FISSION BARRIERS
OF
TWO ODD-NEUTRON HEAVY NUCLEI

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EFFECTIVE INTERACTIONS

The fission barriers of the ^{235}U and ^{239}Pu nuclei
have been calculated within the
Hartree-Fock plus BCS with blocking formalism

Two Skyrme force parametrizations have been considered
SIII and SkM*
They are known to reproduce reasonably well
systematic spin and parity properties
of the ground states of odd nuclei

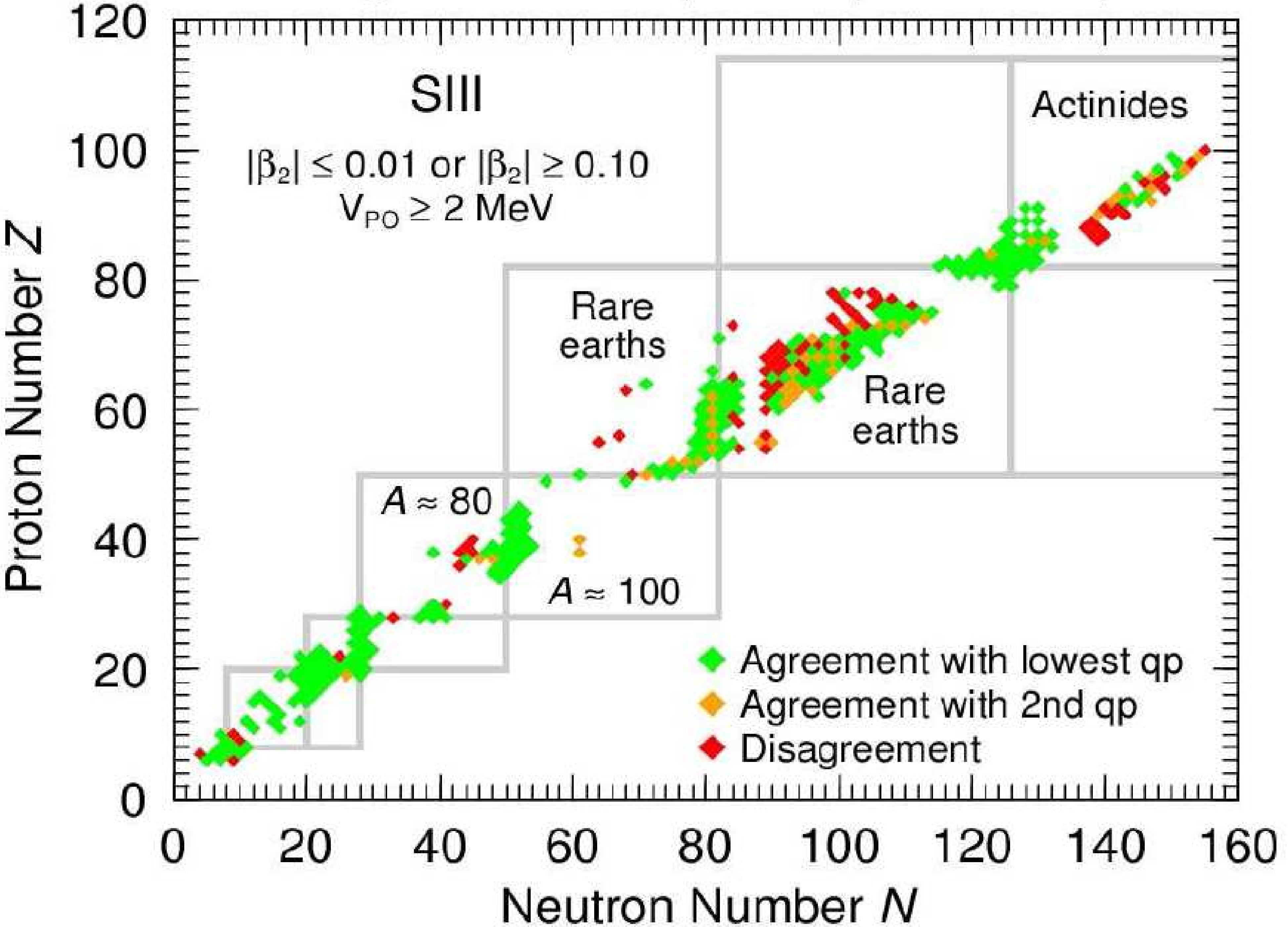
The pairing correlations have been generated
by a seniority force whose parameters
have been fitted to reproduce « experimental » gaps

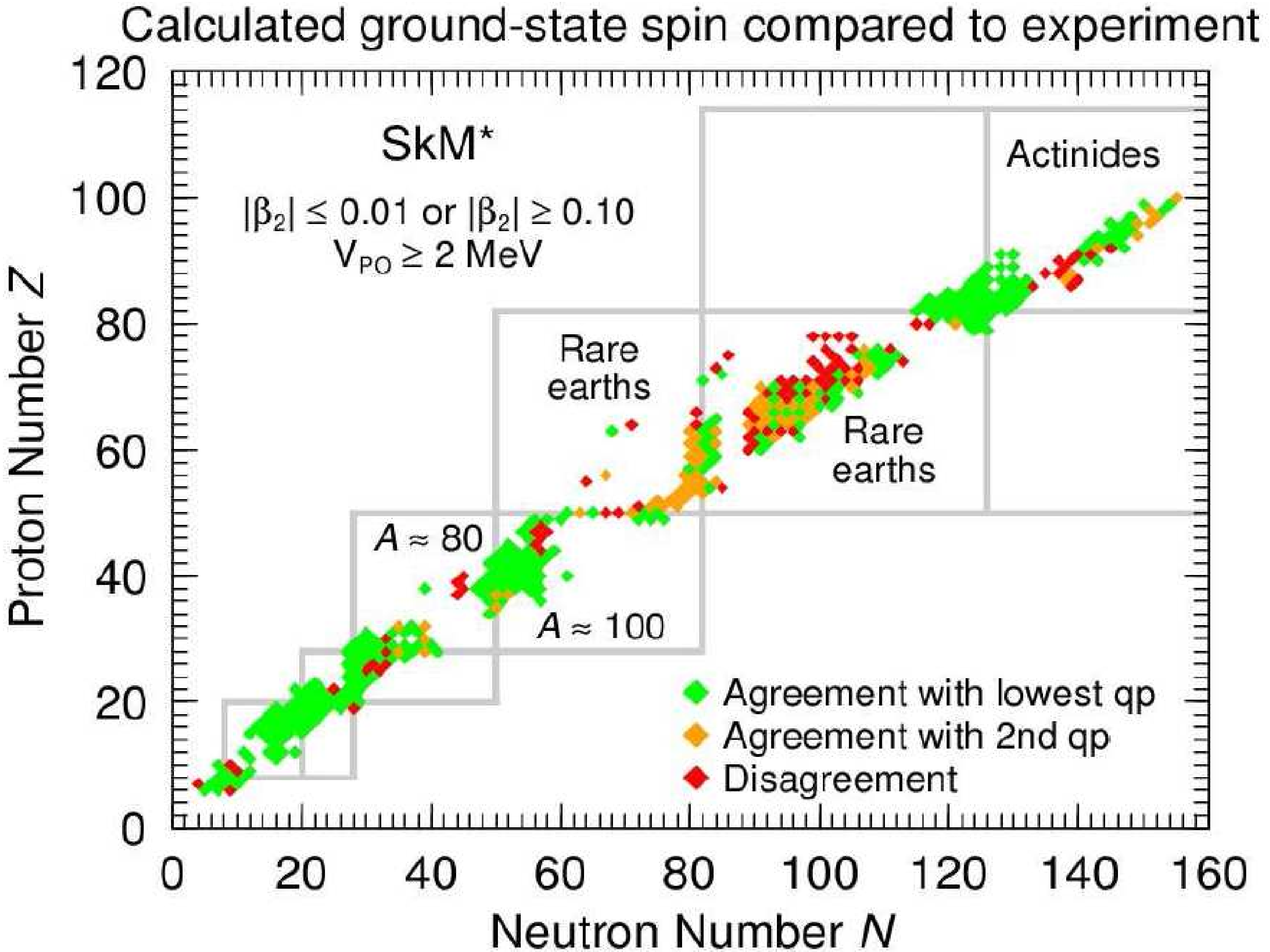
$$\Delta_n(N,Z) = \frac{(-1)^N}{2}\,[S_n(N,Z) - S_n(N+1,Z)] \quad \text{and} \quad \Delta_p(N,Z) = \ldots$$

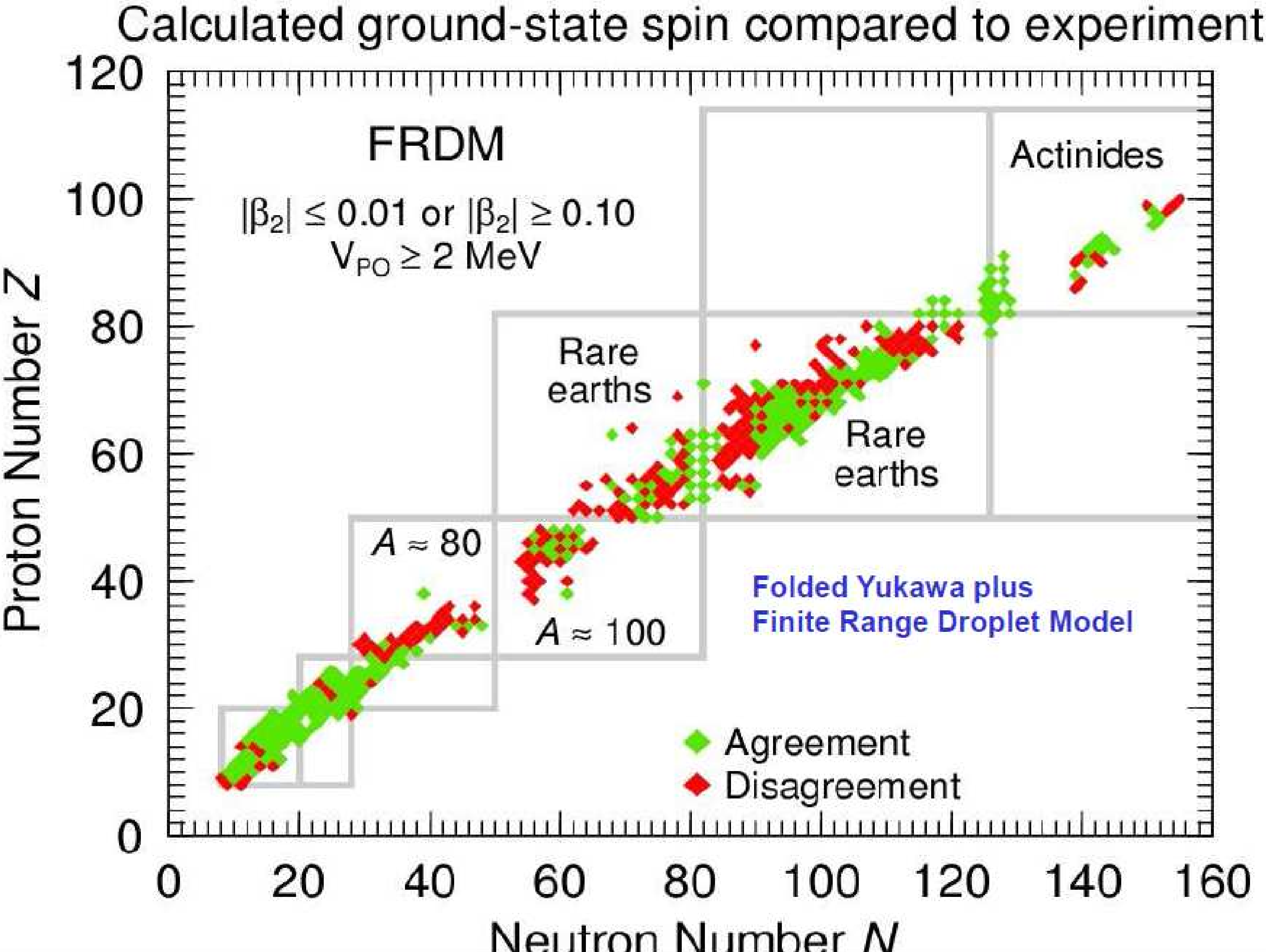
for some well deformed <u>odd</u> nuclei
having reasonably high gaps in the actinide region

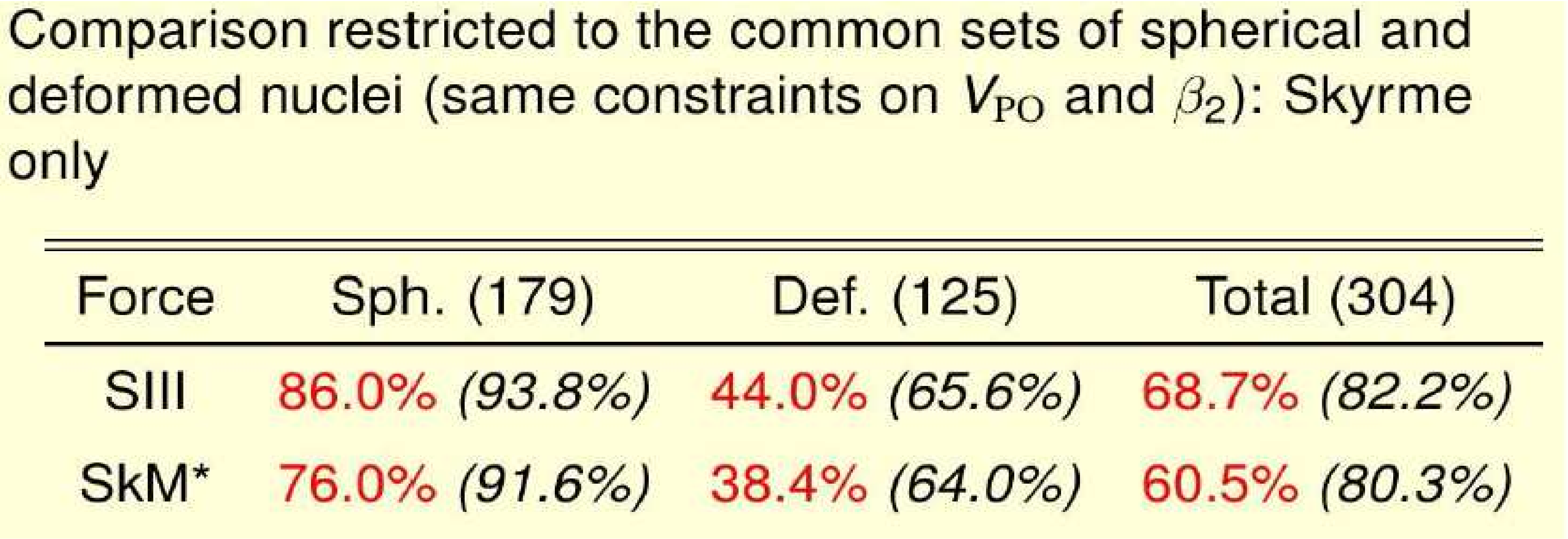
L. Bonneau, P. Quentin, P. Möller, Phys. Rev. C76, 024320 (2007)

Calculated ground-state spin compared to experiment




Calculated ground-state spin compared to experiment
SkM*
$|\beta_2| \leq 0.01$ or $|\beta_2| \geq 0.10$
$V_{PO} \geq 2$ MeV
Actinides
Rare earths
Rare earths
A ≈ 80
A ≈ 100
Agreement with lowest qp
Agreement with 2nd qp
Disagreement
Proton Number Z
Neutron Number N
0
20
40
60
80
100
120
0
20
40
60
80
100
120
140
160


Calculated ground-state spin compared to experiment
FRDM
$|\beta_2| \leq 0.01$ or $|\beta_2| \geq 0.10$
$V_{PO} \geq 2$ MeV
Actinides
Rare earths
Rare earths
$A \approx 80$
$A \approx 100$
Folded Yukawa plus
Finite Range Droplet Model
Agreement
Disagreement
Proton Number Z
Neutron Number N
0
20
40
60
80
100
120
0
20
40
60
80
100
120
140
160



Comparison restricted to the common sets of spherical and deformed nuclei (same constraints on V_{PO} and β_2): Skyrme only

Force	Sph. (179)	Def. (125)	Total (304)
SIII	86.0% *(93.8%)*	44.0% *(65.6%)*	68.7% *(82.2%)*
SkM*	76.0% *(91.6%)*	38.4% *(64.0%)*	60.5% *(80.3%)*

These two interactions provide also reasonably good s.p. wavefunctions
in particular for their magnetic properties
as seen from a recent study on magnetic moments
of some deformed nuclei

L.Bonneau, N. Minkov, Dao Duy Duc, P. Quentin, J. Bartel
Phys. Rev. C91, 054307 (2015)

TABLE VIII. Magnetic moments (in μ_N units) with the SIII parametrization: intrinsic contribution μ_{intr}, collective gyromagnetic ratio $g_R^{(\mathrm{unpol})}$ calculated without core polarization, corresponding total magnetic moment $\mu_{\mathrm{tot}}^{(\mathrm{unpol})}$, collective gyromagnetic ratio $g_R^{(\mathrm{pol})}$ calculated with core polarization, corresponding total magnetic moment $\mu_{\mathrm{tot}}^{(\mathrm{pol})}$, and experimental μ_{exp} values taken from Ref. [30] (by convention, the most recent value is retained when several entries appear).

Nucleus	K^π	μ_{intr}	$g_R^{(\mathrm{unpol})}$	$\mu_{\mathrm{tot}}^{(\mathrm{unpol})}$	$g_R^{(\mathrm{pol})}$	$\mu_{\mathrm{tot}}^{(\mathrm{pol})}$	μ_{exp}
^{99}Sr	$5/2^-$	−0.753	0.262	−0.566	0.302	−0.537	
	$3/2^+$	−0.630		−0.473	0.305	−0.447	−0.261(5)
^{99}Y	$5/2^+$	2.927	0.262	3.114	0.285	3.131	
^{103}Mo	$3/2^+$	−0.624	0.249	−0.475	0.251	−0.473	
	$5/2^-$	−0.734		−0.556	0.213	−0.582	
^{103}Tc	$5/2^+$	2.811	0.249	2.989	0.450	3.132	
	$3/2^-$	1.962		2.111	0.303	2.144	
^{175}Yb	$7/2^-$	0.886	0.338	1.149	0.361	1.167	0.768(8)
^{175}Lu	$7/2^+$	1.452	0.338	1.715	0.352	1.726	2.2323(11)
^{179}Hf	$9/2^+$	−1.000	0.345	−0.718	0.327	−0.732	−0.6409(13)
^{179}Ta	$7/2^+$	1.460	0.345	1.728	0.335	1.721	2.289(9)
	$9/2^-$	5.075		5.357	0.351	5.362	
^{235}U	$7/2^-$	−0.768	0.324	−0.516	0.289	−0.543	−0.38(3)
^{235}Np	$5/2^+$	2.663	0.324	2.894	0.407	2.954	
	$5/2^-$	0.833		1.064	0.354	1.086	
^{237}Np	$5/2^+$	2.744	0.318	2.971	0.407	3.035	3.14(4)
	$5/2^-$	0.831		1.058	0.348	1.080	1.68(8)

These interactions are quite old
SIII (1975), SkM* (1982)
As compared to more recent ones,
they do not include some EDF components
which were not considered in their fitting process
(related e.g. to the square of the spin-current tensor
or including a zero-range tensor component)

Yet
They show no spin instability near saturation
As we saw they seem to yield reasonably good spectroscopic properties
It is therefore interesting to see how good they are
to describe s.p. energy spectra
and consequently fission barrier distributions
according to the spin and parity for a given fissioning nucleus
However we have used sometimes the SLy5* force to see...

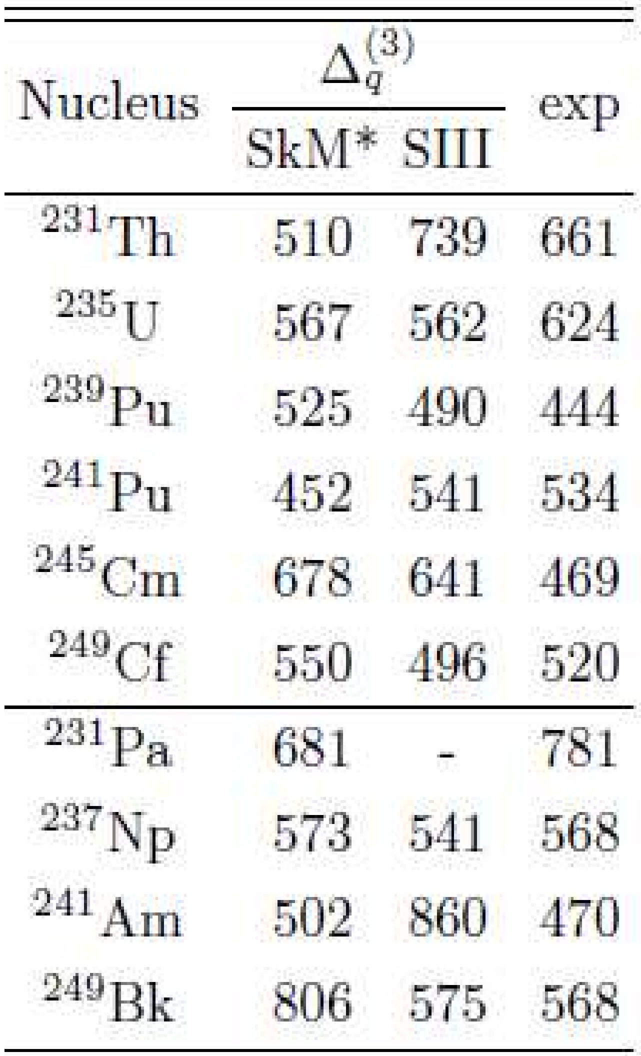
The parameters of the seniority force

Only n-n and p-p pairing
(12 MeV s.p. window
around the chemical potential)

$$\langle i\,\tilde{i}\,|\tilde{v}_{residual}|\,j\,\tilde{j}\,\rangle = \frac{G_q}{11 + N_q}$$

$G_n = -16.0$ MeV, $G_p = -16.0$ MeV for SkM*

$G_n = -17.15$ MeV, $G_p = -14.0$ MeV for SIII.



Nucleus	$\Delta_q^{(3)}$		exp
	SkM*	SIII	
^{231}Th	510	739	661
^{235}U	567	562	624
^{239}Pu	525	490	444
^{241}Pu	452	541	534
^{245}Cm	678	641	469
^{249}Cf	550	496	520
^{231}Pa	681	-	781
^{237}Np	573	541	568
^{241}Am	502	860	470
^{249}Bk	806	575	568

SOME THEORETICAL ASPECTS

The time reversal breaking
due to the presence of the « odd » nucleon
is taken into account self-consistently in the mean field approach

It has been explicitely shown to be perturbative
One can thus define unambiguously « quasi pairs » of states
which are almost time reversal images

From these quasi-pairs we define a Bogoliubov-Valatin-like
restricted Bogoliubov canonical transformation

Only seniority one states have been considered so far
thus limiting ourselves to low energy s.p. excitations

Axial symmetry has been imposed
(a genuine limitation at least
for the description of the inner fission barrier)
Intrinsic parity has not been imposed
(necessary for a fair description of the outer fission barrier)

From calculated mean field energies to nuclear energies

For well deformed nuclei, as the considered actinide nuclei in their ground state and on the way to fission,
we use the Bohr-Mottelson Unified Model ansatz

$$|I\,M\,\alpha\,K\,\pi> = \sqrt{\frac{2I+1}{16\pi}}\;[\,D^{I}_{MK}\,|\Psi^{\alpha}_{K\pi}> + (-1)^{I+K}\,D^{I}_{M-K}\,\hat{T}\,|\Psi^{\alpha}_{K\pi}>]$$

where $|\Psi^{I}_{MK}>$ **is the calculated BCS state**

The Model Hamiltonian is $\hat{H}_{BM} = \hat{H}_{int.} + \frac{\hat{\vec{R}}^{2}}{2\,J_{core}}$ with $\hat{\vec{R}} = \hat{\vec{j}}_{total} - \hat{\vec{j}}_{odd}$

The diagonal matrix element of the intrinsic Hamiltonian $\hat{H}_{int.}$
is not the calculated BCS energy dubbed as

$$<\Psi^{\alpha}_{K\pi}|\;\hat{H}_{Skyrme}|\Psi^{\alpha}_{K\pi}>$$

since the latter includes a spurious rotational energy
due to the mean field approximation

It has been removed according to the Lipkin approximate ansatz

One gets

$$< I\;M\,\alpha\,K\,\pi|\;\hat{H}_{int.}|I\;M\,\alpha\,K\,\pi> =$$

$$<\Psi^{\alpha}_{K\pi}|\;\hat{H}_{Skyrme}|\Psi^{\alpha}_{K\pi}> - \frac{1}{2\,J_{L}}\,[<\Psi^{\alpha}_{K\pi}|\;\hat{\vec{j}}^{\,2}_{total}|\Psi^{\alpha}_{K\pi}> - \hbar^{2}K\left(K+1\right)]$$

One can show that $<\Psi^{\alpha}_{K\pi}|\;\hat{\vec{j}}^{\,2}_{total}|\Psi^{\alpha}_{K\pi}> \approx$

$$<\Psi^{\alpha}_{K\pi}|\;\hat{\vec{j}}^{\,2}_{core}|\Psi^{\alpha}_{K\pi}> + <\alpha\,K\,\pi|\;\hat{\vec{j}}^{\,2}_{odd}|\alpha\,K\,\pi>$$

where on the rhs

the first matrix element is calculated only with core particles

the second is calculated for the s.p. state $|\alpha\,K\,\pi>$

Assuming that $J_{core} \approx J_{L} \equiv J$

one gets for the diagonal matrix element of the Hamiltonian $\hat{H}_{BM}$

$$< I\;M\,\alpha\,K\,\pi|\;\hat{H}_{BM}|I\;M\,\alpha\,K\,\pi> = < I\;M\,\alpha\,K\,\pi|\;\hat{H}_{int.}|I\;M\,\alpha\,K\,\pi>$$

$$\frac{\hbar^{2}}{2\,J}\,\{[\,I\left(I+1\right) - 2\mathrm{K}^{2}] + <\alpha\,K\,\pi|\;\hat{\vec{j}}^{\,2}_{odd}/\hbar^{2}|\alpha\,K\,\pi> + \delta_{K,1/2}\,a\left(-1\right)^{I+1/2}\left(I+1/2\right)\}$$

and finally

$$< I\;M\,\alpha\,K\,\pi|\;\hat{H}_{BM}|I\;M\,\alpha\,K\,\pi> = <\Psi^{\alpha}_{K\pi}|\;\hat{H}_{Skyrme}|\Psi^{\alpha}_{K\pi}> + \frac{\hbar^{2}}{2\,J}$$

$$\{[\,I\left(I+1\right) - K\left(K-1\right)] - <\Psi^{\alpha}_{K\pi}|\;\hat{\vec{j}}^{\,2}_{core}/\hbar^{2}|\Psi^{\alpha}_{K\pi}> + \delta_{K,1/2}\,a\left(-1\right)^{I+1/2}\left(I+1/2\right)\}$$

One gets in particular for the rotational band head $\{\alpha, I = K, \pi\}$

$$E^{b.h.}_{\alpha K \pi} = <\Psi^{\alpha}_{K\pi}|\,\hat{H}_{Skyrme}\,|\Psi^{\alpha}_{K\pi}> + \frac{\hbar^2}{2J}\,\{2K - <\Psi^{\alpha}_{K\pi}|\,\frac{\hat{\vec{j}}^{\,2}_{core}}{\hbar^2}\,|\Psi^{\alpha}_{K\pi}> - \delta_{K,1/2}\,a\}$$

TEST OF THE QUALITY OF THE BAND HEAD SPECTRA

We exclude data pertaining
- **to bands attributed to particle-vibration couplings**
- **to bands with an excitation energy > 650 keV (a typical gap value) since we deal only with seniority 1 states**

We assume that inter-band Coriolis couplings are not significant

Moments of inertia J and decoupling parameters a are calculated using the standard formulae
- **for J, Inglis-Belyaev (neglecting the small time-reversal violation) renomalized to take into account missing Thouless-Valatin terms**

- **for a, the expectation value of the** $\hat{j}_{+}\hat{T}$ **operator for the s.p. state of the « odd » particle, (assuming K = + 1/2)**

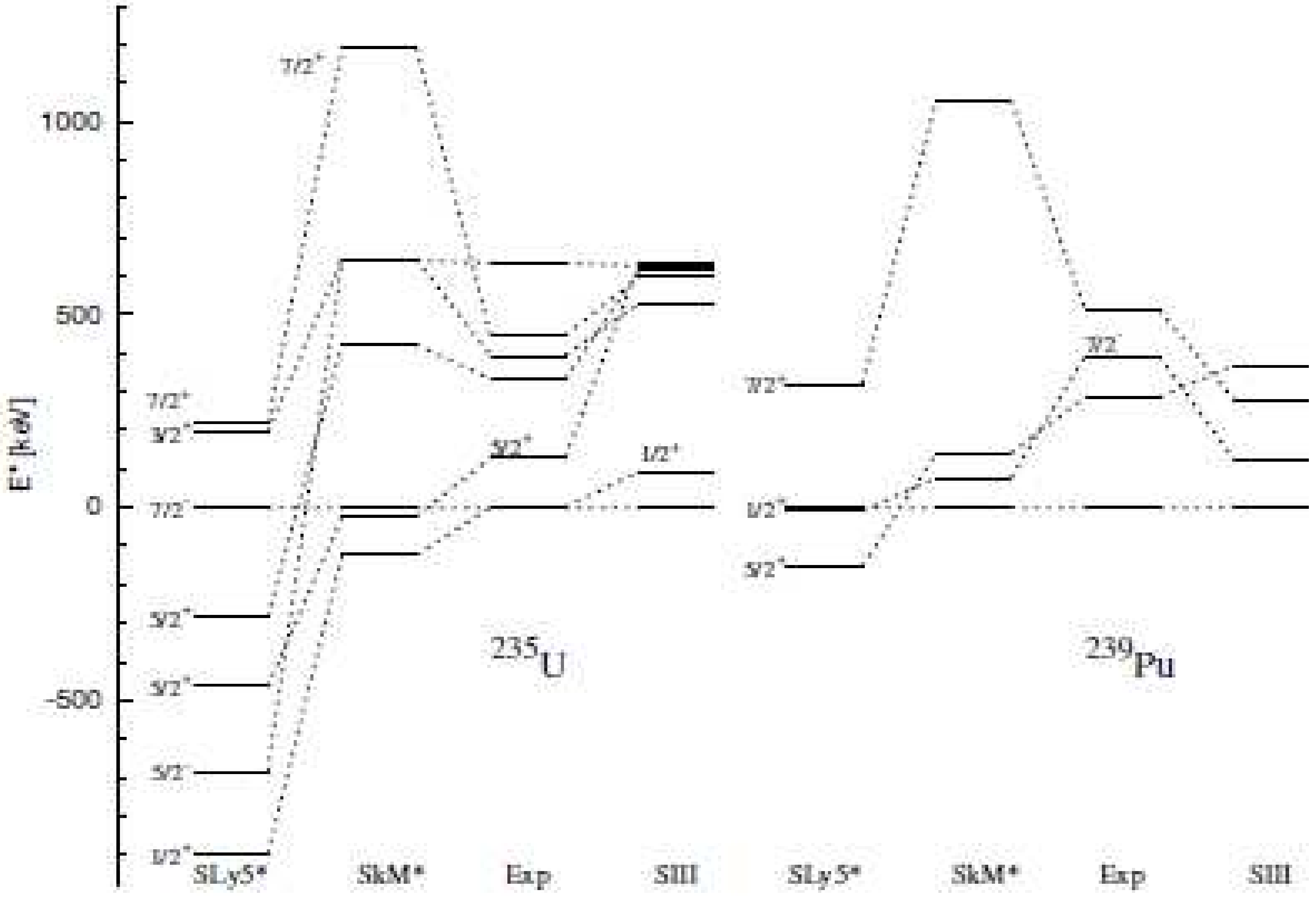


Figure 5.1: Partial band-heads of ^{235}U and ^{239}Pu calculated with the SkM* and SIII interactions without rotational correction in the *minimal time-odd* scheme and the SLy5* in the *full time-odd* scheme with comparison to the experiments.

$$\Delta_{rms}\left(\mathrm{keV}\right) = 250\ (\mathrm{SIII}),\ 350\ (\mathrm{SkM^*}),\ 650\ (\mathrm{SLy5^*})$$

The situation is slightly worse for neighbouring odd-proton nuclei

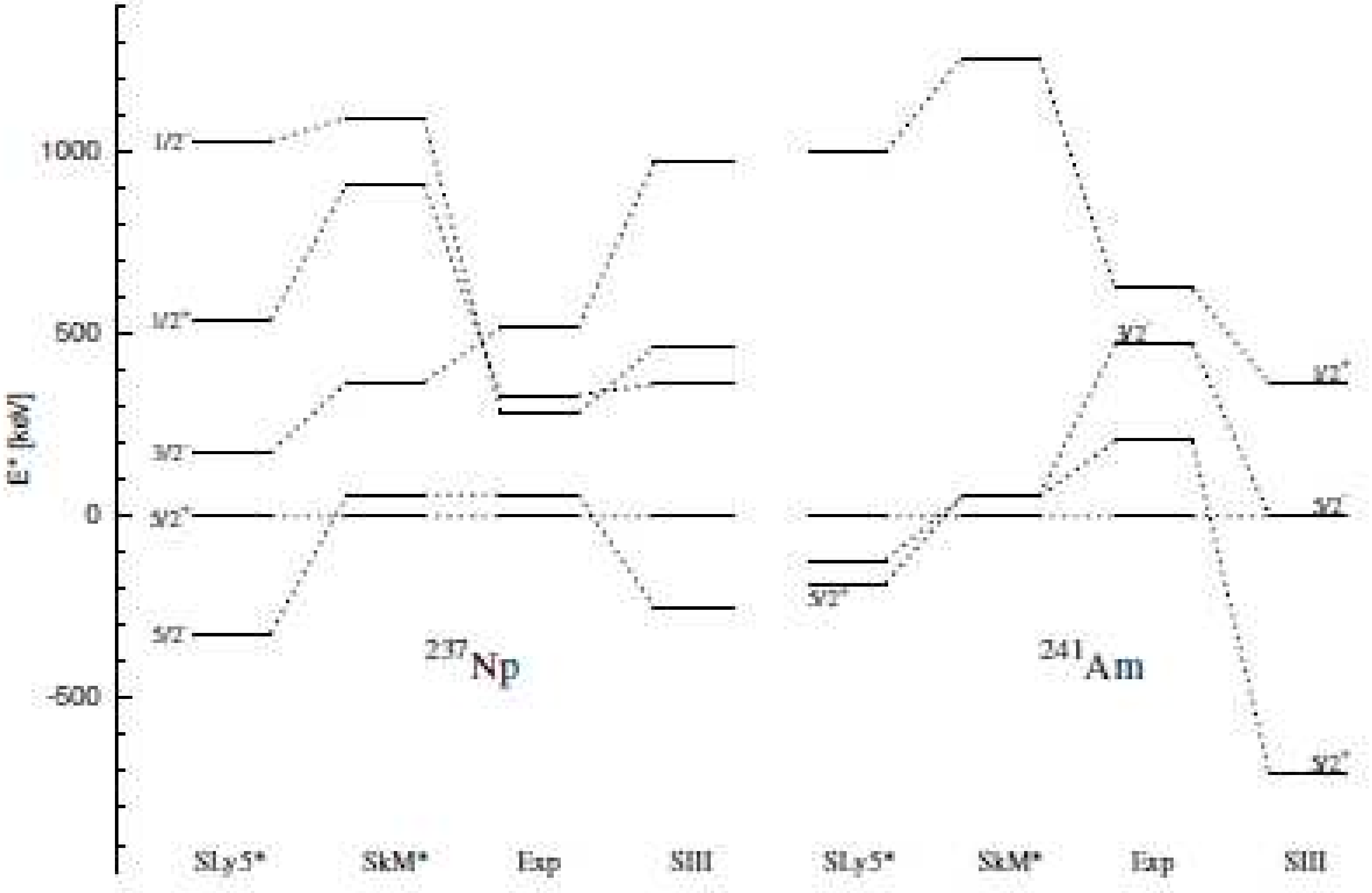


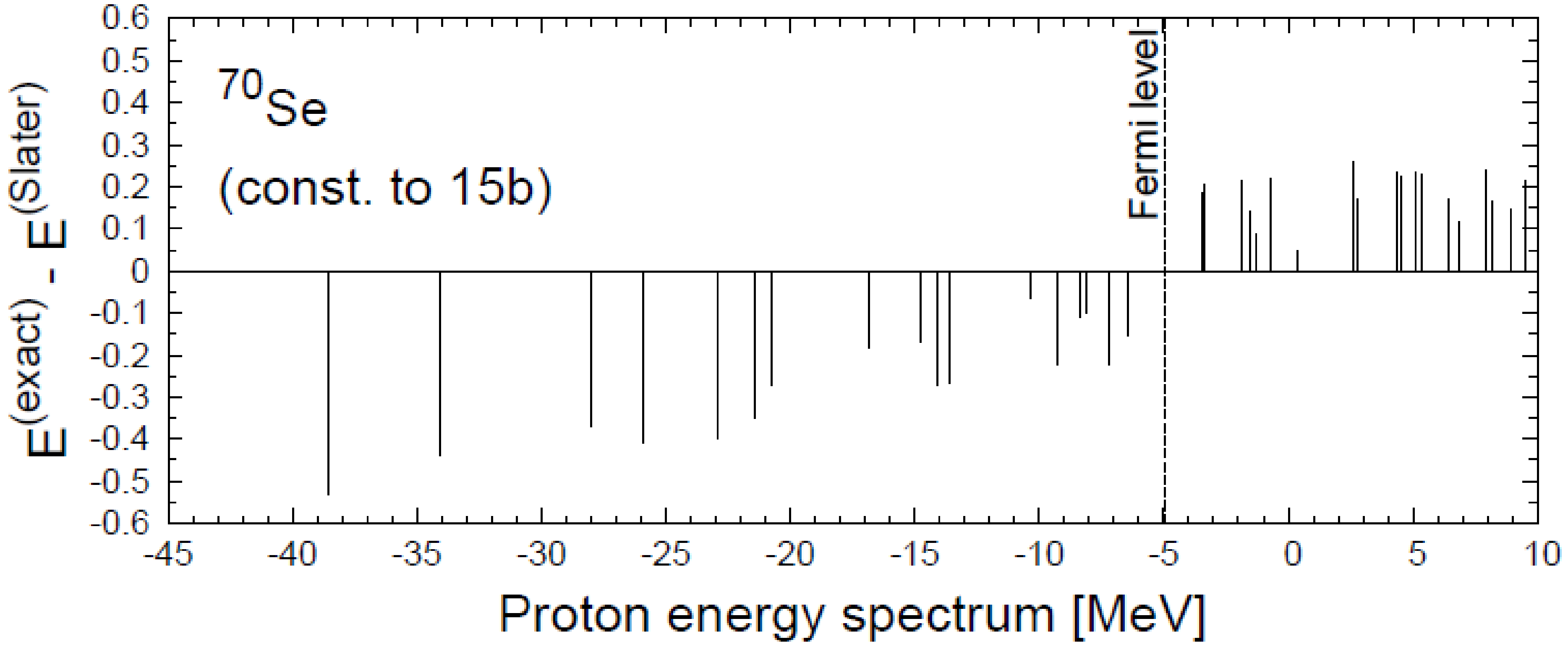
Figure 5.2: Partial band-heads of ^{237}Np and ^{241}Am calculated with the SkM* and SIII interactions without rotational correction in the minimal time-odd scheme while the SLy5* interaction in the *full time-odd* scheme with comparison to the experiments.

$$\Delta_{rms}(\mathrm{keV}) = 450\ (\mathrm{SIII}),\ 500\ (\mathrm{SkM^*}),\ 460\ (\mathrm{SLy5^*})$$

This might be due to the use of the Slater approximation for Coulomb exchange energy and field terms

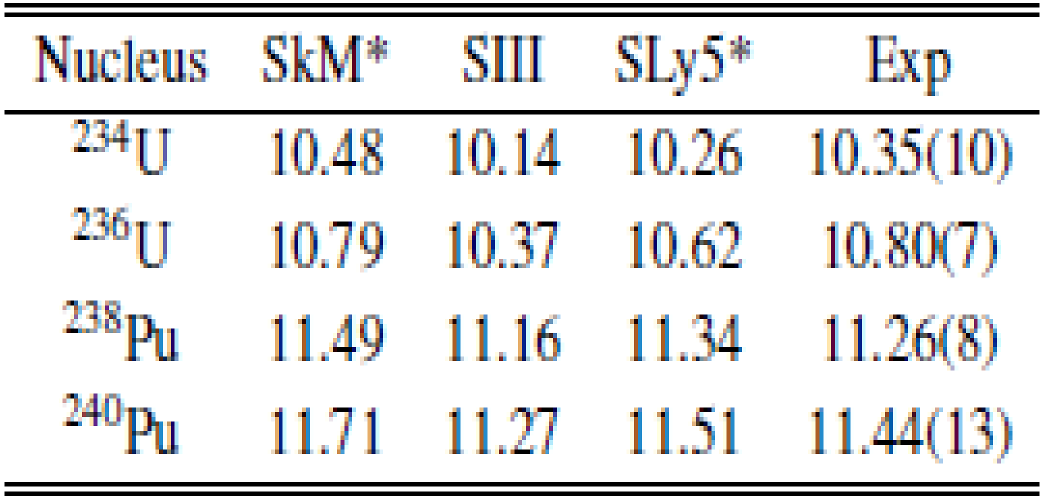
J. Le Bloas, Meng-Hock Koh, P. Quentin, L. Bonneau, J.I.A Ithnin, Phys . Rev. C84, 0143310 (2011)

The Slater approximation pushes systematically s.p. levels upwards (occupied), downwards (unoccupied)



Intrinsic quadrupole moments calculated Q_0(in barns) vs those deduced from experimental B(E2)

for even nuclei in the region

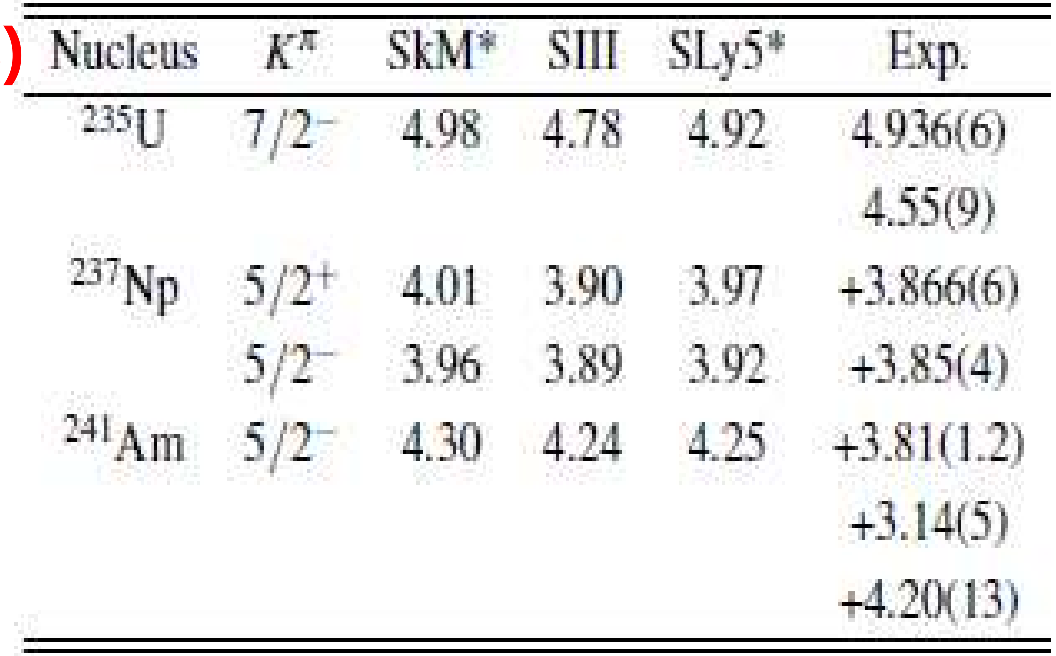


Nucleus	SkM*	SIII	SLy5*	Exp
^{234}U	10.48	10.14	10.26	10.35(10)
^{236}U	10.79	10.37	10.62	10.80(7)
^{238}Pu	11.49	11.16	11.34	11.26(8)
^{240}Pu	11.71	11.27	11.51	11.44(13)

Experimental spectroscopic quadrupole moment $Q^{(S)}$ (in barns) vs those deduced from calculated Q_0

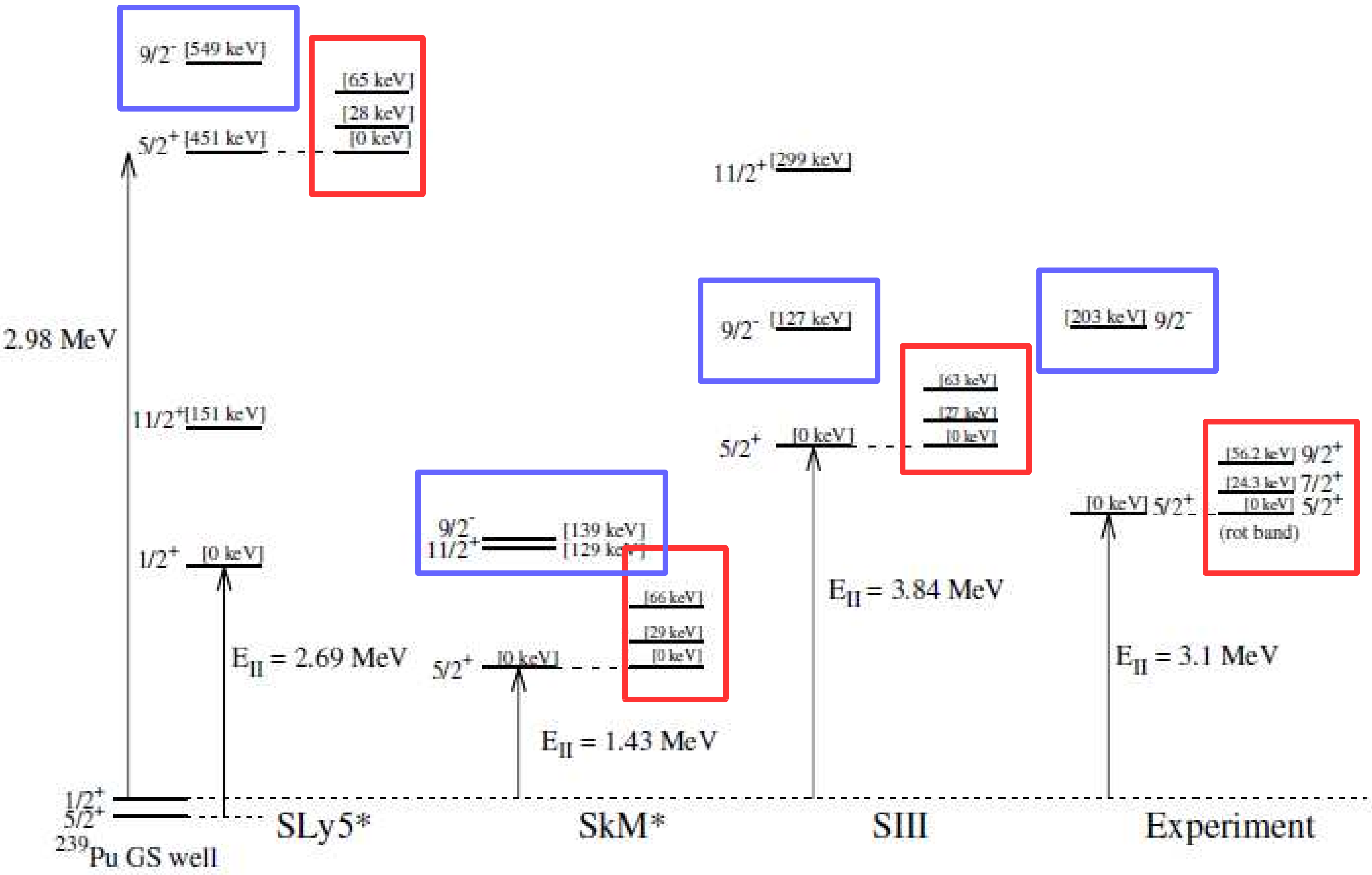
for odd nuclei in the region

$$Q^{(s)} = \frac{3K^2 - I(I+1)}{(K+1)(2I+3)} Q_0$$



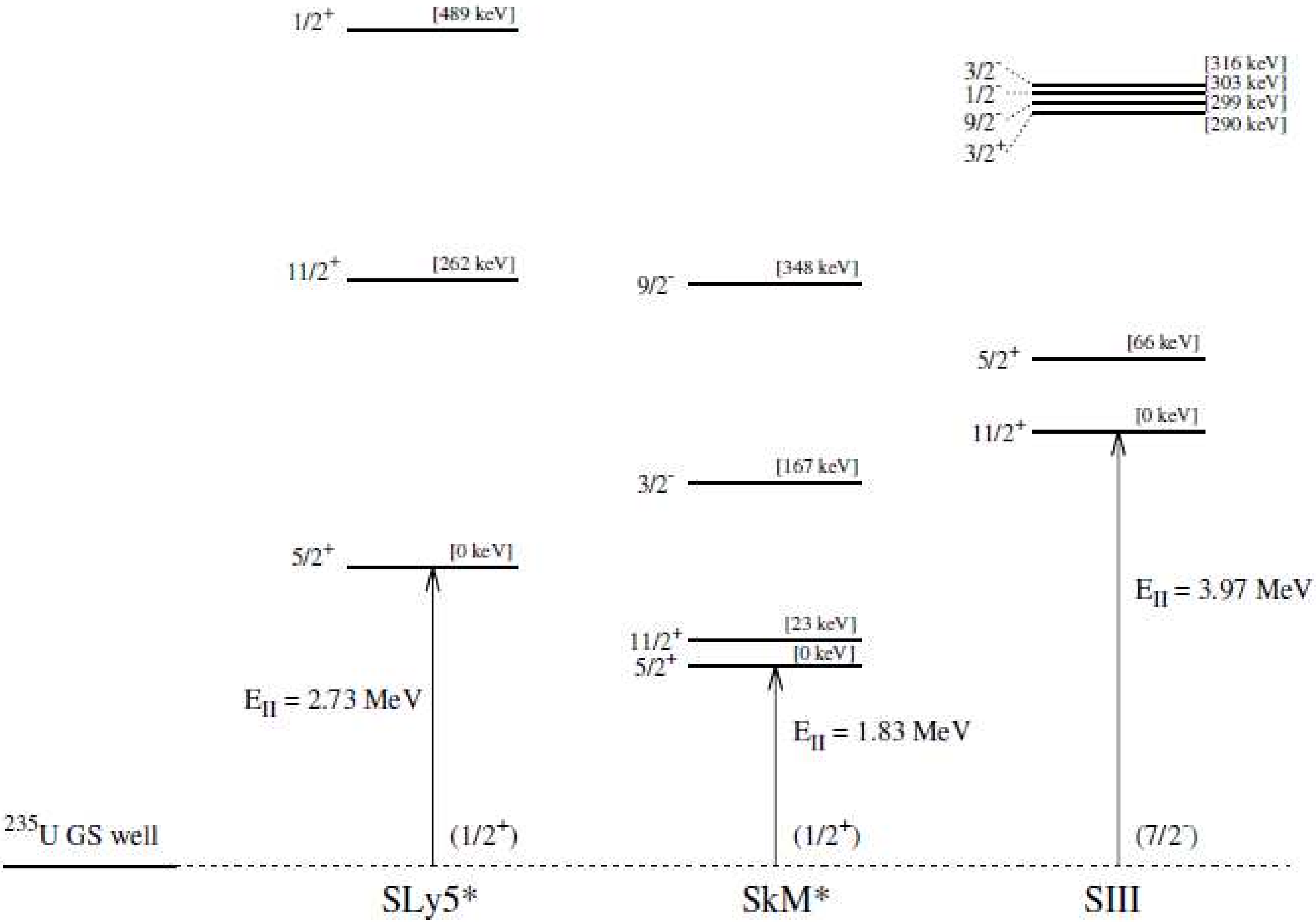
Nucleus	K^π	SkM*	SIII	SLy5*	Exp.
^{235}U	$7/2^-$	4.98	4.78	4.92	4.936(6)
					4.55(9)
^{237}Np	$5/2^+$	4.01	3.90	3.97	+3.866(6)
	$5/2^-$	3.96	3.89	3.92	+3.85(4)
^{241}Am	$5/2^-$	4.30	4.24	4.25	+3.81(1.2)
					+3.14(5)
					+4.20(13)

SPECTRUM IN THE FISSION ISOMERIC WELL (^{239}Pu)

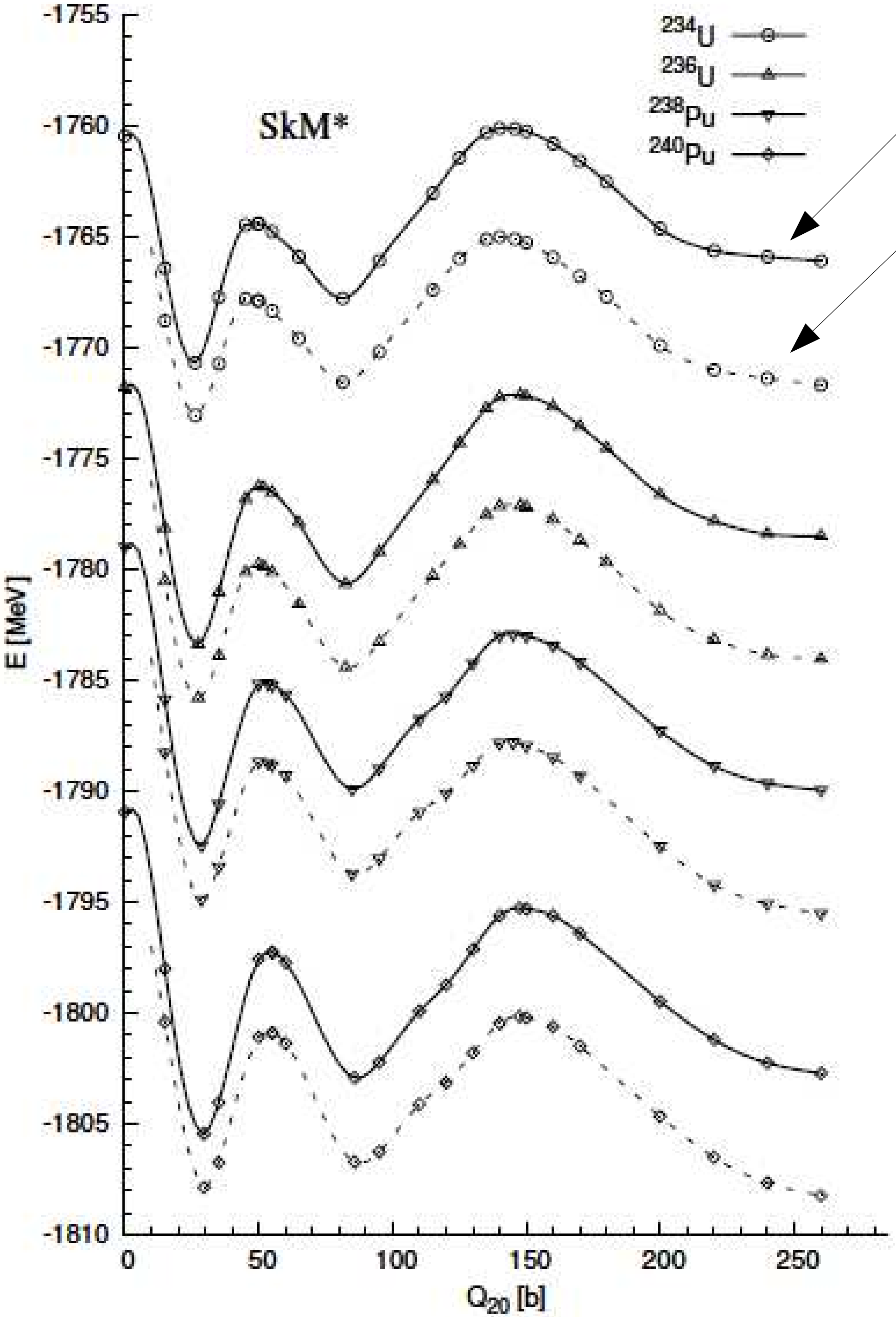


SPECTRUM IN THE FISSION ISOMERIC WELL (^{235}U)

No available data



A SELECTION OF SOME FISSION BARRIER RESULTS



BCS Energy

With Rot. Correction

^{234}U

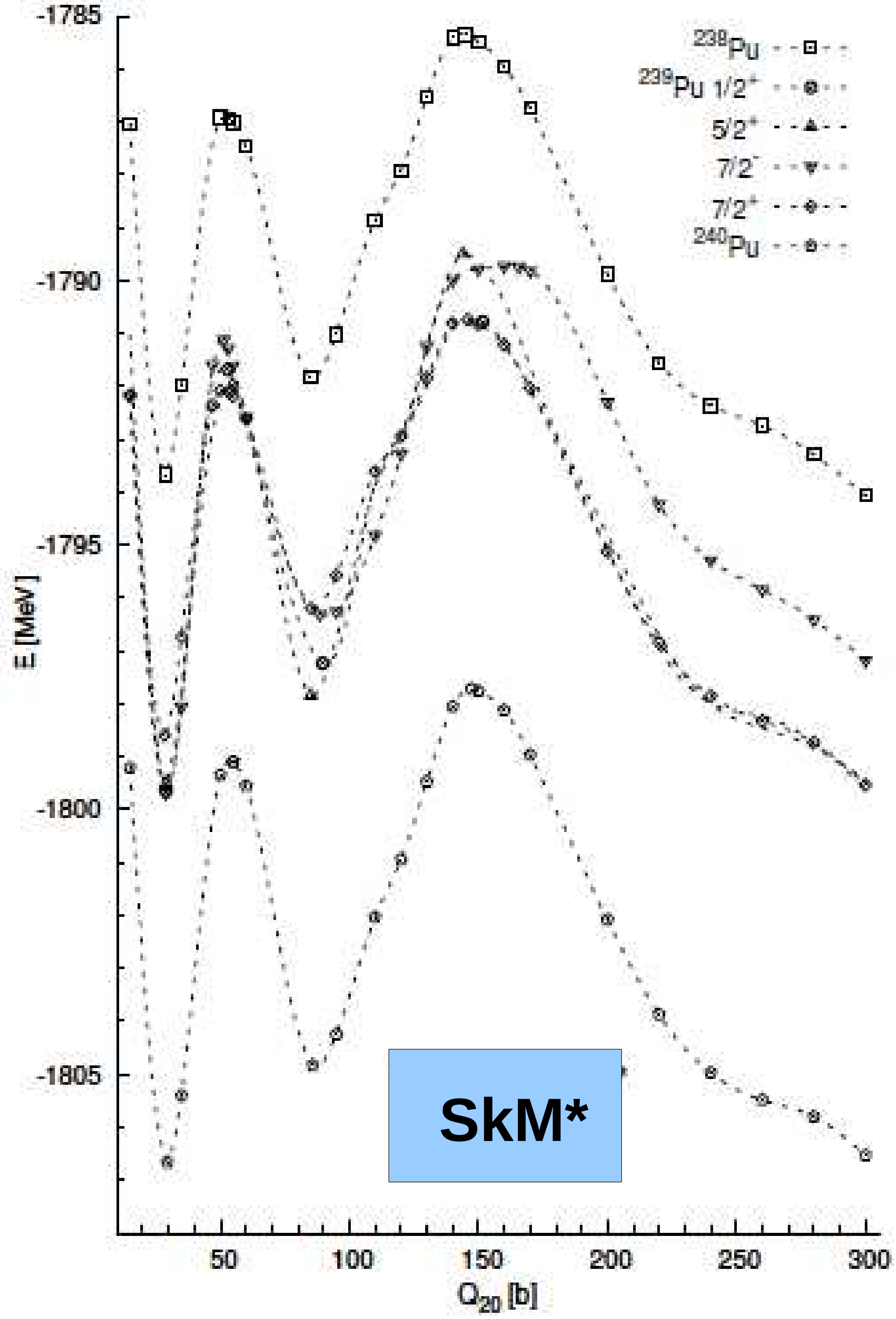
^{236}U

^{238}Pu

^{240}Pu

SkM*
Even-Even Nuclei
Intrinsic Parity Conserved

FISSION BARRIERS OFTHREE PLUTONIUM ISOTOPES



^{240}Pu

^{239}Pu

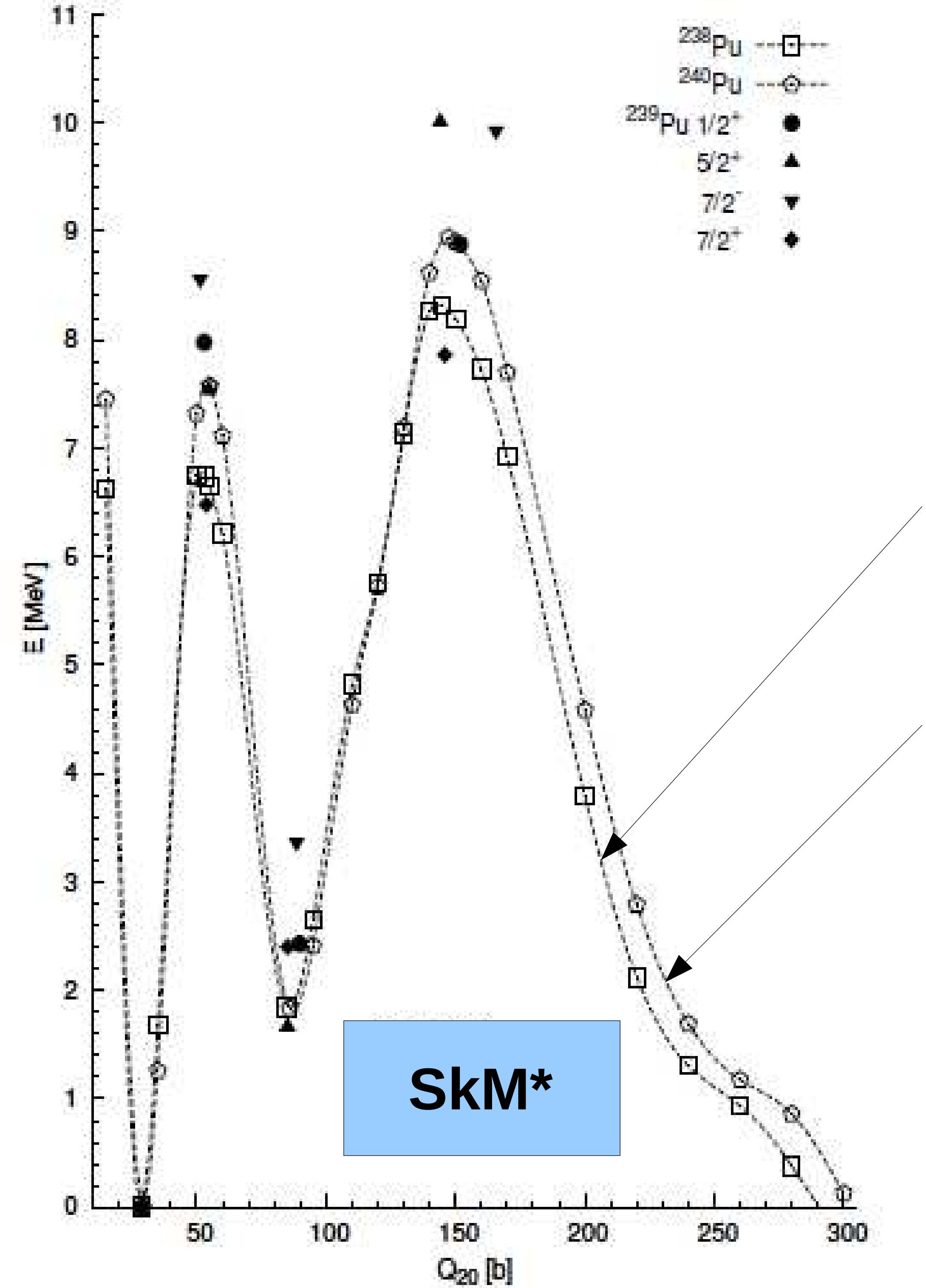
^{238}Pu

Intrinsic Parity Conserved

With Rot. Correction

FISSION BARRIERS OFTHREE PLUTONIUM ISOTOPES

SPECIALIZATION ENERGIES



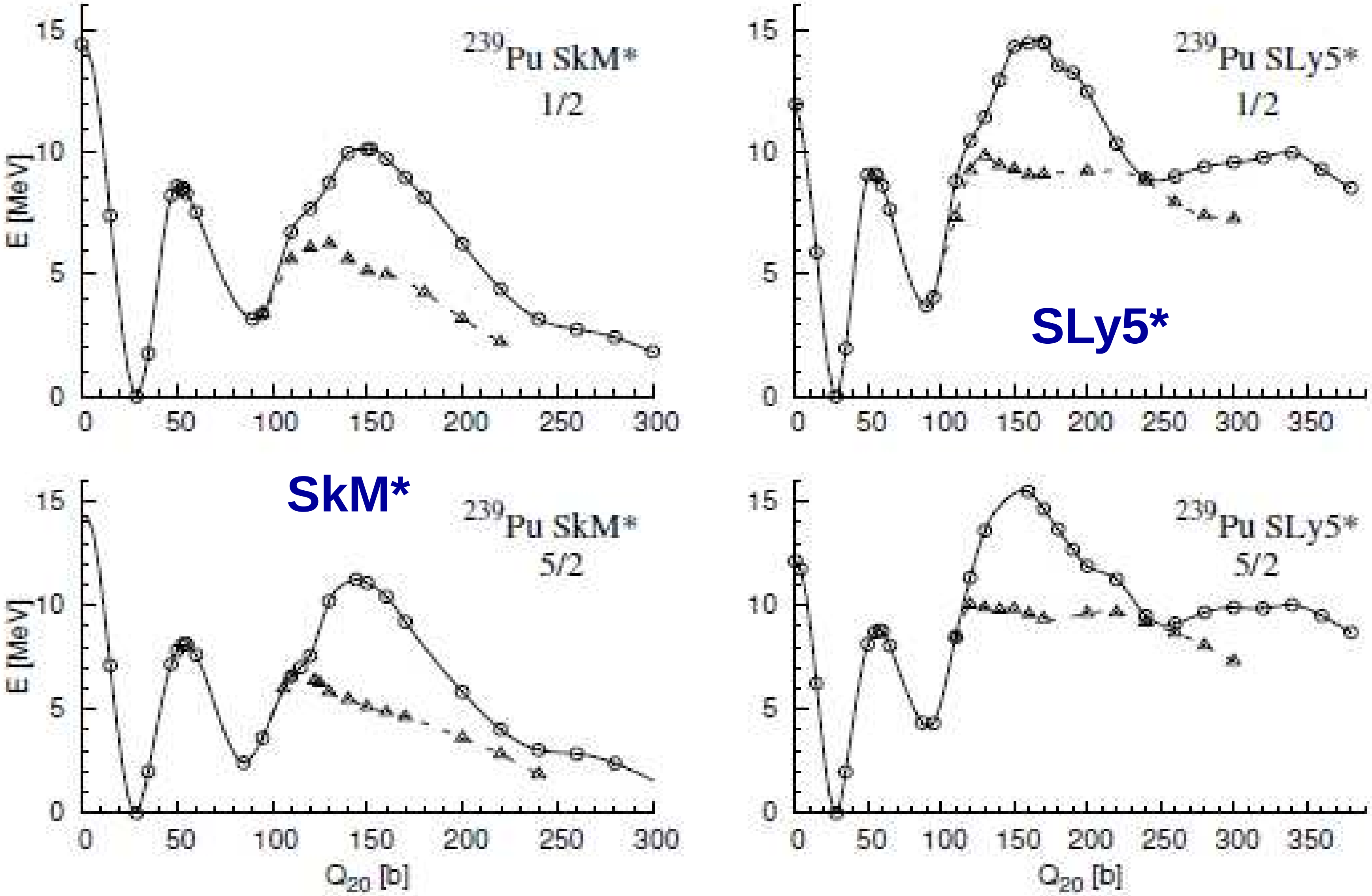
^{238}Pu

^{240}Pu

**Intrinsic Parity Conserved
With Rot. Correction
Energies adjusted at
ground state**

EFFECT OF INTRINSIC PARITY BREAKING ON THE FISSION BARRIERS

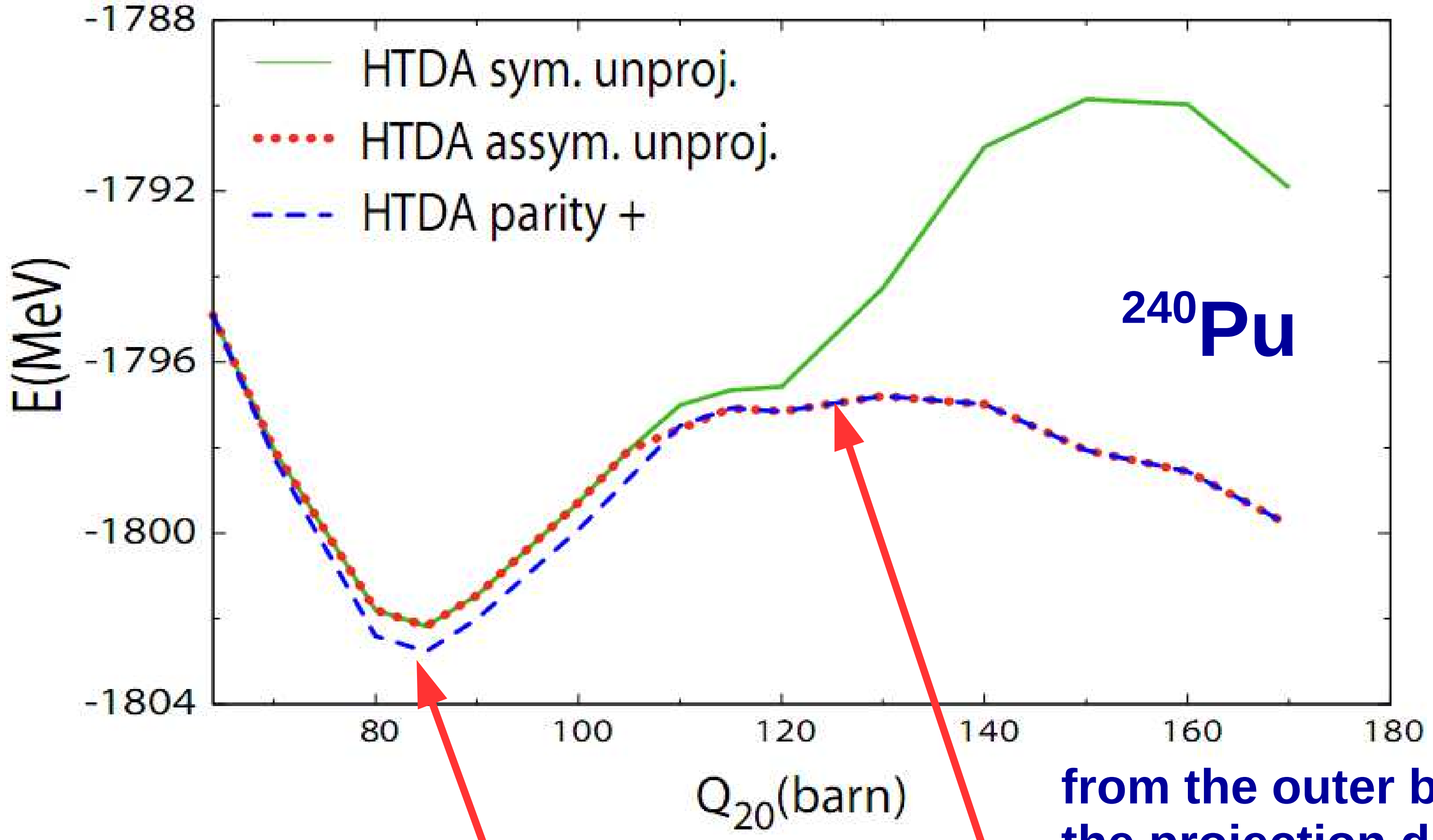
With Rotational Correction



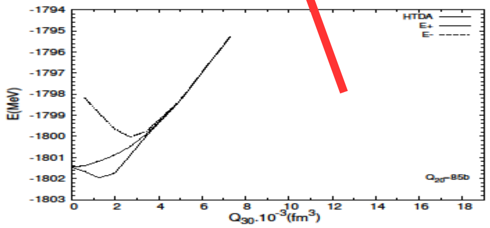
SLy5*

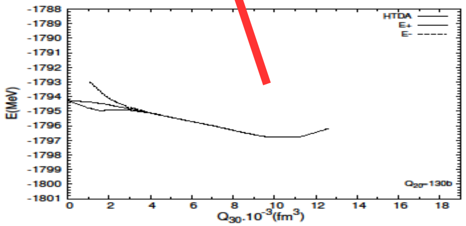
SkM*

PROJECTION ON GOOD PARITY STATES ITS EFFECT ON THE OUTER FISSION BARRIERS



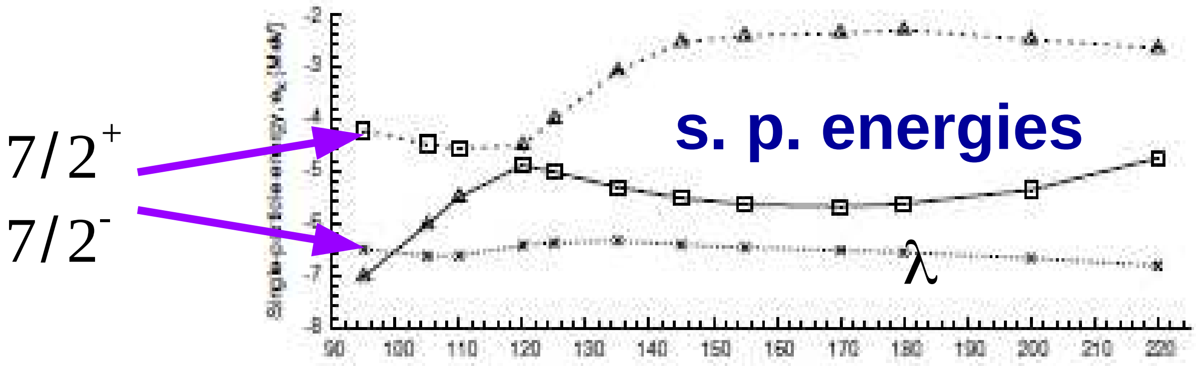
from the outer barrier on
the projection does not affect
the deformation energy

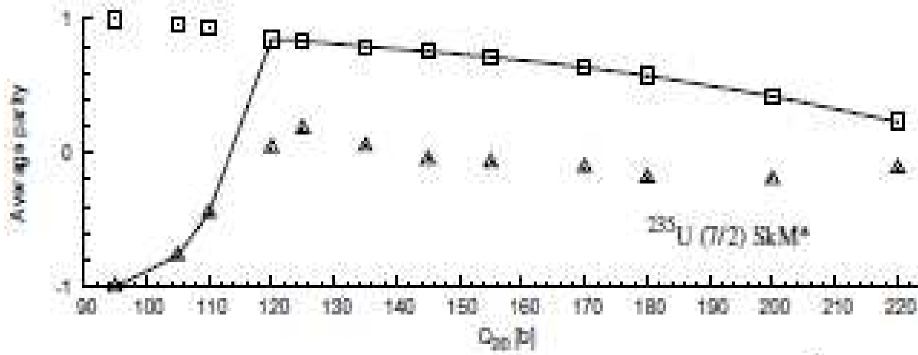




T.V. Nhan Hao, P. Quentin, L. Bonneau, Phys. Rev. C86, 064307 (2012)

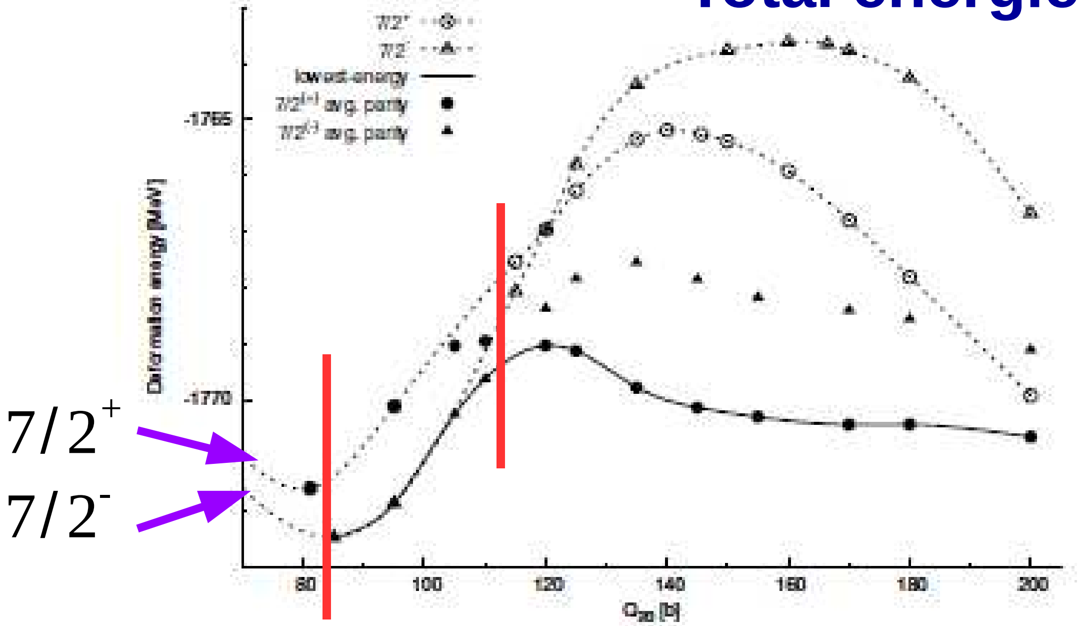
POSSIBLE AMBIGUITY IN NON-PROJECTED CALCULATIONS IN THE INNER PART OF THE OUTER FISSION BARRIERS





Parities

Total energies



^{239}Pu
SkM*

7/2 states

FISSIONING NUCLEUS	E_A (Eval.)	E_A (Calc.)	E_B (Eval.)	E_B(Calc.)
^{234}U	4.80	5.42	5.50	
^{235}U *	5.25	7.18	6.00	5.94
^{236}U	5.00	6.21	5.67	
^{238}Pu	5.60	6.45	5.10	
^{239}Pu **	6.20	7.71	5.70	4.66
^{240}Pu	6.05	7.25	5.15	5.50 ***

SkM*

* $7/2^-$ ** $1/2^+$ *** HTDA Pairing Calculations

Axial symmetry is imposed near inner barriers (an effect of ~1 MeV)

CONCLUSIONS

WHAT HAVE WE LEARNED ?

- « Old » effective interactions provide rather good **spectroscopic properties** (especially SIII) and **fission barrier heights** (especially SkM*)
Yet with error bars at least of a couple of 100 keV

- **Specialization energies** may reach the 1 MeV range

WHAT REMAINS TO BE DONE ?

- Break **the axial symmetry** at least near the inner barrier

- Improve on the treatment of pairing beyond BCS
use **a particle number conserving approach** as the HTDA

- Explore the capacities of **« new » Skyrme parametrizations**
(SLy5* did not prove to be a successful bet)