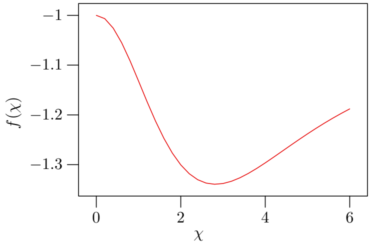
As this linear term does not contribute to $\Delta_{\rm oe}(N, Z)$, we can set $I_{np} = 0$. Then

$$\tilde{E}_{\rm RPA,\tau} = \tfrac{1}{2}\,\Omega_\tau G_\tau f(\chi_\tau),$$

$$f(\chi) = \frac{2\chi}{\pi \sinh \chi} \int_0^\infty \ln\left(\frac{1}{\chi}\tanh^{-1}\left((\tanh\chi)\sqrt{\frac{x^2}{x^2+1}}\right)\right) dx.$$

The function $f(\chi)$ is shown in the next slide.

Function $f(\chi)$



Remember $\chi_\tau = \dfrac{1}{\tilde{g}_\tau G_\tau}$.

When the single nucleon spectrum is diluted, $\tilde{g}_\tau$ decreases, and so χ_τ increases.

For $A \approx 24$ one gets $\chi_\tau \approx 3.8$. So $f'(\chi_\tau) > 0$, and $E_{\mathrm{RPA},\tau}$ increases with the blocking of the Fermi level.

For $A \approx 100$ one gets $\chi_\tau \approx 2.6$, which is slightly less than $\chi = 2.8$, where $f(\chi)$ is minimal. So $f'(\chi_\tau) \approx 0$. Then blocking the Fermi level has little impact on $E_{\mathrm{RPA},\tau}$ and the change may have either sign.

Pairing parameters for the neighbourhood of the Sn isotopic chain

Sample for determination of liquid drop parameters:

Measured doubly even masses for $50 \leq N \leq 88,\ 48 \leq Z \leq 52$.

Pairing parameter ζ kept from $N \approx Z$.

$\bar{G}, \alpha$ adjusted to reproduce on average:

1. The measured $\Delta_{\mathrm{oe}}(N, 50)$ for $51 \leq N \leq 83$.
2. The measured $\Delta_{\mathrm{oe}}(N, 49)$ for $54 \leq N \leq 82$ and $\Delta_{\mathrm{oe}}(N, 51)$ for $54 \leq N \leq 84$.

Result:

$$G_\tau = 5.818 A^{-0.7461}(1 - 0.0170 M_T M_T') \text{ MeV}$$

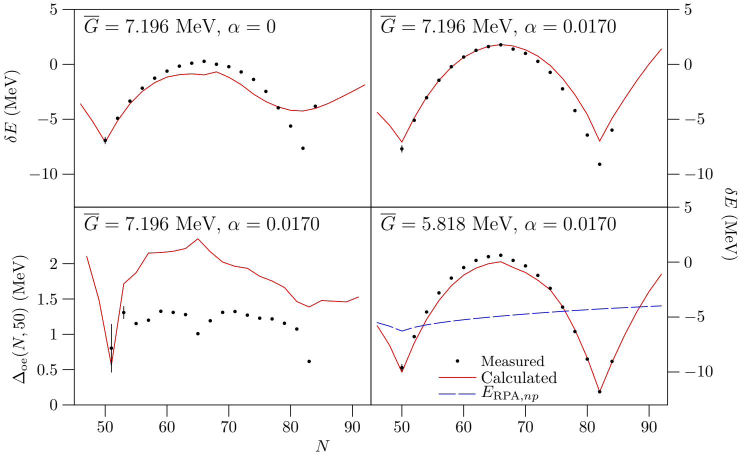
This $\bar{G}$ is 19% lower than the one for $N \approx Z$.

In particular we thus have two determinations of the τ-independent G_τ of ^{100}Sn which differ by this amount.

As the determination from $N \approx Z$ data involves the interpretation of incomplete spectra of ^{82}Nb and ^{86}Tb, the value above is likely to be most reliable.

The next slide illustrates the need both of reducing $\bar{G}$ relative to $N \approx Z$ and of choosing $\alpha > 0$.

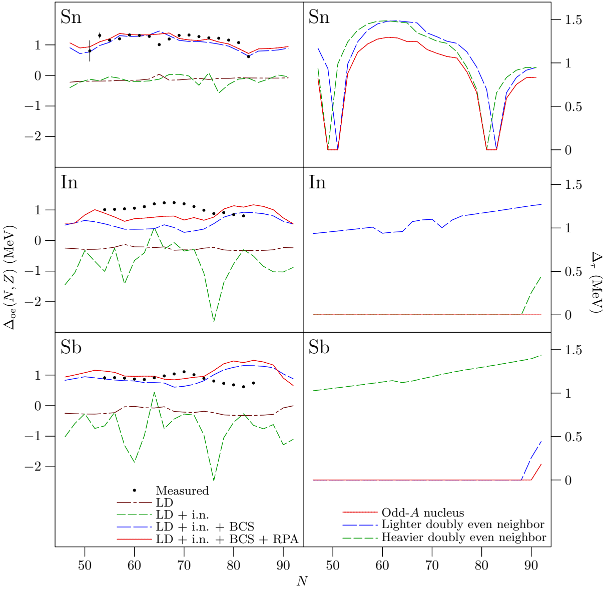
Need of reduced $\bar{G}$ and $\alpha > 0$



$\delta E = E(N, Z) - E_{\rm LD}$, measured and calculated.

Remember that the liquid drop parameters are adjusted for each choice of paring parameters. Therefore the empirical δE differ somewhat between the plots.

Results for the neighbourhood of the Sn isotopic chain



$N \approx 50$: $\chi_\tau \approx 3.2$. (Larger than above because G_τ is smaller.)

$N \approx 90$:

$\chi_n \approx 3.9$, $\chi_{p,np} \approx 2.9$.

All of these are larger than 2.8.

Pairing parameters for the neighbourhood of ^{102}Zr

Region: $60 \leq N \leq 64,\ 38 \leq Z \leq 42$. All these nuclei are well deformed.

Sample for determination of liquid drop parameters:
The doubly even nuclei in the region.

Pairing parameter ζ kept from $N \approx Z$.

$\bar{G}, \alpha$ adjusted to reproduce on average the empirical $\Delta_{\mathrm{oe}}(N, Z)$ in the region separately for odd N and odd Z

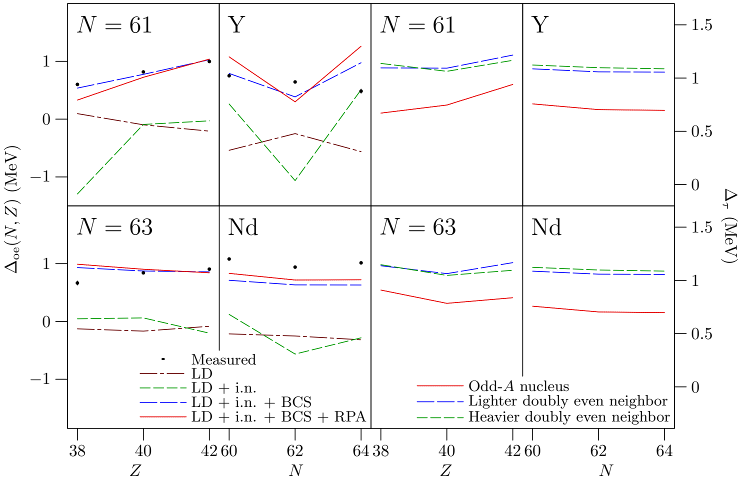
Result:

$$G_\tau = 5.210 A^{-0.7461}(1 - 0.0132 M_T M'_T) \text{ MeV}$$

This $\bar{G}$ is practically the same as for the Sn neighbourhood.

α is significantly smaller.

Results for the neighbourhood of ^{102}Zr



$\chi_n \approx 3.4$, $\chi_{p,np} \approx 3.2$. These are not much larger than 2.8.

Conclusion

The following was observed in the RPA-amended Nilsson-Strutinskij model.

- The RPA correction makes a very signinficant positive contribution to the odd-even mass difference in light nuclei with $Z = N - 1$.
- In heavier nuclei with $Z = N - 1$ as well as in the neighbourhood of the Sn isotopes and in the region of well-deformed nuclei near ^{102}Zr, this contribution is less significant and may have either sign.
- For $Z = N - 1$ in the upper *sd* shell, it makes up about half of the total odd-even mass difference for odd N and about the total for odd Z.
- The different significance of the RPA-correction in the light and heavy nuclei may be understood when its contribtion to the odd-even mass difference is assumed to result from the dilution of the single-nucleon by the blocking of the Fermi level in the odd-A nucleus.
- The smooth RPA energy in any channel of two-netron, two-proton or neutron-proton interaction indeed has a minimum at $\chi = 2.8$, where χ is the avarage level spacing at the Fermi level in units of the pair coupling constant.
- In the lighter nuclei, χ has values somewhat above this value, so the RPA energy increases with the blocking of the odd-A Fermi level.
- In the heavier nuclei, χ is closer to the point of minimum.

Interpolation

$E_{\mathrm{RPA},\tau\tau'}$ is interpolated when

$$(1) \quad \tau = \tau', \quad (2) \quad \tau\tau' = np \text{ and } N = Z.$$

Interpolation interval in terms of a parameter w:

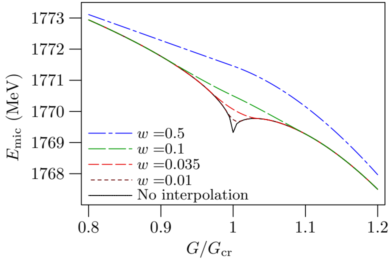
$$G_{\mathrm{min},\tau\tau'} < G_{\tau\tau'} < G_{\mathrm{max},\tau\tau'}$$
$$G_{\mathrm{min},\tau\tau'} = (1 - w)\min(G_{\mathrm{cr},\tau}, G_{\mathrm{cr},\tau'}),$$
$$G_{\mathrm{max},\tau\tau'} = (1 + w)\max(G_{\mathrm{cr},\tau}, G_{\mathrm{cr},\tau'}).$$

Note:

1. $G_{\substack{\mathrm{min}\\\mathrm{max}},\tau\tau} = (1 \mp w) G_{\mathrm{cr},\tau}$.
2. No interpolation when $G_{\mathrm{max},\tau\tau'} = 0$.
   This happens for $\tau = \tau'$ when $G_{\mathrm{cr},\tau} = 0$.
   As mentioned previously, this occurs when the nucleus is spherical and has an open subshell of nucleons of the kind τ.
   Conversely, $G_{\mathrm{cr},\tau}$ is particularly large in magic nuclei such as ^{56}Ni and ^{100}Sn, and actually close to G_τ in these two nuclei.

The next slide shows the influence of the interpolation parameter w on some calculated results.

Dependence of E_{mic} on the interpolation parameter w



^{100}Sn. (So all G_τ are equal $:= G$).

Levels $(\epsilon_{kn} + \epsilon_{kp})/2$ used for both neutrons and protons. (So $G_{\text{cr,n}} = G_{\text{cr,p}} := G_{\text{cr}}$.)

Seen: The choice of w can make a difference of 1–2 MeV in E_{mic}.

The graph for ^{56}Ni is similar.

Previous calculations (Bentley *et al.*, *op. cit.*, Neergård, *op. cit.* 2017) used $w = 0.5$.

Presently, we have chosen to take the RPA seriously unless there is a clear reason not to do so.

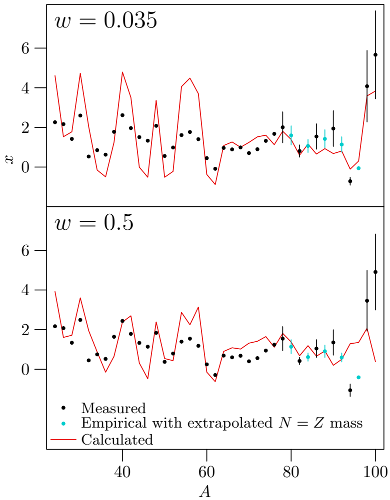
Such a reason is given by the observation that the exact minimum of H is a monotonic function of G.

Therefore, this should hold for E_{mic}.

As illustrated, this suggest $w = 0.035$.

This value was then chosen.

Wigner x



Definition of the Wigner x:

$$E(N,Z) = E_0 + \frac{|M_T|(|M_T|+x)}{2\theta} + a_c \frac{Z(Z-1)}{A^{1/3}} B_c,$$

$$|M_T| = 0, 2, 4 \text{ for } A \equiv 0 \mod 4,$$

$$|M_T| = 1, 3, 5 \text{ for } A \equiv 2 \mod 4.$$

Empirically, x has local maxima as a function of A at the doubly magic mass numbers 40, 56 and 100.

This is true in the calculations when $w = .035$ but not when $w = 0.5$.

Of course this does not prove that the former gives the best approximation to the exact minimum of H.

Extra slides

Ansatz states in a single-j shell

Quasi-neutrons $1 \dots n/2$ and quasi-protons $n/2+1 \dots n$ inhabit a single-j shell.

The symbols below indicate the coupling of their angular momenta $j_1, \dots, j_n$, all of which are equal to j.

$\mathcal{A}$ = antisymmetrisation in the quasi-neutrons and in the quasi-protons and normalisation.

$n = 4$ or 8:

$(v = 0)$ = unique state with isospin and seniority 0.

$n = 4$:

$(J = 2j)^2 = \mathcal{A}\,[(j_1 j_3)2j\ (j_2 j_4)2j\ ]0$, (Danos, Gillet) $(J = 1)^2 = \mathcal{A}\,[(j_1 j_3)1\ (j_2 j_4)1\ ]0$.

$n = 8$:

$(J = 2j)^4_{4j-2} = \mathcal{A}\,\{[(j_1 j_5)2j\ (j_2 j_6)2j\ ]4j{-}2\ [(j_3 j_7)2j\ (j_4 j_8)2j\ ]4j{-}2\ \}0$, (Danos, Gillet)

$(J = 2j)^4_0 = \mathcal{A}\,[(j_1 j_5)2j\ (j_2 j_6)2j\ ]0 \otimes [(j_3 j_7)2j\ (j_4 j_8)2j\ ]0$, (Van Isacker)

$(J = 2j)^4$ = span $\mathcal{A}\,[(j_1 j_5)2j\ (j_2 j_6)2j\ (j_3 j_7)2j\ (j_4 j_8)2j\ ]0$,
(dimensions 2 and 3 for $j = 7/2$ and $9/2$)

$(n = 4)^2 = \mathcal{A}\,\psi(j_1, j_2, j_5, j_6) \otimes \psi(j_3, j_4, j_7, j_8)$,
$\psi(j_1, j_2, j_3, j_4) = (n = 4$ ground state with the same interaction), (Qi)

$(J = 1)^4$ = unique state $\mathcal{A}\,[(j_1 j_5)1\ (j_2 j_6)1\ (j_3 j_7)1 (j_4 j_8)1\ ]0$.

Some of these were examined in Neergård, Phys. Rev. C 88, 034329 (2013); 90, 014318 (2014).

Overlaps

$n=4, 1f_{7/2}$	$(J=2j)^2$	$(J=1)^2$
$v=0$	0.62	0.19
$(J=2j)^2$		0.66

$n=4, 1g_{9/2}$	$(J=2j)^2$	$(J=1)^2$
$v=0$	0.52	0.11
$(J=2j)^2$		0.54

$n=8, 1f_{7/2}$	$(J=2j)^4_{4j-2}$	$(J=2j)^4_0$	$(J=2j)^4$ [a]	$(n=4)^2$ [b]	$(J=1)^4$
$v=0$	0.49	0.67	0.67	0.87	0.20
$(J=2j)^4_{4j-2}$		0.74		0.71	0.69
$(J=2j)^4_0$				0.94	0.67
$(J=2j)^4$ [a]				0.94	0.73
$(n=4)^2$ [b]					0.47

$n=8, 1g_{9/2}$	$(J=2j)^4_{4j-2}$	$(J=2j)^4_0$	$(J=2j)^4$ [a]	$(n=4)^2$ [c]	$(J=1)^4$
$v=0$	0.25	0.47	0.47	0.80	0.06
$(J=2j)^4_{4j-2}$		0.54		0.50	0.40
$(J=2j)^4_0$				0.87	0.45
$(J=2j)^4$ [a]				0.87	0.50
$(n=4)^2$ [c]					0.25

[a] The space $(J=2j)^4$, which contains the states $(J=2j)^4_{4j-2}$ and $(J=2j)^4_0$.

[b] Interaction ZR I. [c] Interaction QLW.

Overlaps with calculated states, $n = 4$

Interaction	$v = 0$	$(J = 2j)^2$	$\perp (v = 0),(J = 2j)^2$	$(J = 1)^2$	$\perp (v = 0),(J = 1)^2$
$1f_{7/2}$					
SchTr, emp.	0.78	0.97	1.5×10^{-3}	0.58	5×10^{-2}
SchTr, fit	0.82	0.95	7×10^{-4}	0.54	4×10^{-2}
ZR I	0.83	0.95	3×10^{-4}	0.52	4×10^{-2}
ZR II	0.76	0.98	1.7×10^{-5}	0.57	7×10^{-2}
$1g_{9/2}$					
SchTr, emp.	0.77	0.93	1.4×10^{-3}	0.43	8×10^{-2}
SchTr, fit	0.77	0.93	2×10^{-3}	0.44	8×10^{-2}
QLW	0.78	0.92	1.1×10^{-4}	0.38	1.0×10^{-1}
ZE I	0.88	0.84	1.7×10^{-3}	0.35	4×10^{-2}
ZE II	0.79	0.92	9×10^{-4}	0.41	8×10^{-2}
ZE III	0.89	0.83	9×10^{-4}	0.28	6×10^{-2}
ZE IV	0.83	0.89	3×10^{-6}	0.36	7×10^{-2}
CCGI	0.82	0.89	4×10^{-3}	0.42	5×10^{-2}
SLGT0	0.80	0.91	1.4×10^{-3}	0.41	7×10^{-2}
GF	0.76	0.93	1.3×10^{-3}	0.44	9×10^{-2}
ZI	0.77	0.93	1.5×10^{-3}	0.43	8×10^{-2}

Overlaps with calculated states, $n = 8$

Interaction	$v = 0$	$(J = 2j)^4_{4j-2}$	$(J = 2j)^4_0$	$(J = 2j)^4$	$(n = 4)^2$	$(J = 1)^4$
$1f_{7/2}$						
SchTr, emp.	0.75	0.78	0.93	0.95	0.97	0.50
SchTr, fit	0.79	0.77	0.93	0.94	0.97	0.48
ZR I	0.80	0.77	0.92	0.93	0.98	0.47
ZR II	0.73	0.80	0.92	0.94	0.96	0.50
$1g_{9/2}$						
SchTr, emp.	0.70	0.65	0.86	0.89	0.96	0.30
SchTr, fit	0.70	0.63	0.87	0.89	0.97	0.30
QLW	0.70	0.66	0.84	0.88	0.95	0.28
ZE I	0.83	0.50	0.80	0.80	0.99	0.22
ZE II	0.72	0.61	0.86	0.88	0.97	0.28
ZE III	0.85	0.44	0.76	0.76	0.98	0.17
ZE IV	0.76	0.61	0.82	0.85	0.97	0.25
CCGI	0.76	0.56	0.84	0.86	0.98	0.27
SLGT0	0.73	0.63	0.85	0.88	0.97	0.28
GF	0.68	0.67	0.86	0.90	0.95	0.31
ZI	0.70	0.64	0.86	0.89	0.96	0.30