Pairing theory of the Wigner energy

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What is the Wigner energy?

Myers, Swiatecki, Nucl. Phys. 81, 1 (1966):

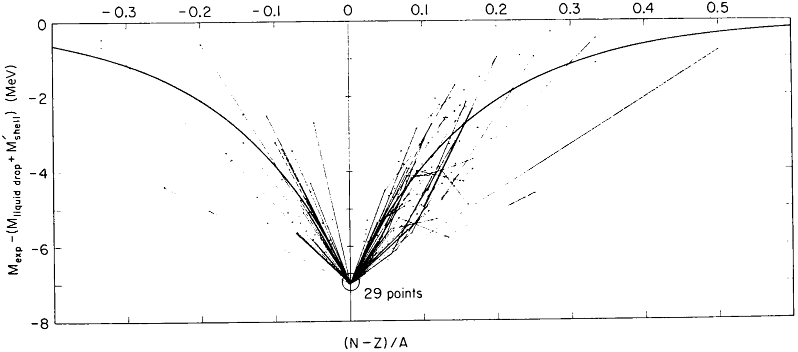


Fig. 14. The sharp trough along $N = Z$, occurring in the masses of the lighter nuclei, is illustrated. The experimental masses in the range $A = 4$ to $A = 58$ were corrected for all known effects (liquid-drop binding and shell effects deduced from nuclei with $N = Z$) and the remainder plotted as a function of $(N-Z)/A$. Lines connect even mass isobars, dots correspond to odd values of A. The smooth curve is the exponential function $-7\exp(-6|N-Z|/A)$.

Their "liquid-drop binding" has (N-Z)-quadratic symmetry energy.

Explanations of the Wigner energy

Myers and Swiatecki cite (hence name):

Wigner, Phys. Rev. 51, 947 (1937)
(twelve years before the discovery of the nuclear spin-orbit splitting):
Spin-isospin $SU(4)$ symmetry
$\Rightarrow$ INTERACTION part of symmetry energy $\propto T(T+4)$.
T = isospin, in N, Z even ground states = $T_z = |N - Z|/2$.
KINETIC part $\propto T^2$ (Thomas-Fermi approximation).

Neergård, Phys. Rev. C 80, 044313 (2009):
Redoes Wigner's derivation but for isospin $SU(2)$ symmetry.
Gets interaction part $\propto T(T+1)$.
$\Rightarrow$ TOTAL symmetry energy $\propto T(T+X)$, $X < 1$.

Many attempts of explanation by Myers and Swiatecki and others.
Review in Neergård, *op. cit.*

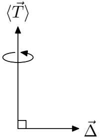
Superfluid isorotation

Duflo, Zuker, Phys. Rev. C 52, R23 (1995):
Semi-empirical mass formula with symmetry terms $\propto T(T+1)$.

Frauendorf, Sheikh, Nucl. Phys. A 645, 509 (1999);
Phys. Scr. T 88, 162 (2000):
This looks like axially symmetric rotor spectrum.
What deformation? Answer: superfluidity. Measured by gaps $\Delta_{n,p}$.
Isovector $\vec{\Delta}$:

$$\Delta_x + i\Delta_y = \sqrt{2}\Delta_p\,, \qquad \Delta_x - i\Delta_y = -\sqrt{2}\Delta_n\,,$$
$$\Delta_z \propto \langle \text{sum of } np \text{ pair annihilators} \rangle\,.$$

In a product of n and p BCS states, $\langle T_x \rangle = \langle T_y \rangle = \Delta_z = 0$.
Thus isorotation on an axis perpendicular to $\vec{\Delta}$.



NOTE: $\vec{\Delta}$ is a *complex* vector.
Its real and imaginary parts may have different directions.
$\vec{\Delta}^* \propto \langle$isovector of sums of pair *creators*$\rangle$.

Hartree-Bogolyubov + Random Phase model

Neergård, Phys. Lett. B 537, 287 (2002); 572, 159 (2003); *op.cit.* (2009):

Hamiltonian: $H = \sum_i h_i - G\,\vec{P}^\dagger\!\cdot\vec{P} + \kappa \sum_{i<j} \vec{t}_i\cdot\vec{t}_j$.

$$\begin{array}{lcl} i & = & \text{nucleon label.} \\ \vec{t} & = & \text{single-nucleon isospin .} \\ h & = & \text{single-nucleon Hamiltonian, } [h, \vec{t}\,] = 0\,. \\ \vec{P} & = & \text{isovector of such sums of pair annihilators that} \\ & & \vec{\Delta} = G\langle\vec{P}\rangle \text{ in the quasinucleon vacuum.} \end{array}$$

Routhian: $R = \langle\sum_i h_i\rangle - G|\langle\vec{P}\rangle|^2 + \frac{1}{2}\kappa|\langle\vec{T}\rangle|^2 - \lambda_n\langle N\rangle - \lambda_p\langle Z\rangle$.

No exchange terms! That is, Hartree-Bogolyubov without "Fock".

Minimised with Bogolyubov quasinucleon vacuum.
$\langle N\rangle, \langle Z\rangle$ identified with N, Z. Result: BCS.

Ground state energy. Goldstone modes

RPA corresponding to small oscillations about the Hartree-Bogolyubov minimum. Ground state energy:

$$E = \sum v^2 \epsilon - |\vec{\Delta}|^2 / G + \tfrac{1}{2} \kappa T^2 + c + \tfrac{1}{2} \left(\sum \omega - \sum \omega_0 \right) .$$

ϵ	$=$	eigenvalue of h, counted with multiplicity.
v^2	$=$	BCS occupancy, possibly different for neutrons and protons.
c	$=$	constant *containing omitted exchange terms*. T-independent.
ω / ω_0	$=$	perturbed/unperturbed RPA frequency.

Goldstone and quasi-Goldstone modes:

$\omega = 0$ from conservation of N, Z. (Only for $\Delta_{n,p} > 0$.)

IMPORTANT: $\omega = |\lambda_n - \lambda_p|$ from $[-\lambda_n N - \lambda_p Z, T_-] = (\lambda_n - \lambda_p) T_-$.
(Only for $T > 0$ or $T = 0$ and $\Delta_n = \Delta_p > 0$.)

This gives energy contribution essentially linear in T.

The symmetry force

Symmetry force: $\kappa \sum_{i<j} \vec{t}_i \cdot \vec{t}_j$.

Only contributes to E:

$$E = E(\kappa = 0) + \tfrac{1}{2}\kappa \left(T(T+1) - \frac{3A}{4} \right) \quad \text{(the exact eigenvalue)}.$$

No influence on BCS state or composition of RPA modes except the quasi-Goldstone mode.

$\Rightarrow$ Corresponding term in E may be added *a posteriori*.

NOTE: The symmetry force is *attractive* in the $T = 0$ *two-particle* and *two-hole* channels (though acting here in the *particle-hole* channel):

$$\vec{t}_1 \cdot \vec{t}_2 = \begin{cases} -\frac{3}{4}\,, & T = 0 \\ \frac{1}{4}\,, & T = 1 \end{cases}$$

This is how isoscalar attraction enters this model.

Equidistant case

Equidistant four-fold degenerate ϵ:

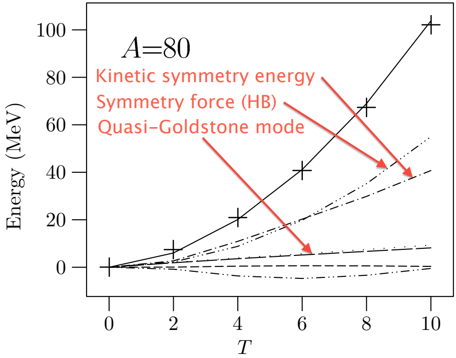
$$E = E(T=0) + \tfrac{1}{2}(D+\kappa)T(T+1)\,, \quad D = \text{level spacing}\,,$$

(in a very good approximation).

The term $\frac{1}{2}DT$ requires the spontaneous breaking of the isobaric invariance by the pairing force.

Absent for $G = 0$.
Weakened for $G < G_{\text{crit}} =$ lower limit for $\Delta > 0$:
First order perturbation theory: Linear term $\frac{1}{2}GT$.
Note: $G_{\text{crit}} \approx D\big/\big(2 + \log(\Omega/2)\big) \ll D\,, \quad \Omega = \text{number of levels}\,.$
(Neergård, *op. cit.* 2003.)

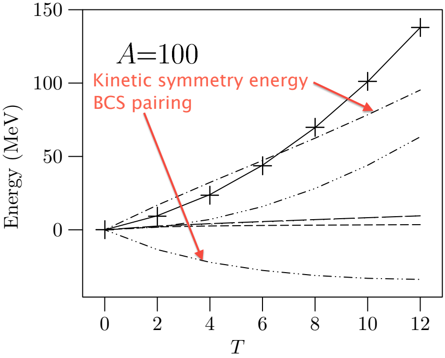
Deformed case

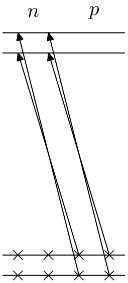


$+$ = empirical Coulomb reduced relative mass.
— $= E - E(T = 0)$. Broken line = individual term.
Kinetic symmetry energy $= \sum v^2 \epsilon$ relative to $T = 0$,
Symmetry force (HB) $= \frac{1}{2}\kappa T^2$.
Quasi-Goldstone mode $= \frac{1}{2}|\lambda_n - \lambda_p|$.
For $T = 2$, the latter/$(E - E(T = 0)) \approx 1/3 = T/(T(T + 1))$.
Neutron Woods-Saxon levels, $\beta = 0.342$ (from $E_{2^+}(^{80}\mathrm{Zr})$), $\Omega = 40$,
$G = 0.264$ MeV (from $\Delta_{n,p}(T = 0) = 12\ \mathrm{MeV}/\sqrt{A}$), $\kappa = 1.1$ MeV.

Doubly magic case

Yet another mechanism!





BCS pairing $= -|\vec{\Delta}|^2/G$ relative to $T = 0$.
$\beta = 0, \Omega = 41$ (one more major shell),
$G = 0.2$ MeV ($\Rightarrow \Delta_{n,p}(T > 0) \approx 12$ MeV$/\sqrt{A}$), $\kappa = 0.8$ MeV.

Conclusions of the Hartree-Bogolyubov + Random Phase analysis

- On *average*, represented by the equidistant case, superfluid isorotation gives a symmetry energy $\propto T(T+1)$.
- Shell structure modifes this average behaviour.

The analysis in terms of Goldstone modes is inspired by Marshalek, who did it for spatial rotation, Nucl. Phys. A 275, 416 (1977). Marshalek cites Ginocchio, Wesener, Phys. Rev. 170, 859 (1968), whose model and analysis is the same as the present one except for the symmetry force.

Exact minimisation of the Hamiltonian

Bentley, Frauendorf, Phys. Rev. C 88, 014322 (2013):

Concerned with the accuracy of the RPA for $G \approx G_{\text{crit}}$.
Relevant to medium mass nuclei.
Therefore: Exact minimisation of the Hamiltonian for each A, T, T_z.

Only feasible for small Ω.
The authors include $\Omega = 7$ neutron-proton average Nilsson levels about the Fermi level.

Individual deformations for each N, Z are taken from a Nilsson-Strutinsky calculation.
This is unlike Neergård, *op. cit.*, who keeps the Hamiltonian constant for each A.
Breaks insignificantly the isobaric invariance in $T = 1$ multiplets.

Analysis in the case of exact minimisation

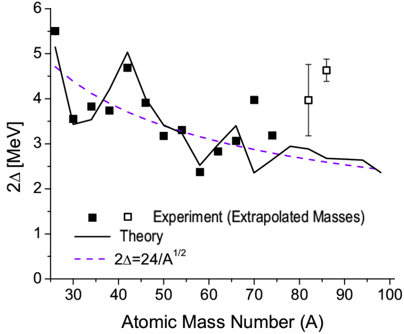
The following combinations of empirical and calculated $E(A, T, T_z)$ are considered. The empirical $E(A, T, T_z)$ is the mass reduced by the Coulomb energy relative to $T_z = 0$:

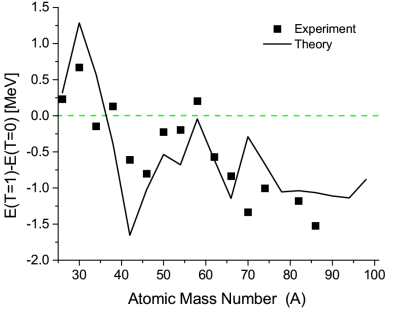
- $T = 0$ doubly odd-doubly even mass differences: "2Δ" $= E(A,0,0) - \big(E(A-2,0,0) + E(A+2,0,0)\big)/2$, odd $A/2$.
- Isospin splitting in the doubly odd $N = Z$ nuclei: $E(A,1,0) - E(A,0,0)$, odd $A/2$.
- Constants θ, X in $E(A, T, T) = \text{constant} + \dfrac{T(T+X)}{2\theta}$ from: $T = 0,2,4$ for even $A/2$. $T = 1,3,5$ for odd $A/2$.

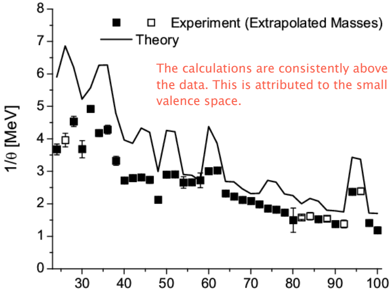
Parameters fitted to the $T = 0$ doubly odd-doubly even mass differences and the isospin splittings:

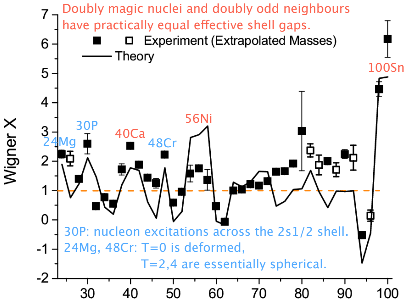
$$G = 13.9A^{-3/4}\ \text{MeV}\,, \quad \kappa = 119.8A^{-1}\ \text{MeV}\,.$$

Results of exact minimisation



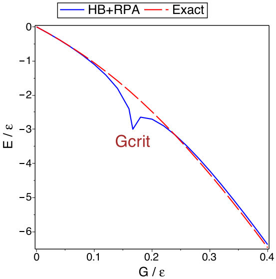


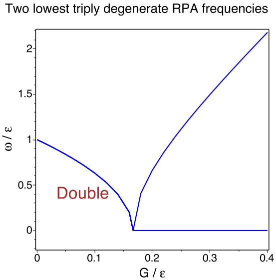


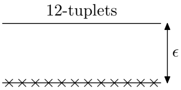


Comparison with HB + RPA

Bentley, Neergård, Frauendorf, Phys. Rev. C 89, 034302 (2014):
The exact minimisation allows a test of HB+RPA.
Found good except in a narrow region about G_{crit}.
The plot in the middle shows the origin of the singularity:







Similar results for one type of nucleon:
Hung, Dang, Phys. Rev. C 76, 054302 (2007).

The singularity can be remedied by interpolation.
The case shown is the most extreme one among those studied; configuration on the right.

Nilsson-Strutinsky + HB + (interpolated) RPA (1)

Bentley, Neergård, Frauendorf, *op. cit.*:

Strutinsky energy expression:

$$E = E_{\mathrm{LD}} + E_{\mathrm{s.p.}} - \tilde{E}_{\mathrm{s.p.}} + P - \tilde{P}\,.$$

E_{LD}	$=$	deformed liquid drop energy.
$E_{\mathrm{s.p.}}$	$=$	sum of occupied single-nucleon levels.
P	$=$	pairing energy.
$\tilde{E}_{\mathrm{s.p.}}, \tilde{P}$	$=$	smooth counterterms.

Nilsson-Strutinsky + HB + (interpolated) RPA (2)

$$E_{\mathrm{LD}} = -\left(a_v - a_{vt}\frac{T(T+1)}{A^2}\right)A + \left(a_s - a_{st}\frac{T(T+1)}{A^2}\right)A^{2/3}B_s$$
$$+\, a_c\frac{Z(Z-1)}{A^{1/3}}B_c\,, \qquad B_s, B_c \text{ are functions of the deformation.}$$

This absorbs the symmetry force.

$E_{\mathrm{s.p.}} + P$ from HB + (interpolated) RPA, $\Omega = A/2$.

In doubly odd $T = 0$ states the Fermi level is blocked to the pairing force.

h as in Bentley, Frauendorf, *op. cit.*, except that states with equal T, "isobaric analogues", are assumed to have the same deformation, the one calculated for $T_z = T$. Thus, except for the liquid drop Coulomb term, the last term in E_{LD}, we now have exact isobaric invariance also for $T = 1$.

Nilsson-Strutinsky + HB + (interpolated) RPA (3)

$\tilde{E}_{\text{s.p.}}$ by standard Strutinsky smoothing:
3rd order. Smoothing parameter $41A^{-1/3}$ MeV.

$\tilde{P}$ by replacing sums with integrals:
$\tilde{P} = \tilde{P}_{\text{BCS}} + \tilde{P}_{\text{RPA}}$, where:

$$\tilde{P}_{\text{BCS}} = -\sum_{n,p} \frac{\Omega\tilde{\Delta}}{2\exp a},$$

$$\begin{aligned}\tilde{P}_{\text{RPA}} &= \sum_{n,p,np} \frac{2\tilde{\Delta}}{\pi} \int_0^\infty \log\left(\frac{1}{2a}\log\frac{\cosh(x+a)}{\cosh(x-a)}\right)\cosh x\,dx \\ &\quad + |\tilde{\lambda}_n - \tilde{\lambda}_p|/2,\end{aligned}$$

$$\tilde{\Delta} = \frac{\Omega}{2\tilde{g}(\tilde{\lambda})\sinh a}, \quad a = \frac{1}{\tilde{g}(\tilde{\lambda})G}, \quad n, p, np.$$

$\tilde{g}(\epsilon) =$ smooth level density. $\tilde{\lambda}_n, \tilde{\lambda}_p, \tilde{\lambda}_{np}$ correspond to $N, Z, A/2$.
The last term in $\tilde{P}_{\text{RPA}}$ cancels the kinetic contribution to the T-linear term in E_{LD} so that the actual kinetic contribution is due to the quasi-Goldstone term in P_{RPA}.

Nilsson-Strutinsky + HB + (interpolated) RPA (4)

With the *complete* expression for the total energy, the liquid drop parameters were fitted to the 112 measured doubly even masses with $24 \leq A \leq 100$, $0 \leq N - Z \leq 10$. Asymptotic Duflo-Zuker parameters were considered but miss quite a lot the masses in the upper part of this region. The parameters in MeV shown below are insignificantly different from those published due to an improved RMSD minimisation. The minimum is RMSD = 0.950 MeV. Both sets are similar to the most recent asymptotic Duflo-Zuker parameters.

a_v	a_{vt}	a_s	a_{st}	a_c
15.15	108.6	16.24	128.3	0.6583

E_{LD} with symmetry energy $\propto T^2$: RMSD = 1.193 MeV
E_{LD} with symmetry energy $\propto T(T+4)$: RMSD = 1.430 MeV
This confirms the bulk $T(T+1)$ proportionality.

Nilsson-Strutinsky + HB + (interpolated) RPA (5)

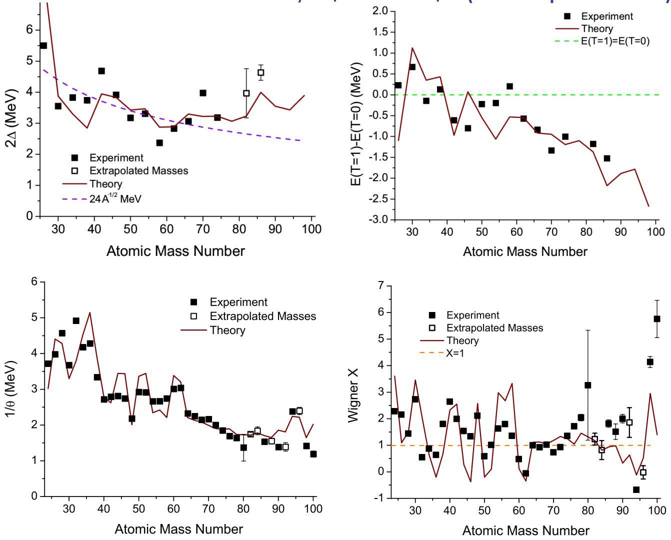
Fitted to the $T = 0$ doubly odd-doubly even mass differences:

$$G = 8.6A^{-4/5}\ \text{MeV}\,.$$

Analysis as in Bentley, Frauendorf, *op. cit.* with the following modifications.

- Doubly odd-doubly even mass differences are derived from the empirical and calculated *total* masses.
- In the calculations of $E(A,1,0) - E(A,0,0)$, $1/\theta$ and X, the liquid drop Columb energy is subtracted from both.

Results of Nilsson-Strutinsky + HB + (interpolated) RPA



Now, *both* $E(A,1,0) - E(A,0,0)$ and $1/\theta$ are reproduced on average. Shell effects as before.

Remake of a shell model calculation

$A = 48$. Effective interactions from the literature.
Original calculation in the *fp* shell: Satuła *et al.*, Phys. Lett. B 407, 103 (1997).
Remake in the $1f7/2$ shell: Bentley, Neergård, Frauendorf, *op. cit.*

J of included interactions								$1/\theta$ (MeV)	X	X/θ (MeV)
0	1	2	3	4	5	6	7	2.41	1.31	3.17
0		2	3	4	5	6	7	2.23	1.07	2.37
0		2		4	5	6	7	1.86	1.23	2.29
0		2		4		6	7	1.38	1.75	2.42
0		2		4		6		0.25	1.71	0.42

Satuła *et al.* noticed the drop of X/θ when the $T = 0$ interaction is quenched and concluded that the $T = 0$ interaction is responsible for the Wigner energy. It is seen that the drop of X/θ is due to a drop of $1/\theta$ and X increases.

Leaving $T \approx 0$

It was a point above to keep the isobaric invariance. In particular, neutron-proton average Nilsson levels were employed. This cannot be upheld in moving away from $T \approx 0$ towards a general theory.

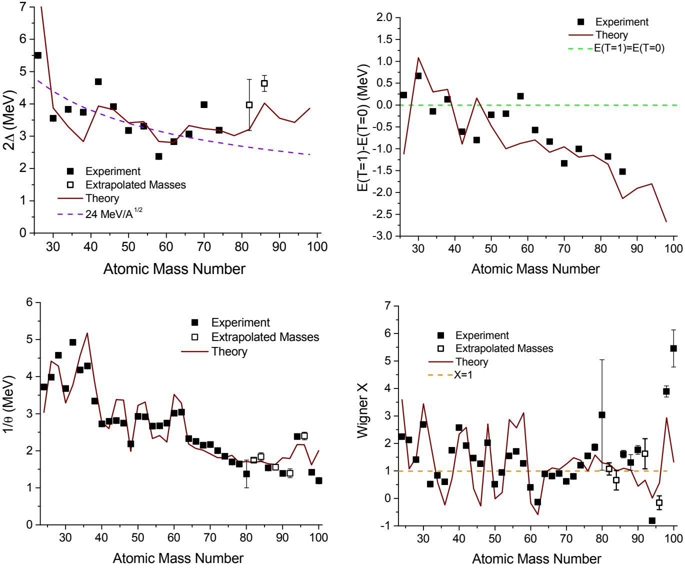
Modifications to allow different neutron and proton spectra *keeping the calculations simple*:

- The difference between the *state vectors* of a single neutron and a single proton in orbits with equal ordinal number from the bottom is neglected. That is, only the *energies* are assumed different. Then the formulas for P_{RPA} remain the same.
- In $\tilde{P}_{\mathrm{RPA}}$, the smooth level density $\tilde{g}(\tilde{\lambda}_{np})$ is replaced with $(\tilde{g}(\tilde{\lambda}_{n0}) + \tilde{g}(\tilde{\lambda}_{p0}))/2$, where $\tilde{\lambda}_{n0}$ and $\tilde{\lambda}_{p0}$ are the smooth neutron and proton chemical potentials for $T = 0$.
- In $\tilde{P}_{\mathrm{RPA}}$, the term $|\tilde{\lambda}_n - \tilde{\lambda}_p|/2$ is replaced with $|\tilde{\lambda}_n - \tilde{\lambda}_{n0} + \tilde{\lambda}_{p0} - \tilde{\lambda}_p|/2$.

Results with different neutron and proton spectra (1)

- Upon refit of the liquid drop parameters, the RMSD of the previous 112 masses drops from 0.950 MeV to 0.870 MeV.
- The changes in the combinations of masses are invisible in the plots. See the next slide.

Results with different neutron and proton spectra (2)



Conclusion of Strutinsky calculations and an outlook

- The Hartree-Bogolyubov plus Random Phase scheme is an excellent approximation to the exact minimisation of the paring force Hamiltonian except near the critical values of the pairing force constant G.
- The singularities at the critical G can be remedied by interpolation.
- Strutinsky renormalisation of the resulting theory enables an accurate description of the masses near $N = Z$ and the isospin splitting in the $N = Z$ doubly odd nuclei *including a microscopic Wigner energy*.
- The variation with A of the Wigner X is well understood from the shell structure.
- Easy modifications allow the theory to be extended to the entire chart of nuclides and improve the fit to the masses near $N = Z$.
- It is conceivable to replace the Strutinsky renormalisation with a Hartree-Fock approach.