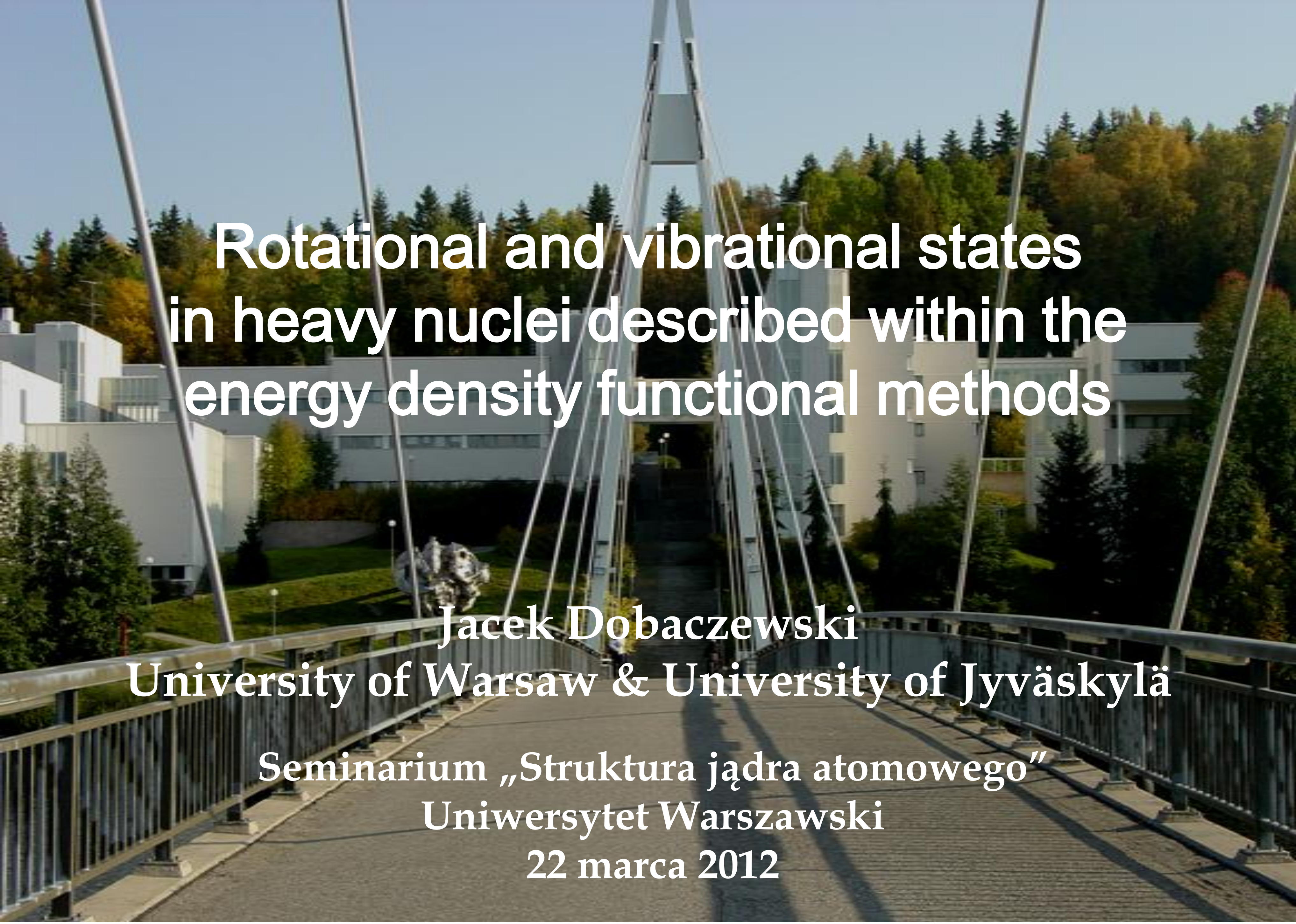
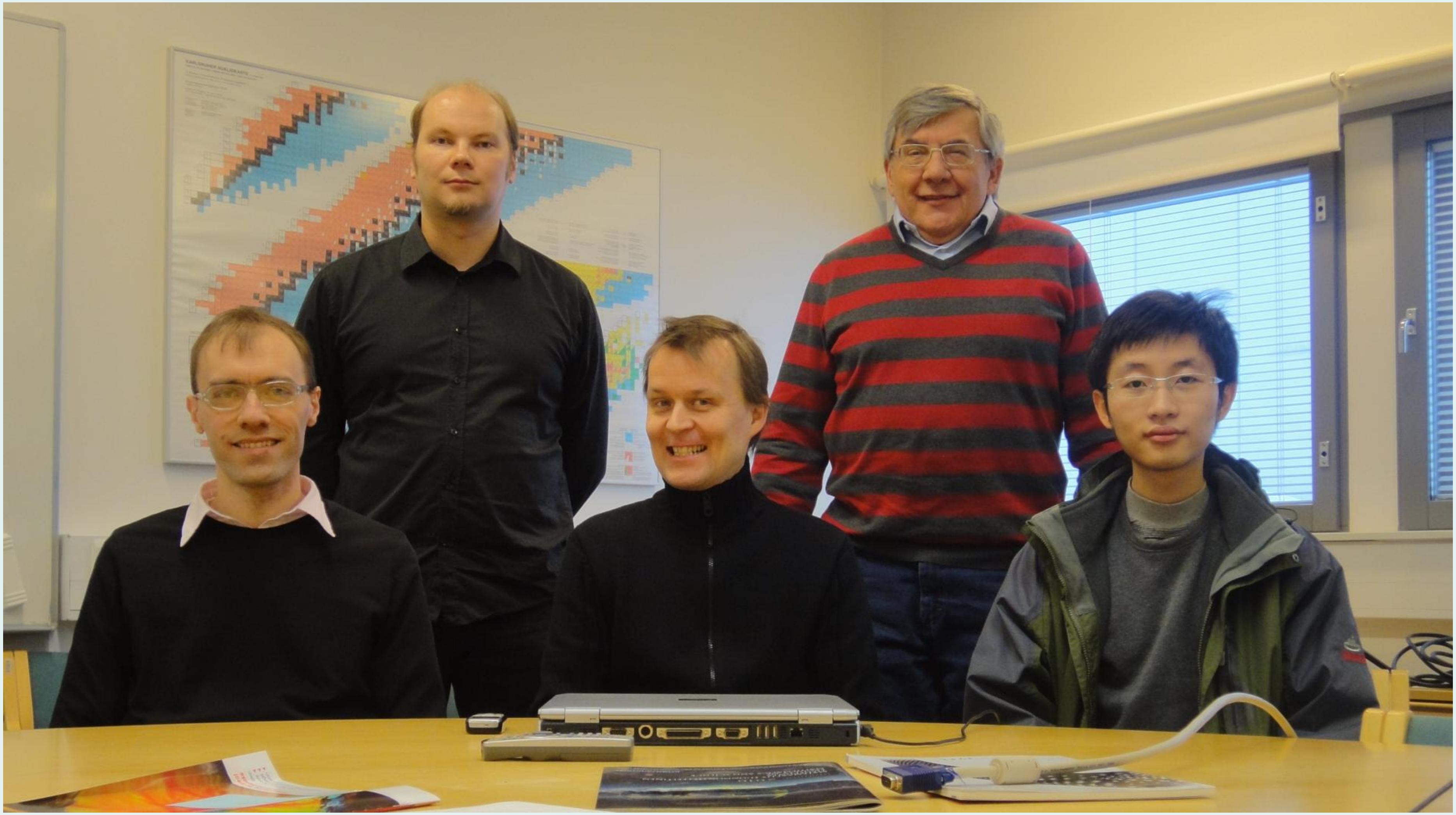


Rotational and vibrational states in heavy nuclei described within the energy density functional methods

Jacek Dobaczewski
University of Warsaw & University of Jyväskylä

Seminarium „Struktura jądra atomowego"
Uniwersytet Warszawski
22 marca 2012



The Jyväskylä theory team on January 10, 2012

Standing, from left: Markus Kortelainen, Jacek Dobaczewski
Seated, from left: Francesco Raimondi, Jussi Toivanen, Yuan Gao
Newcomer: Vaia Prassa
Former members: Gillis Carlsson, Alessandro Pastore, Nicolas Michel, Petr Veselý
Visitors: Dimitar Tarpanov, Yue Shi, Karim Bennaceur,Tamara Nikšić


ntosali 1
ture room 1
FL345
Valvomo

Projects

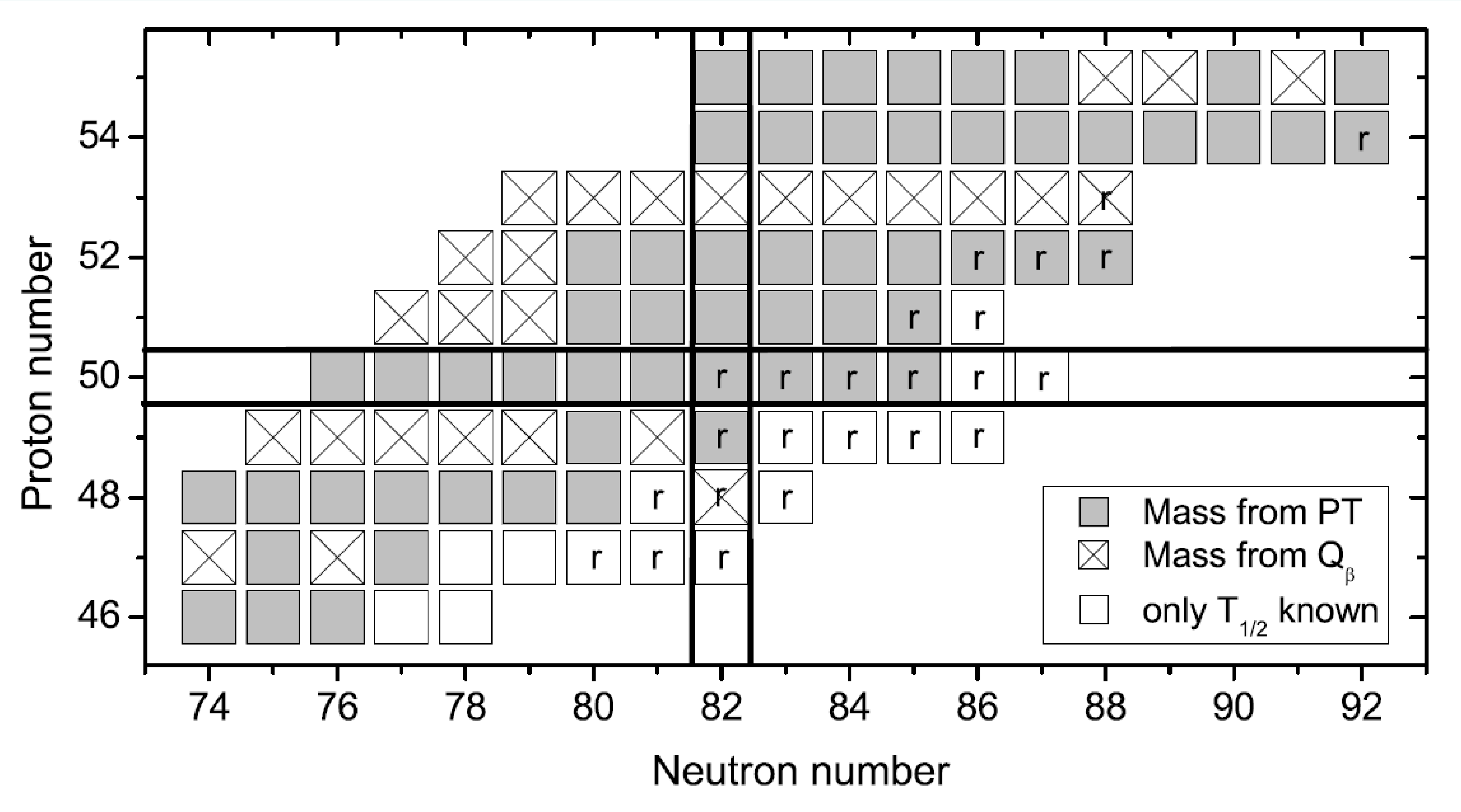
- ❑ Precise Penning-trap mass measurements beyond ^{132}Sn
- ❑ Tilted-axis cranking determination of ultra-high-spin triaxial rotational bands in ^{158}Er
- ❑ Incompressibility of finite nuclei studied within modern QRPA calculations
- ❑ Rotational bands in superheavy nuclei around ^{252}No
- ❖ Low-lying vibrational (2^+ and 3^-) states in semi-magic nuclei (Calsson, Toivanen)
- ❖ QRPA correlation energies up to multipolarity 7 (Calsson, Toivanen)
- ❖ Beta-decay rates in spherical nuclei (Veselý)
- ❖ Beta-decay rates in deformed nuclei (Toivanen, Pastore)
- ❖ Pseudopotentials and equation of continuity in higher-order EDF's (Raimondi)
- ❖ Adjustments of higher-order functionals to data (Prassa, Carlsson, Veselý, Kortelainen)
- ❖ Error propagation in EDF approach (Gao)
- ❖ Approximate restoration of broken symmetries by the Lipkin method (P. Toivanen, Gao)
- ❖ Particle- and Quasiparticle-phonon coupling (Tarpanov, Toivanen)
- ❖ Regularization of zero-range effective interactions (Bennaceur, Raimondi)

Precise Penning-trap mass measurements beyond ^{132}Sn

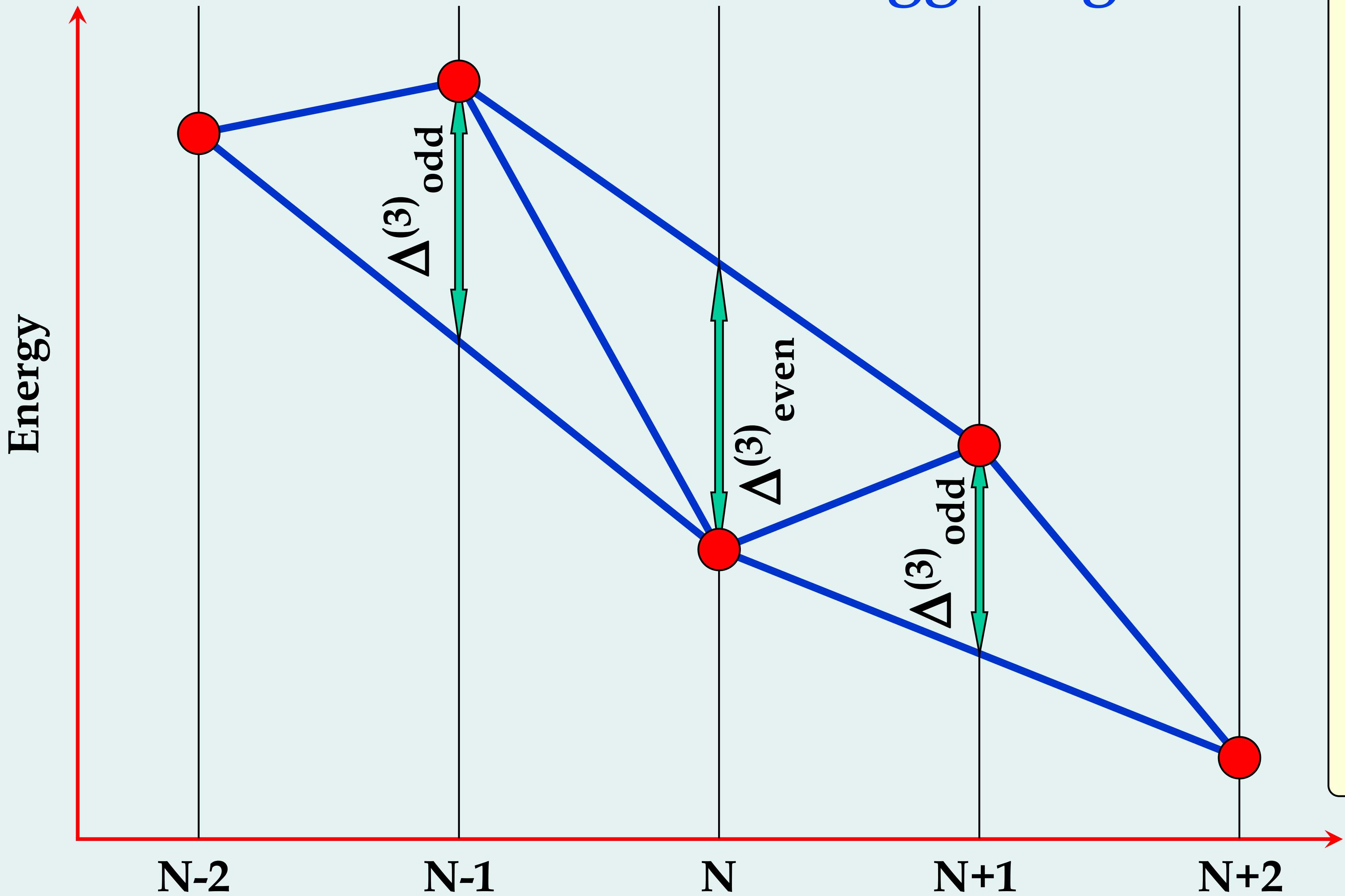
Precision Mass Measurements beyond ^{132}Sn: Anomalous behaviour of odd-even staggering of binding energies

J. Hakala,* J. Dobaczewski, D. Gorelov, T. Eronen,† A. Jokinen, A. Kankainen, V.S. Kolhinen, M. Kortelainen, I. D. Moore, H. Penttilä, S. Rinta-Antila, J. Rissanen, A. Saastamoinen, V. Sonnenschein, and J. Äystö‡
Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland
(Dated: March 7, 2012)

arXiv:1203.0958v2 [nucl-ex] 6 Mar 2012

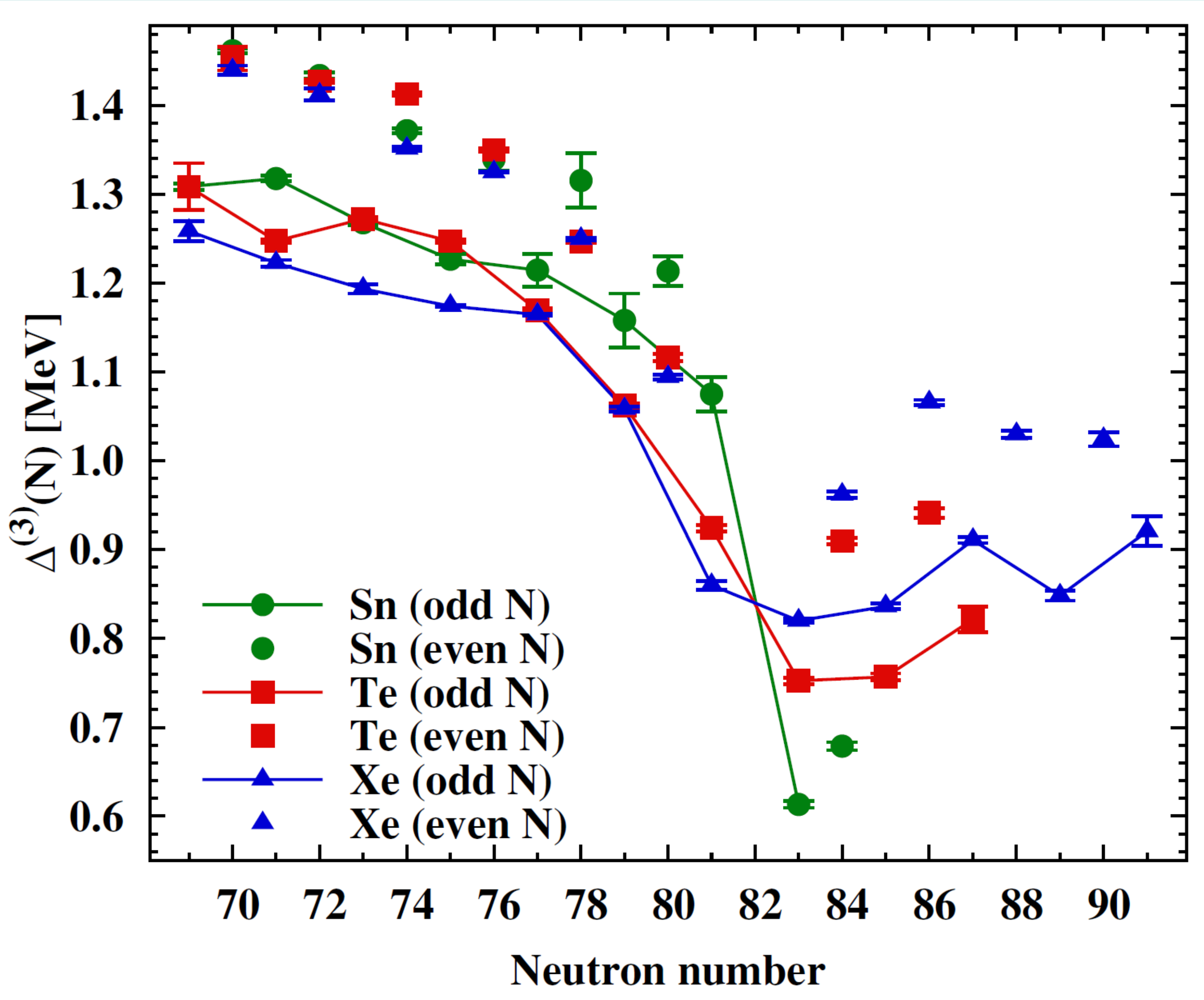


Odd-even mass staggering

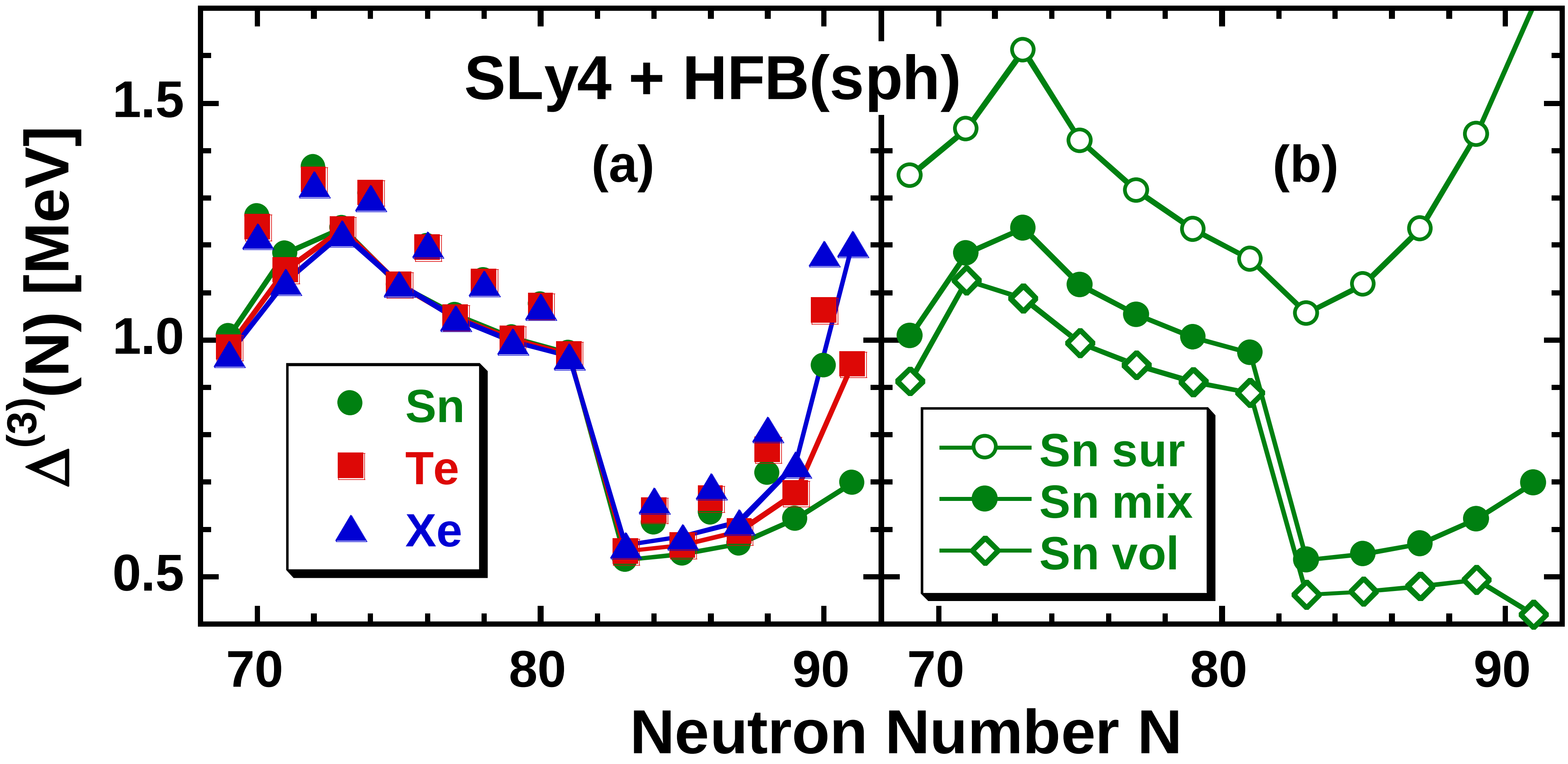


W. Satuła *et al.*, Phys. Rev. Lett. 81, 3599 (1998)

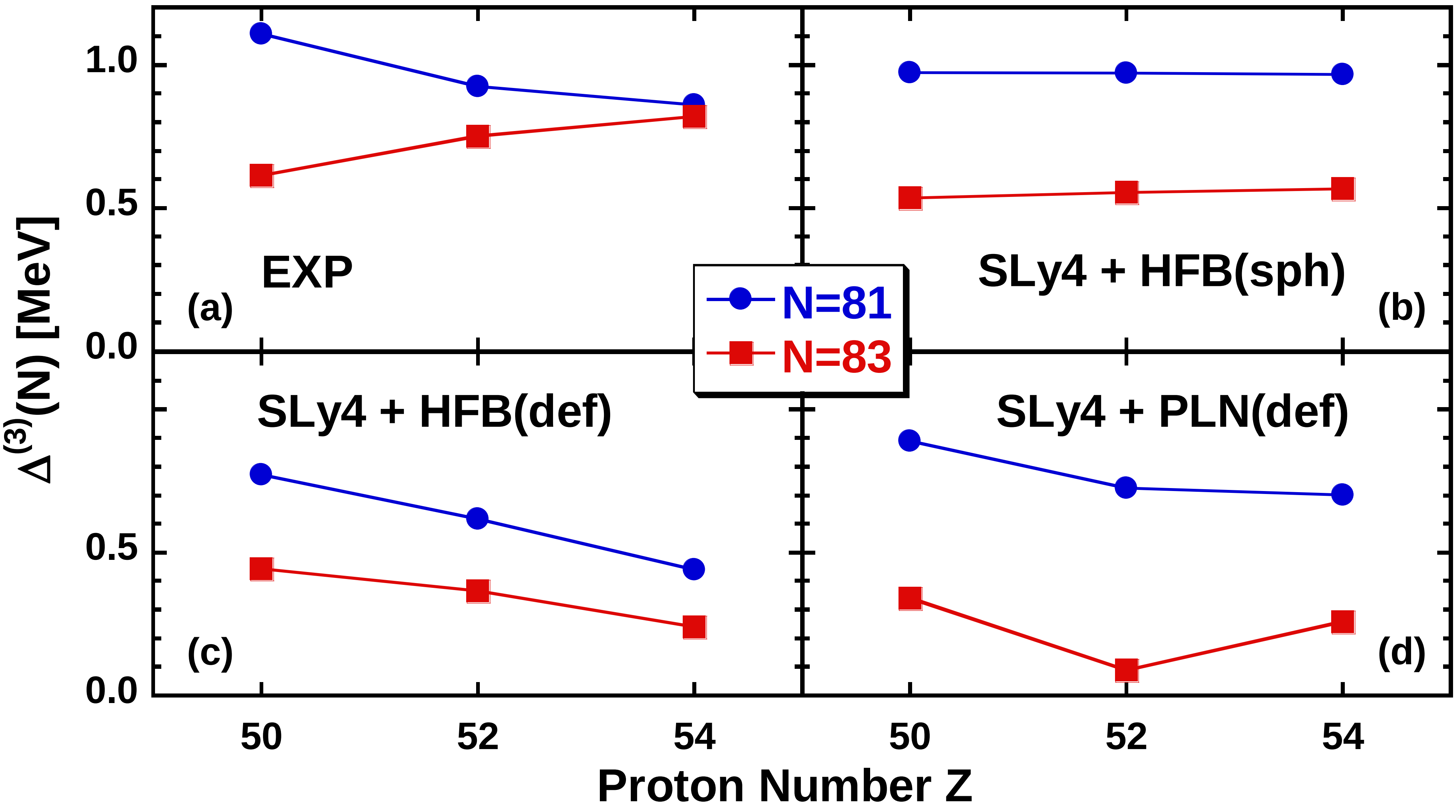
Experimental data around ^{132}Sn



Spherical EDF calculations around ^{132}Sn



Odd-even mass staggering in N=81 & 83

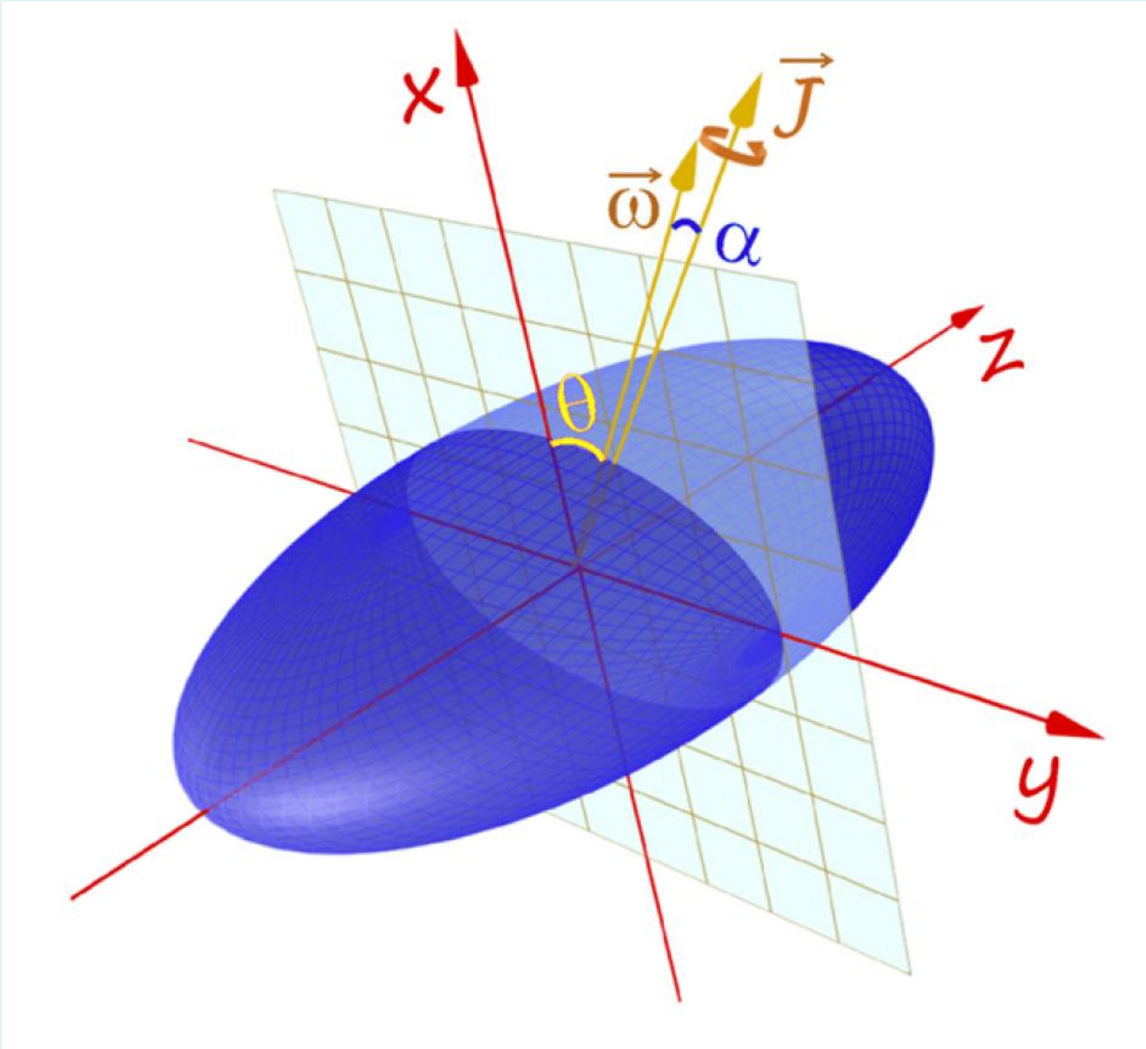


Tilted-axis cranking determination of ultra-high-spin triaxial rotational bands in ^{158}Er

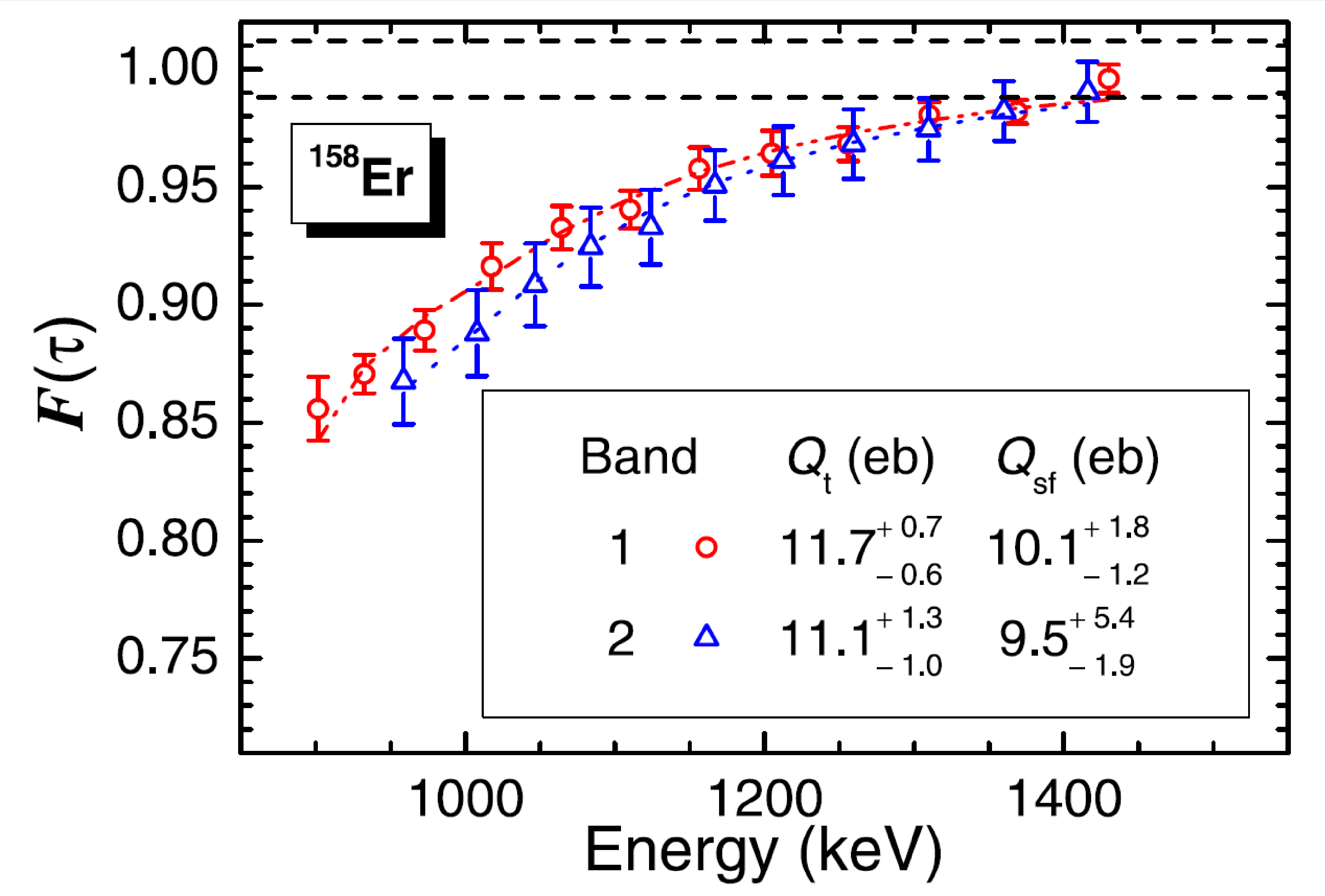
PRL **108,** 092501 (2012) PHYSICAL REVIEW LETTERS week ending 2 MARCH 2012

Self-Consistent Tilted-Axis-Cranking Study of Triaxial Strongly Deformed Bands in ^{158}Er at Ultrahigh Spin

Yue Shi,[1,2,3,4] J. Dobaczewski,[5,4] S. Frauendorf,[6] W. Nazarewicz,[2,3,5] J. C. Pei,[7,2,3] F. R. Xu,[1] and N. Nikolov[2]

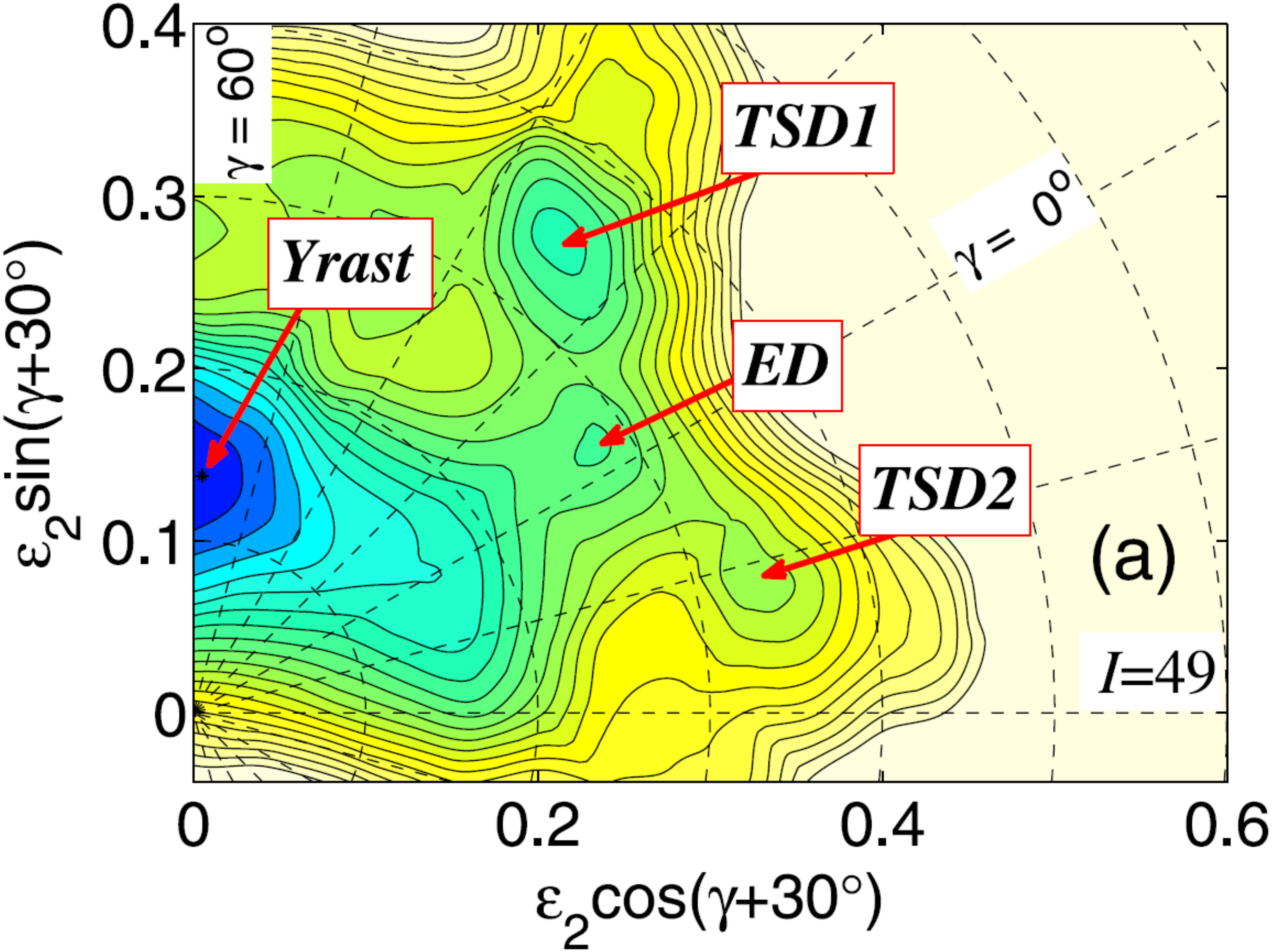


DSAM life-time measurements



X. Wang et al., Phys. Lett. B702, 127 (2011)

Cranked Nilsson–Strutinsky (CNS) model

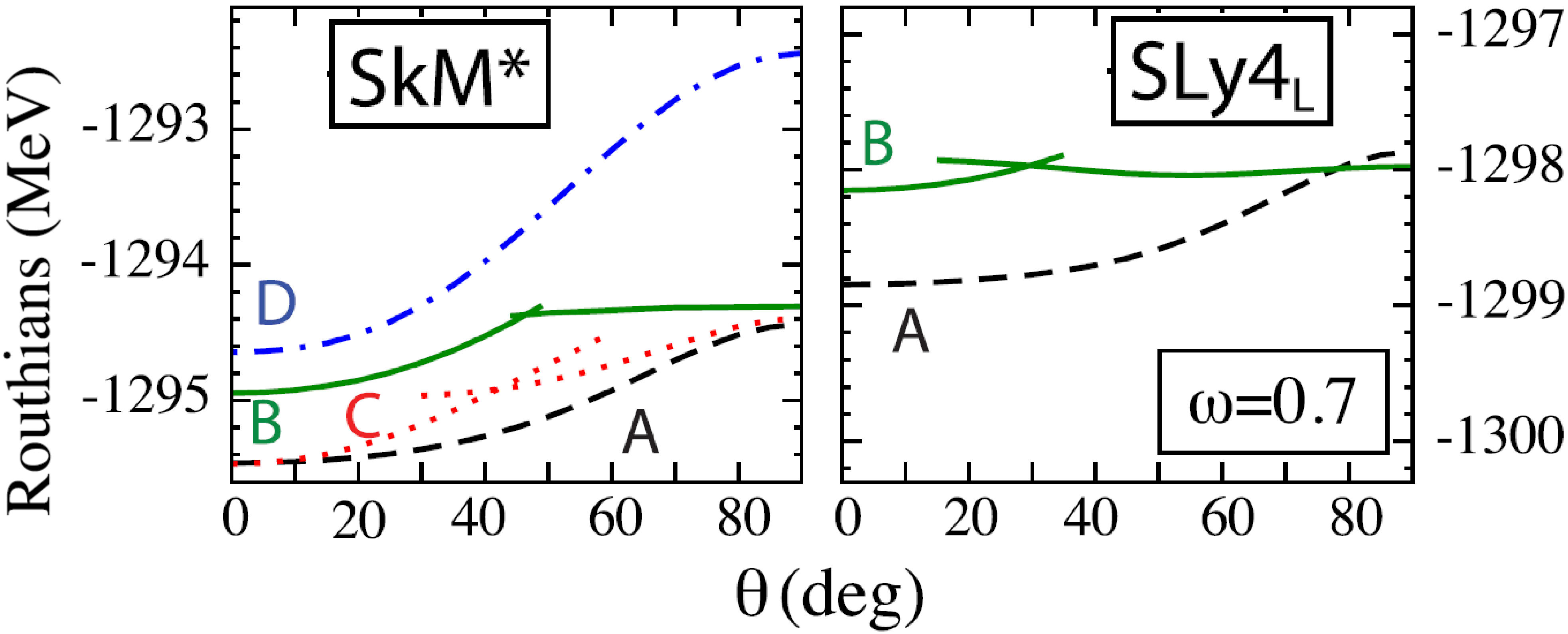


X. Wang et al., Phys. Lett. B702, 127 (2011)

Tilted-axis cranking

Kerman-Onishi theorem

$$\hat{H} - L_{22}\Im\hat{Q}_{22} - \vec{\omega}\cdot\vec{J} \quad\Longrightarrow\quad L_{22} = -\frac{\left(\vec{\omega}\times\vec{J}\right)_z}{2Q_{22}}$$

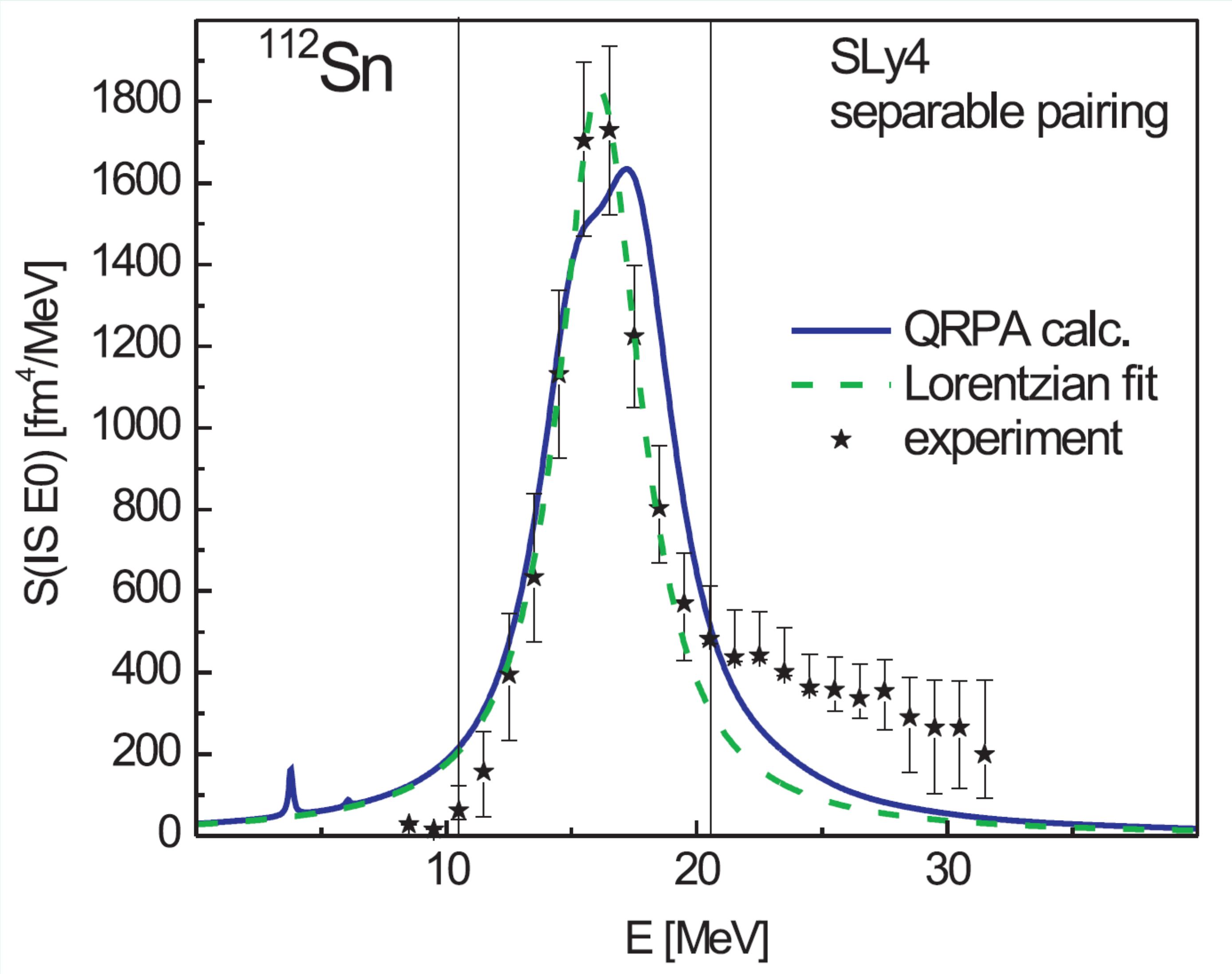


Incompressibility of finite nuclei studied within modern QRPA calculations

Giant Monopole Resonances and nuclear incompressibilities studied for the zero-range and separable pairing interactions.

P. Veselý,[1] J. Toivanen,[1] B. G. Carlsson,[2] J. Dobaczewski,[1,3] N. Michel,[1] and A. Pastore[4]

arXiv:1202.5617 [nucl-th] 25 Feb 2012



Experimental data from:
T. Li, U. Garg, Y. Liu, et al.,
Phys. Rev. Lett. 99, 162503 (2007);
Phys. Rev. C 81, 034309 (2010))

Fast RPA and QRPA + Arnoldi method

Within RPA, let ρ denote the one-body projective density matrix, $\rho^2 = \rho$, and $h(\rho) = \partial E/\partial\rho$ denote the mean-field Hamiltonian calculated for ρ. The TDHF equation for $\rho(t)$ then reads:

$$i\hbar\frac{d}{dt}\rho = [h(\rho), \rho].$$

The RPA method approximates the TDHF solution by a single-mode vibrational state $\rho(t)$ in the vibrating mean field $h(t) = h(\rho(t))$:

$$\rho(t) = \rho_0 + \tilde{\rho}e^{-i\omega t} + \tilde{\rho}^{+}e^{i\omega t}, \qquad h(t) = h_0 + \tilde{h}e^{-i\omega t} + \tilde{h}^{+}e^{i\omega t}$$

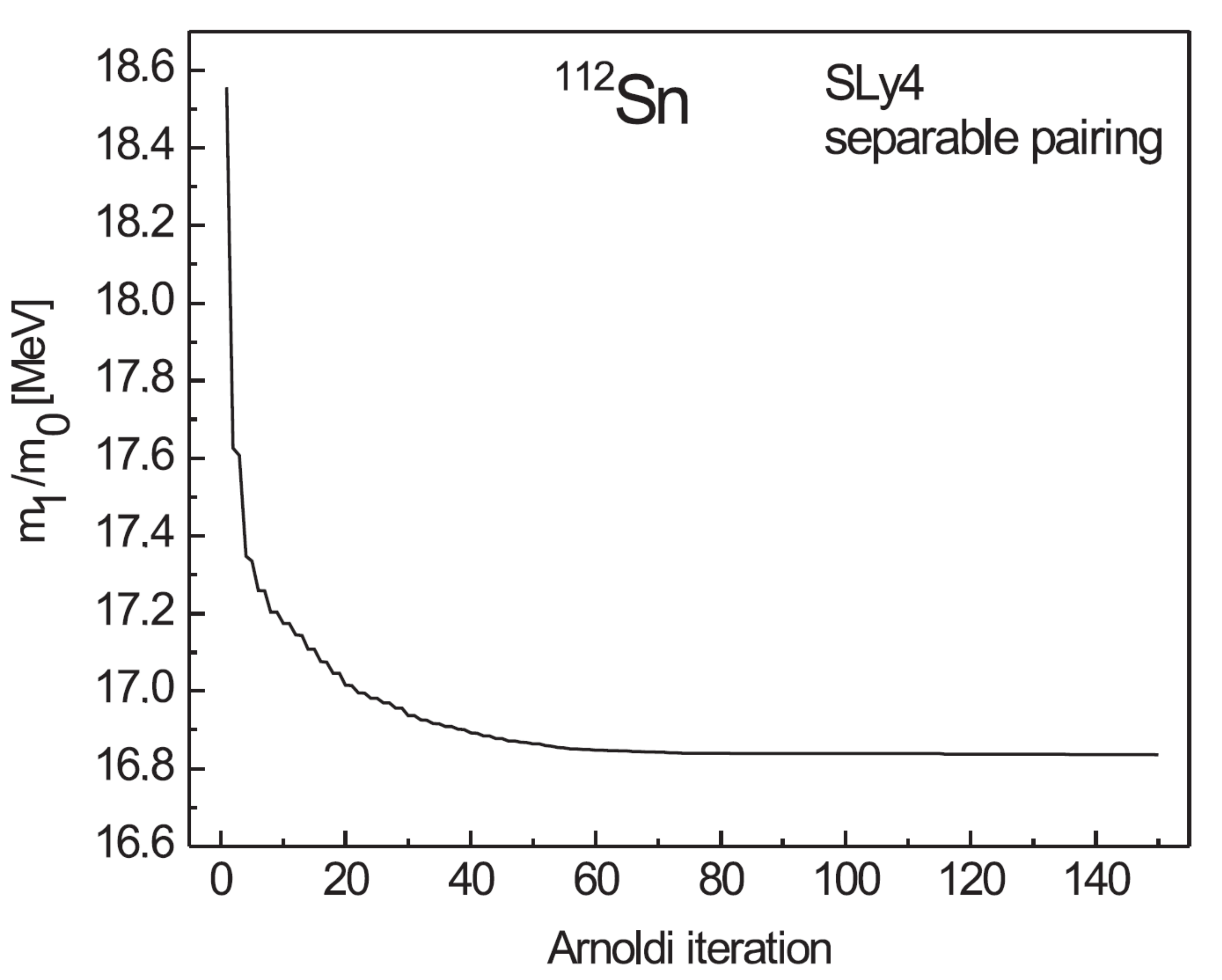
where ρ_0 is the self-consistent solution, $[h_0, \rho_0] = 0$ for $h_0 = h(\rho_0)$, $\tilde{\rho}$ is the RPA amplitude, and $\tilde{h} = h(\tilde{\rho})$. This allows for transforming the TDHF into the RPA equation in the form

$$\hbar\omega\tilde{\rho} = \mathtt{H}_0\tilde{\rho} = [h_0, \tilde{\rho}] + [\tilde{h}, \rho_0],$$

by which the right-hand side becomes a linear operator $\mathtt{H}_0$ depending on ρ_0 and acting on $\tilde{\rho}$.

J. Toivanen *et al.*, Phys. Rev. C 81, 034312 (2010)

Convergence of the Arnoldi method



Finite-range separable pairing interaction

$$\begin{aligned}\hat{V}(\vec{r}_1 s_1 t_1, \vec{r}_2 s_2 t_2; \vec{r}_1' s_1' t_1', \vec{r}_2' s_2' t_2') = \\ &- \; G_0 \delta(\vec{R} - \vec{R}') P(r) P(r') \tfrac{1}{2}(1 + \hat{P}_\sigma) \tfrac{1}{2}(1 - \hat{P}_\tau) \\ &- \; G_1 \delta(\vec{R} - \vec{R}') P(r) P(r') \tfrac{1}{2}(1 - \hat{P}_\sigma) \tfrac{1}{2}(1 + \hat{P}_\tau),\end{aligned}$$

where $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ denotes the centre of mass coordinate, $\vec{r} = \vec{r}_1 - \vec{r}_2$ is the relative coordinate, $r = |\vec{r}|$, and function $P(r)$ is a sum of m Gaussian terms,

$$P(r) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{(4\pi a_i^2)^{3/2}} \mathrm{e}^{-\frac{r^2}{4a_i^2}}.$$

For such a pairing interaction, the pairing energy acquires fully separable form,

$$\begin{aligned}E_{pair}^{sep} = \; - \; \tfrac{1}{2} G_0 \sum_{JN\lambda} & \Big(\sum_{\mu\nu} V_{0;\mu\nu}^{J,N\lambda} \langle \Psi_{\alpha_\mu j_\mu} || \kappa_{T=0}^{J} || \Psi_{\alpha_\nu j_\nu} \rangle \Big) \\ & \times \Big(\sum_{\mu'\nu'} V_{0;\mu'\nu'}^{J,N\lambda} \langle \Psi_{\alpha_{\mu'} j_{\mu'}} || \kappa_{T=0}^{\prime J+} || \Psi_{\alpha_{\nu'} j_{\nu'}} \rangle \Big) \\ - \; \tfrac{1}{2} G_1 \sum_{JN} & \Big(\sum_{\mu\nu} V_{1;\mu\nu}^{NJ} \langle \Psi_{\alpha_\mu j_\mu} || \kappa_{T=1}^{J} || \Psi_{\alpha_\nu j_\nu} \rangle \Big) \\ & \times \Big(\sum_{\mu'\nu'} V_{1;\mu'\nu'}^{NJ} \langle \Psi_{\alpha_{\mu'} j_{\mu'}} || \kappa_{T=1}^{\prime J+} || \Psi_{\alpha_{\nu'} j_{\nu'}} \rangle \Big)\end{aligned}$$

Y. Tian, Z.Y. Ma, P.Ring, Phys. Lett. B676, 44 (2009)

Nuclear incompressibility

The incompressibility of the infinite nuclear matter is defined as

$$K_\infty = 9\rho^2 \frac{\mathrm{d}^2}{\mathrm{d}\rho^2}\left(\frac{E}{A}\right)_{\rho=\rho_{nm}}$$

where ρ_{nm} is the saturation density of nuclear matter.

The incompressibility of the finite nucleus, K_A, is related to the centroid of the giant monopole resonance, E_{GMR}, by the relation

$$E_{GMR} = \sqrt{\frac{\hbar^2 K_A}{m < r^2 >}}$$

where $< r^2 >$ is square root radius of the nucleus. The centroid of the giant monopole resonance can be extracted, e.g., as the ratio of the first and zero moment of the 0^+ strength function,

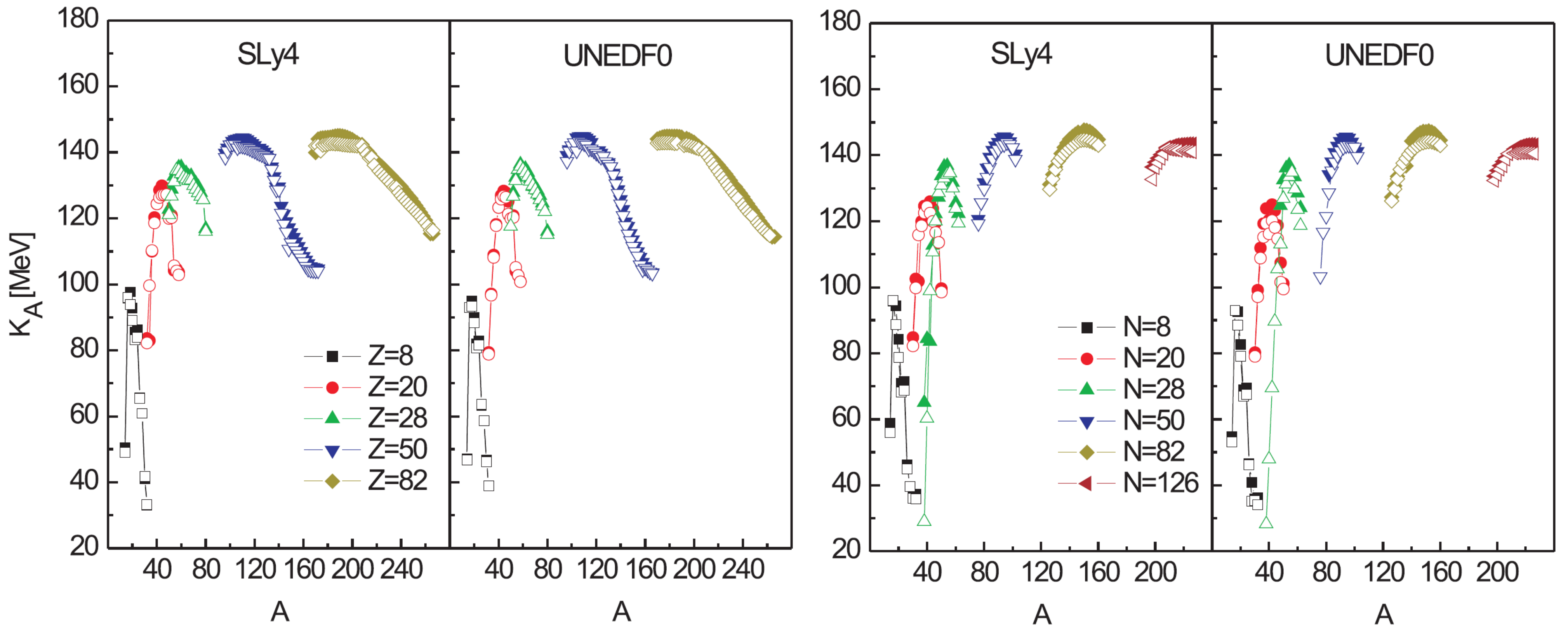
$$E_{GMR} = \frac{m_1}{m_0}.$$

In the analogy to the Weizsäcker formula for the nuclear masses we can introduce similar relation for the nuclear incompressibilities,

$$K_A = K_V + K_S A^{-1/3} + (K_\tau + K_{S,\tau} A^{-1/3})\frac{(N-Z)^2}{A^2} + K_C \frac{Z^2}{A^{4/3}} .$$

J. P. Blaizot, Phys. Rep. 64, 171 (1980)

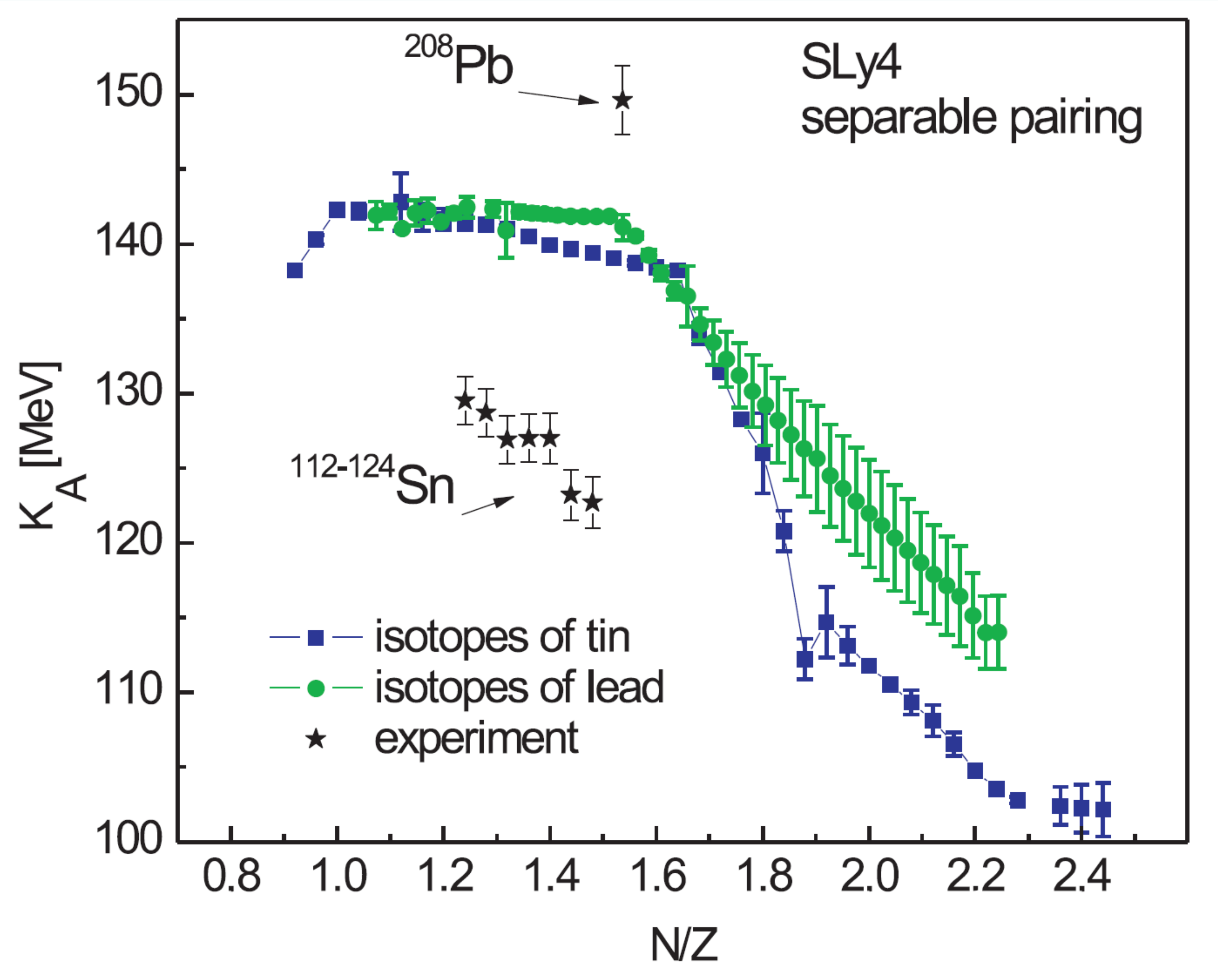
Nuclear incompressibility



Full (empty) symbols correspond to the zero-range (separable) pairing force

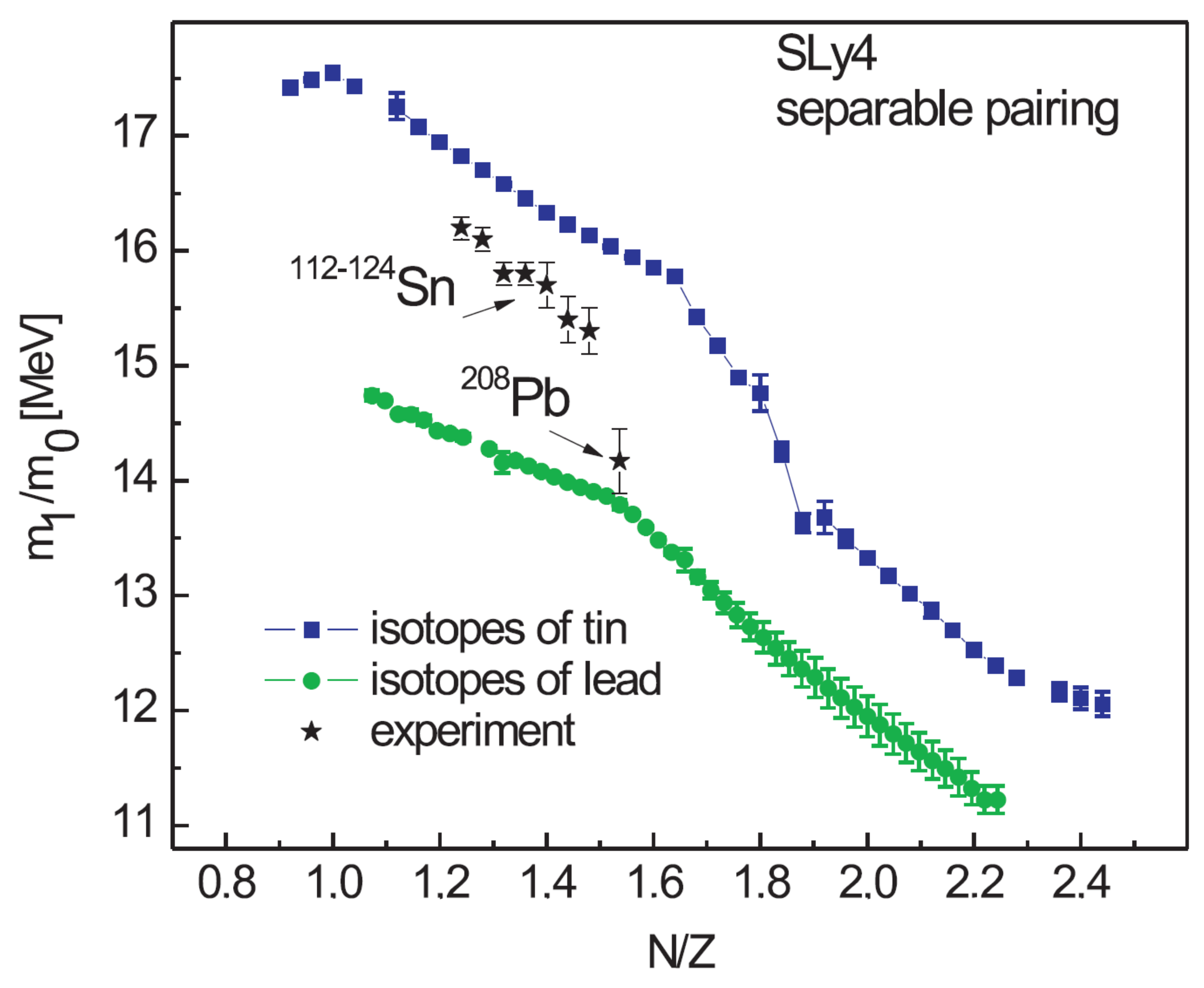
P. Veselý, *et al.*, arXiv:1202.5617

Nuclear incompressibility



P. Veselý, *et al.*, arXiv:1202.5617

Centroids of GMR



P. Veselý, *et al.*, arXiv:1202.5617

Nuclear incompressibility – liquid drop

TABLE I: Parameters (in MeV) of the liquid-drop formula (32) with standard errors, obtained by a fit to the values of K_A calculated in M semi-magic nuclei across the mass chart. The parameter χ was determined as the square root of the sum of fit residuals squared divided by the number of fit degrees of freedom ($M - 5$ in our case).

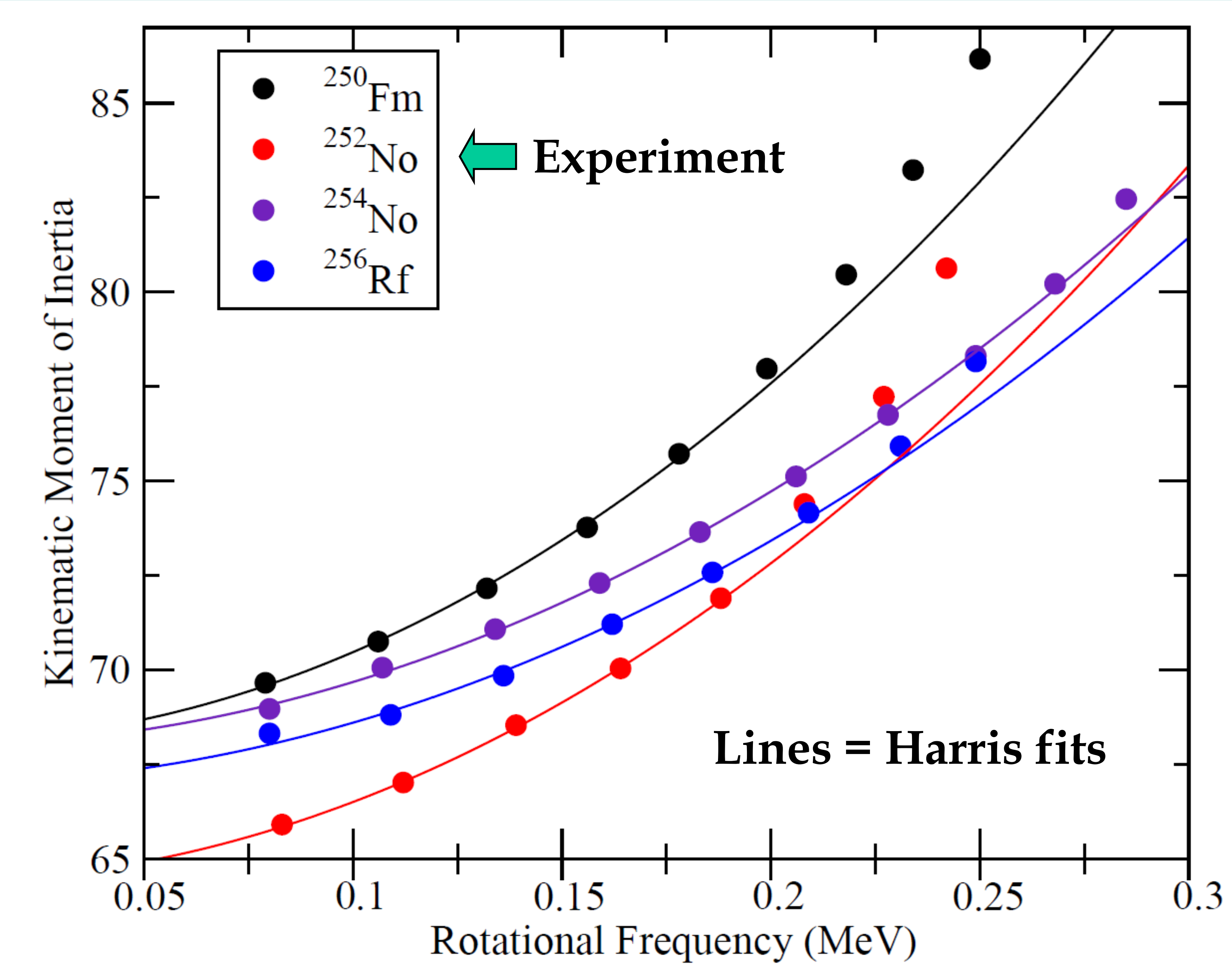
	SLy4		UNEDF0	
	separable	zero-range	separable	zero-range
K_V	252±5	258±5	249±5	257±4
K_S	−391±14	−406±13	−397±14	−412±13
K_τ	−460±30	−500±30	−510±30	−550±30
$K_{S,\tau}$	410±110	560±100	570±120	740±100
K_C	−5.2±0.4	−5.4±0.4	−4.5±0.4	−5.1±0.4
M	210	211	204	195
χ	5.0	4.7	5.3	4.4

P. Veselý, *et al.*, arXiv:1202.5617

Rotational bands in superheavy nuclei around ^{252}No (preliminary)

(with Yue Shi and Paul Greenlees)

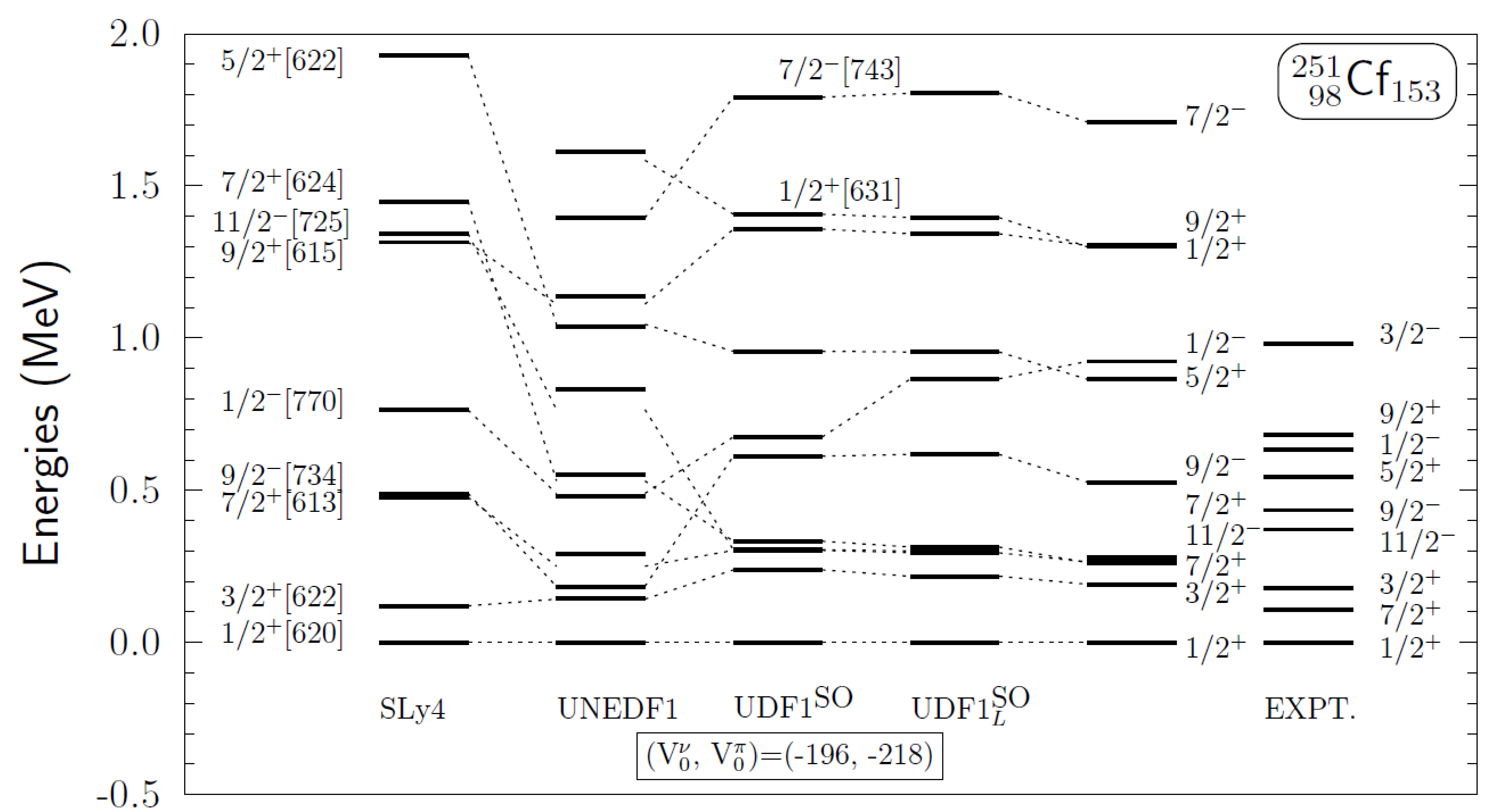
Rotational bands in N=150 & 152 isotones



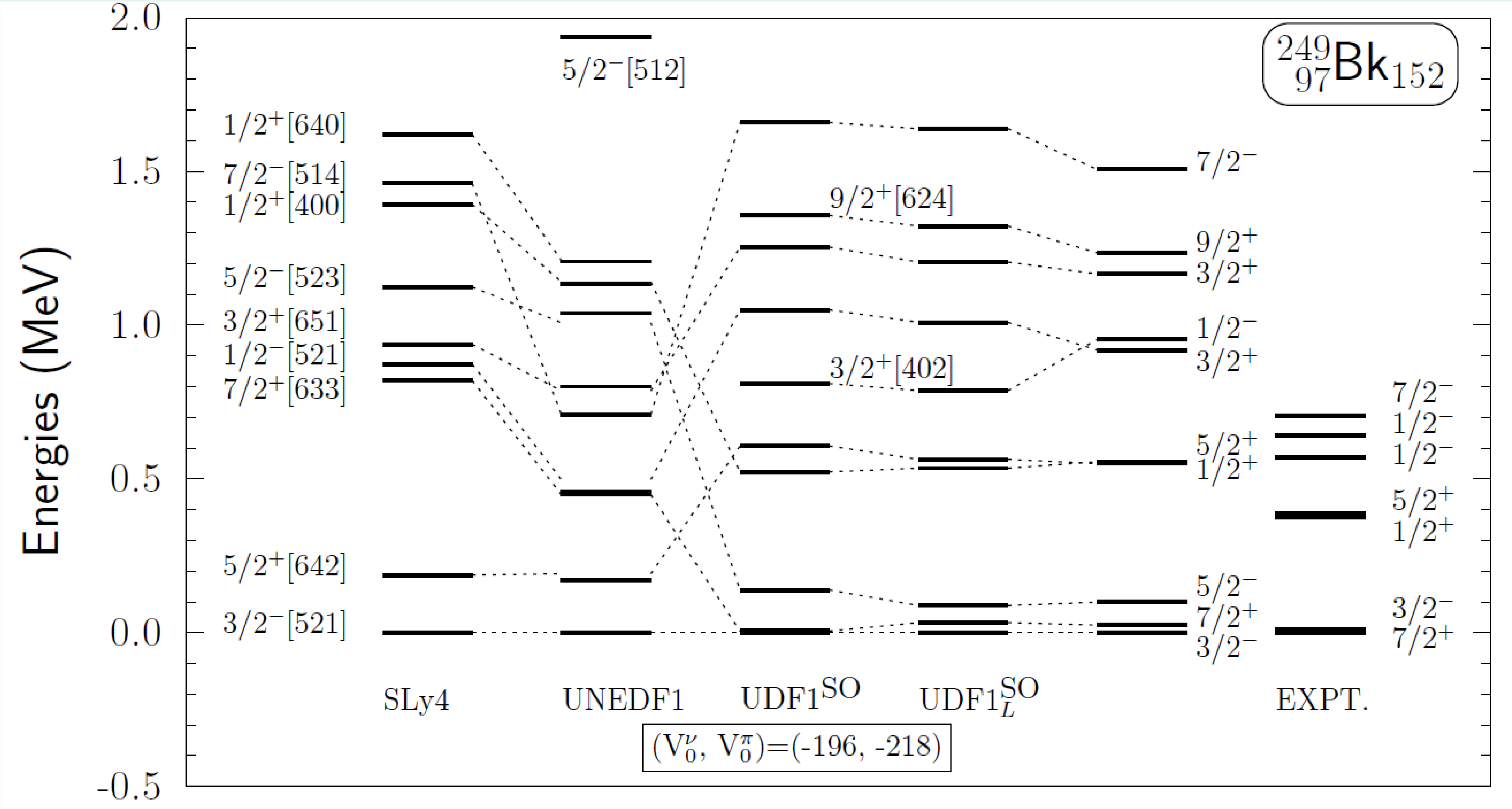
P. Greenlees, *et al.*, to be published

Neutron quasiparticle spectra in $^{251}Cf_{153}$

UNEDF1 = new parameterization adjusted to heavy deformed nuclei
M. Kortelainen et al., Phys. Rev. C85, 024304 (2012)



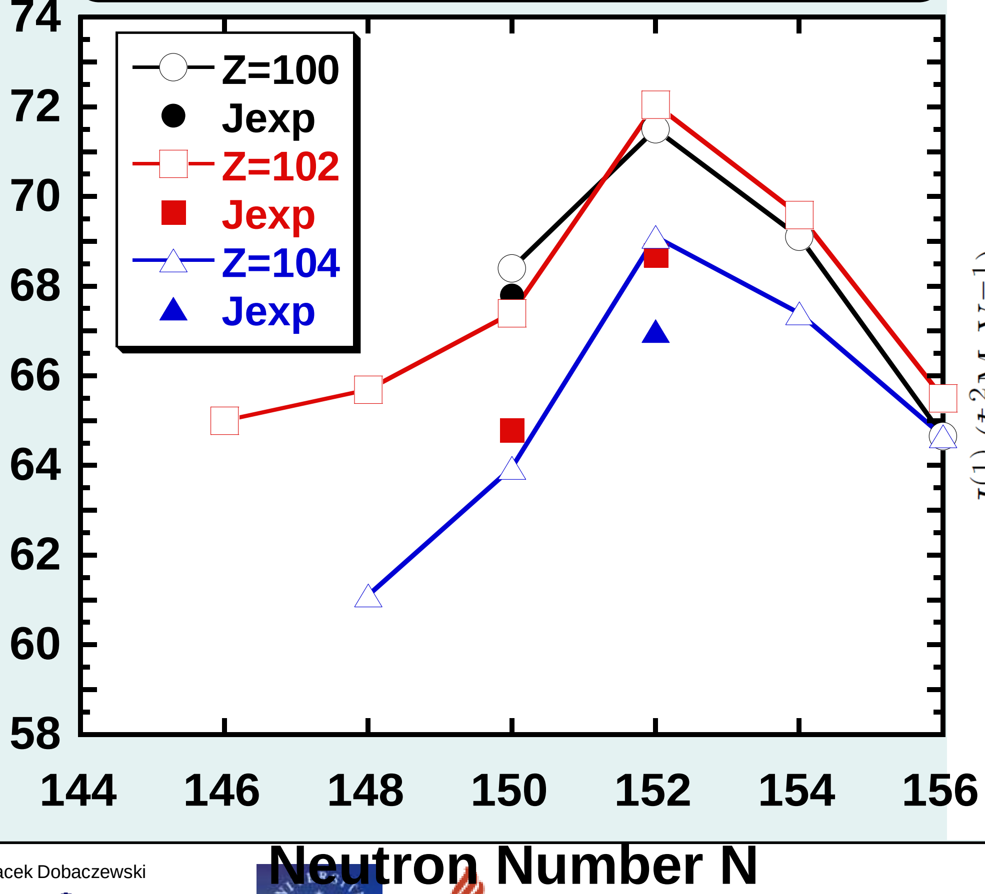
Proton quasiparticle spectra in $^{249}Bk_{152}$



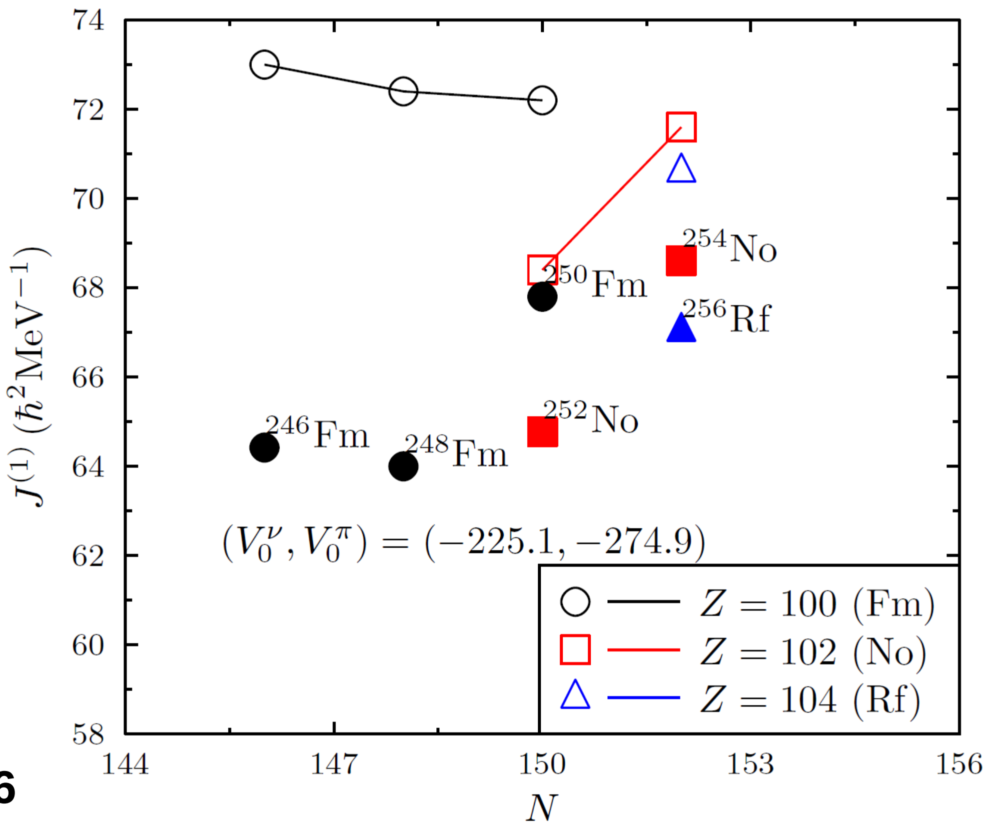
$J^{(1)}$ in N=150 & 152 isotones

Without Lipkin-Nogami
Woods-Saxon & BCS

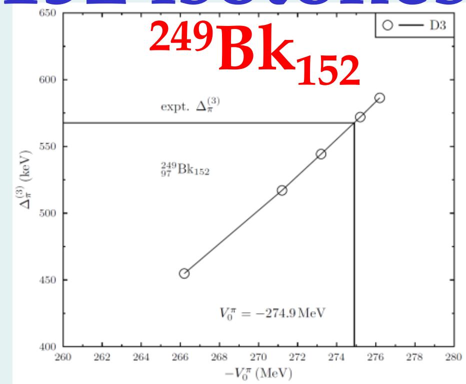
A. Sobiczewski, I. Muntian, Z. Patyk
Phys. Rev. C63, 034306 (2001)

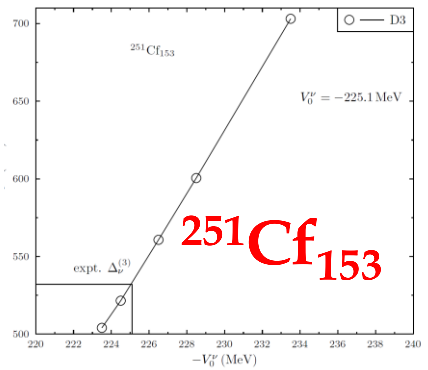


Without Lipkin-Nogami

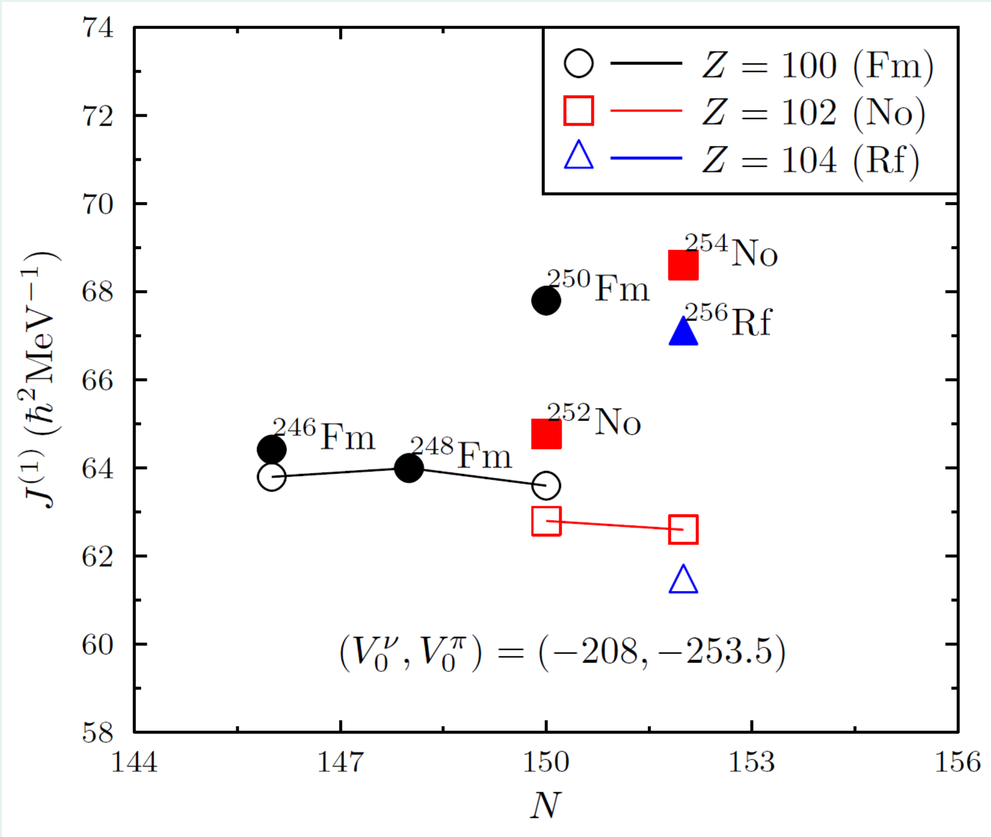


$J^{(1)}$ in N=150 & 152 isotones

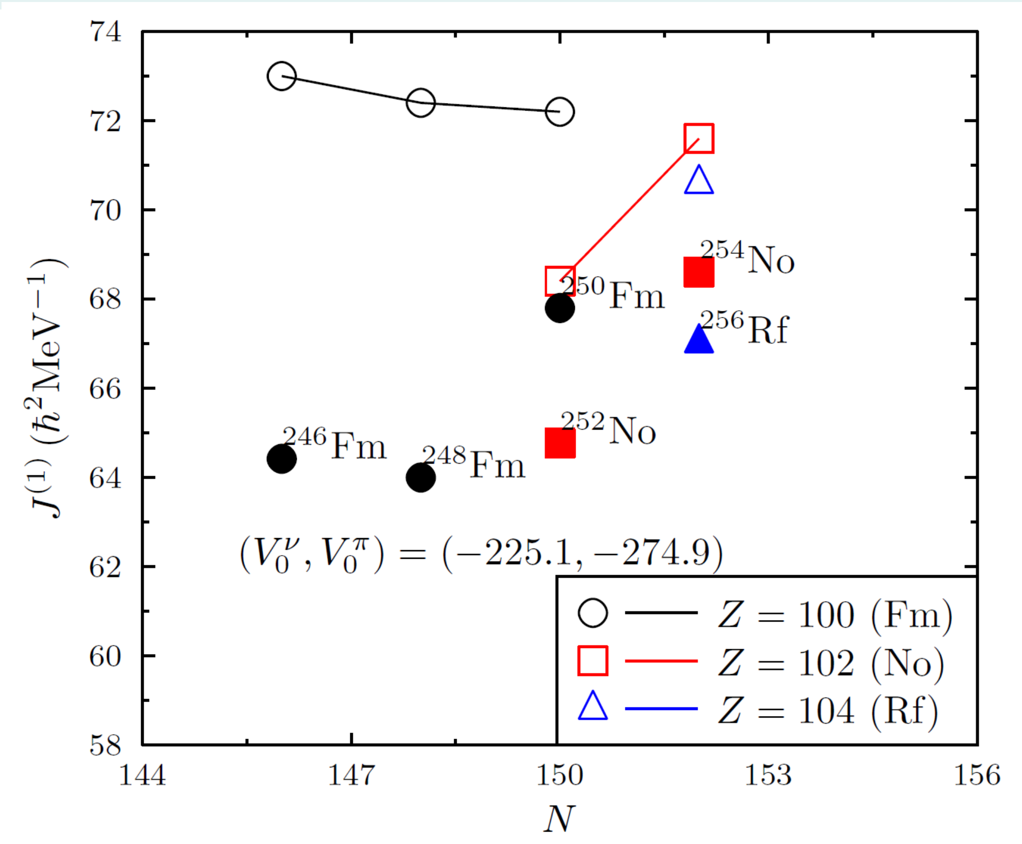




With Lipkin-Nogami



Without Lipkin-Nogami



Conclusions

1. Precise Penning-trap mass measurements beyond ^{132}Sn call for an improved analysis of correlations in odd nuclei
2. Tilted-axis cranking determination of ultra-high-spin triaxial rotational bands in ^{158}Er proves the instability of excited configurations.
3. Incompressibilities of finite nuclei studied within modern QRPA calculations do not provide answer to the question “Why tin is so soft”
4. Rotational bands in superheavy nuclei around ^{252}No challenge current approaches to pairing.

Thank you

What is DFT?

Density Functional Theory:

A variational method that uses observables as variational parameters.

$$\delta \langle \hat{H} - \lambda \hat{Q} \rangle = 0$$
$$\Downarrow$$
$$E = E(Q)$$

$$\text{for} \quad E(\lambda) \equiv \langle \hat{H} \rangle \qquad \text{and} \qquad Q(\lambda) \equiv \langle \hat{Q} \rangle$$

Rayleigh-Ritz Variational Method

$$\hat{H}|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$\Downarrow$$

$$|\Psi\rangle = a_0|\Psi_0\rangle + a_1|\Psi_1\rangle + a_2|\Psi_2\rangle + \ldots$$

$$\langle\Psi|\hat{H}|\Psi\rangle = E_0|a_0|^2 + E_1|a_1|^2 + E_2|a_2|^2 + \ldots$$

$$\Downarrow$$

$$\min_{|\Psi\rangle}\langle\Psi|\hat{H}|\Psi\rangle = E_0 \quad \Longleftarrow \text{Rayleigh-Ritz}$$

Which DFT?

$$\delta\langle\hat{H}-\lambda\hat{Q}\rangle=0 \Longrightarrow E=E(Q)$$

$$\delta\langle\hat{H}-\textstyle\sum_k\lambda_k\hat{Q}_k\rangle=0 \Longrightarrow E=E(Q_k)$$

$$\delta\langle\hat{H}-\int\mathrm{d}q\,\lambda(q)\hat{Q}(q)\rangle=0 \Longrightarrow E=E[Q(q)]$$

$$\delta\langle\hat{H}-\int\mathrm{d}\vec{r}\,\lambda(\vec{r})\hat{\rho}(\vec{r})\rangle=0 \Longrightarrow E=E[\rho(\vec{r})]$$

$$\text{for}\quad \hat{\rho}(\vec{r}) \;=\; \textstyle\sum_{i=1}^{A}\delta(\vec{r}-\vec{r}_i)$$

$$\delta\langle\hat{H}-\int\!\!\int\mathrm{d}\vec{r}\mathrm{d}\vec{r}\,'\,\lambda(\vec{r},\vec{r}\,')\hat{\rho}(\vec{r},\vec{r}\,')\rangle=0 \Longrightarrow E=E[\rho(\vec{r},\vec{r}\,')]$$

What is the DFT good for?

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$
$$\Downarrow$$
$$E = E(Q)$$

Energy E is a function(al) of Q

1) **Exact:** Minimization of E(Q) gives the exact E and exact Q
2) **Impractical:** Derivation of E(Q) requires the full variation δ (bigger effort than to find the exact ground state)
3) **Inspirational:** Can we build useful models E′(Q) of the exact E(Q)?
4) **Experiment-driven:** E′(Q) works better or worse depending on the physical input used to build it.

How the nuclear EDF is built?

$$E'[\rho(\vec{r})] = \int d\vec{r}\, \mathcal{H}(\rho(\vec{r}))$$

LDA

Local energy density is a function of local density

$$E'[\rho(\vec{r},\vec{r}\,')] = \int\int d\vec{r} d\vec{r}\,'\, \mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

Gogny, M3Y,...

Non-local energy density is a function of non-local density

$$\mathcal{H}(\rho(\vec{r},\vec{r}\,')) = V(\vec{r}-\vec{r}\,')\Big[\rho(\vec{r})\rho(\vec{r}\,') - \rho(\vec{r},\vec{r}\,')\rho(\vec{r}\,',\vec{r})\Big]$$

How the nuclear EDF is built?

$$E' = \int \mathrm{d}\vec{r}\, \mathcal{H}(\rho(\vec{r}), \tau(\vec{r}), \Delta\rho(\vec{r}), \ldots)$$

Skyrme, BCP, point-coupling,...

Quasi-local energy density is a function of local densities and gradients

$$E' = \int\int \mathrm{d}\vec{r}\mathrm{d}\vec{r}'\, \mathcal{H}(\rho(\vec{r}), \rho(\vec{r}'))$$

RMF (Hartree)

Non-local energy density is a function of local densities

Collectivity

beyond mean field, ground-state correlations, shape coexistence, symmetry restoration, projection on good quantum numbers, configuration interaction, generator coordinate method, multi-reference DFT, etc....

$$E = \langle\Psi|\hat{H}|\Psi\rangle \simeq \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

$$\text{for}\quad \rho(\vec{r},\vec{r}\,') = \frac{\langle\Psi|a^+(\vec{r}\,')a(\vec{r}\,')|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

True for mean field $\Downarrow$

$$\langle\Psi_1|\hat{H}|\Psi_2\rangle \simeq \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho_{12}(\vec{r},\vec{r}\,'))$$

$$\text{for}\quad \rho_{12}(\vec{r},\vec{r}\,') = \frac{\langle\Psi_1|a^+(\vec{r}\,')a(\vec{r}\,')|\Psi_2\rangle}{\langle\Psi_1|\Psi_2\rangle}$$

Extensions

☆ **I. Range separation and exact long-range effects**

$$\mathcal{H}(\rho) = \mathcal{H}_{\text{long}}(\rho) + \mathcal{H}_{\text{short}}(\rho)$$

☆ **II. Derivatives of higher order:**

$$\mathcal{H}(\rho) = \mathcal{H}(\rho, \tau, \tau_4, \tau_6, \Delta\rho, \Delta^2\rho, \Delta^3\rho, \ldots)$$

☆ **III. Products of more than two densities:**

$$\mathcal{H}(\rho) = \mathcal{H}(\rho^2, \rho^3, \tau^2, \tau^3, \rho\tau, \rho^2\tau, \ldots)$$

Finite-range separable pairing interaction

The interaction matrix elements $V_{T;\mu\nu}^{NJ}$ are defined as follows

$$
\begin{aligned}
V_{0;\mu\nu}^{J,N\lambda} &= \sqrt{(12\pi)(2\lambda+1)(2j_\mu+1)(2j_\nu+1)}\left\{\begin{array}{ccc} l_\mu & l_\nu & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_\mu & j_\nu & J \end{array}\right\} \\
&\times\ M_{n_\mu l_\mu n_\nu l_\nu}^{N\lambda n0}\frac{2^{1/4}}{b^{3/2}}\sqrt{\frac{\pi^{1/2}(2n+1)!}{2(2^n n!)^2}} \\
&\times\ \frac{1}{m}\sum_{i=1}^{m}\frac{1}{(4\pi a_i^2)^{3/2}}\left(\frac{2a_i^2b^2}{1+a_i^2b^2}\right)^{3/2}\left(\frac{1-a_i^2b^2}{1+a_i^2b^2}\right)^{n}\delta_{2n,2n_\mu+l_\mu+2n_\nu+l_\nu-2N-\lambda}, \\
V_{1;\mu\nu}^{NJ} &= \sqrt{(4\pi)(2J+1)(2j_\mu+1)(2j_\nu+1)}\left\{\begin{array}{ccc} l_\mu & l_\nu & J \\ \frac{1}{2} & \frac{1}{2} & 0 \\ j_\mu & j_\nu & J \end{array}\right\} \\
&\times\ M_{n_\mu l_\mu n_\nu l_\nu}^{NJn0}\frac{2^{1/4}}{b^{3/2}}\sqrt{\frac{\pi^{1/2}(2n+1)!}{2(2^n n!)^2}} \\
&\times\ \frac{1}{m}\sum_{i=1}^{m}\frac{1}{(4\pi a_i^2)^{3/2}}\left(\frac{2a_i^2b^2}{1+a_i^2b^2}\right)^{3/2}\left(\frac{1-a_i^2b^2}{1+a_i^2b^2}\right)^{n}\delta_{2n,2n_\mu+l_\mu+2n_\nu+l_\nu-2N-J}
\end{aligned}
$$

where we used the standard notation of the Talmi-Moshinski coefficients $M_{n_\mu l_\mu n_\nu l_\nu}^{N\lambda n0}$.

Nuclear incompressibility

Table 1: Parameters (in MeV) of the liquid-drop formula, obtained by a fit to the values of K_A calculated in M semi-magic nuclei across the mass chart. The standard parameter χ is detrmined as the rms deviation per fit degree of freedom.

	SLy4		UNEDF0	
	separable	zero-range	separable	zero-range
K_V	252±5	258±5	249±5	257±4
K_S	−391±14	−406±13	−397±14	−412±13
K_τ	−460±30	−500±30	−510±30	−550±30
$K_{S,\tau}$	410±110	560±100	570±120	740±100
K_C	−5.2±0.4	−5.4±0.4	−4.5±0.4	−5.1±0.4
M	210	211	204	195
χ	5.0	4.7	5.3	4.4

P. Veselý, *et al.*, arXiv:1202.5617