Potential energy surfaces of super-heavy nuclei in the 4D Fourier parameter space

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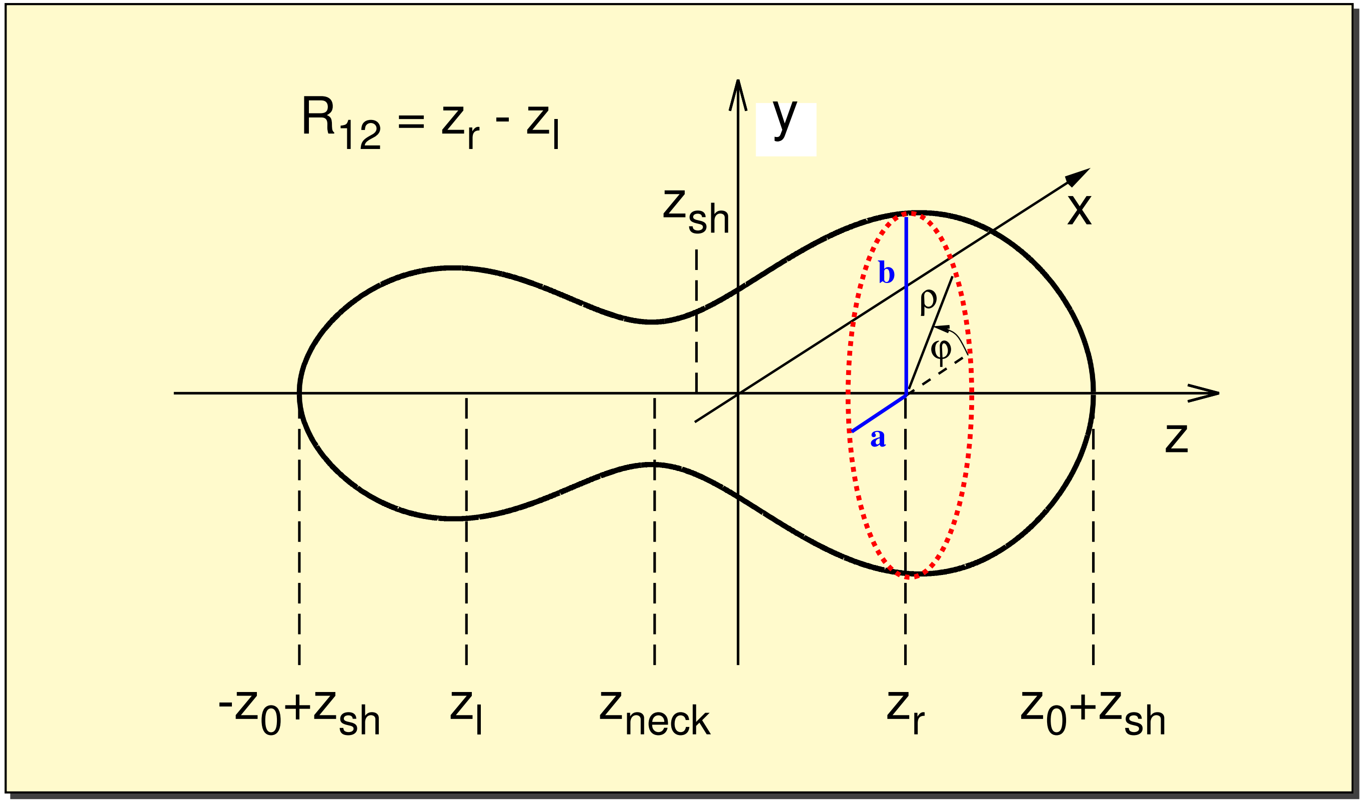
My collaborators:

- **Bożena Nerlo-Pomorska**, Maria Curie Skłodowska University, Lublin,
- **Johann Bartel**, IPHC and University of Strasbourg,
- **Christelle Schmitt**, IPHC, Strasbourg.

Program:

- Fourier parametrization of nuclear shapes,
- Potential energy surfaces of heavy and super-heavy nuclei,
- Systematics of the ground state deformations,
- Fission barrier height and Q_α systematics,
- α-decay and spontaneous fission half-lives in a simple WKB model,
- Summary.

Fourier expansion of nuclear shapes *



$$(x, y, z) \to (\rho, \varphi, z)$$

Nonaxial shapes:

$$\eta = \frac{b-a}{a+b}$$

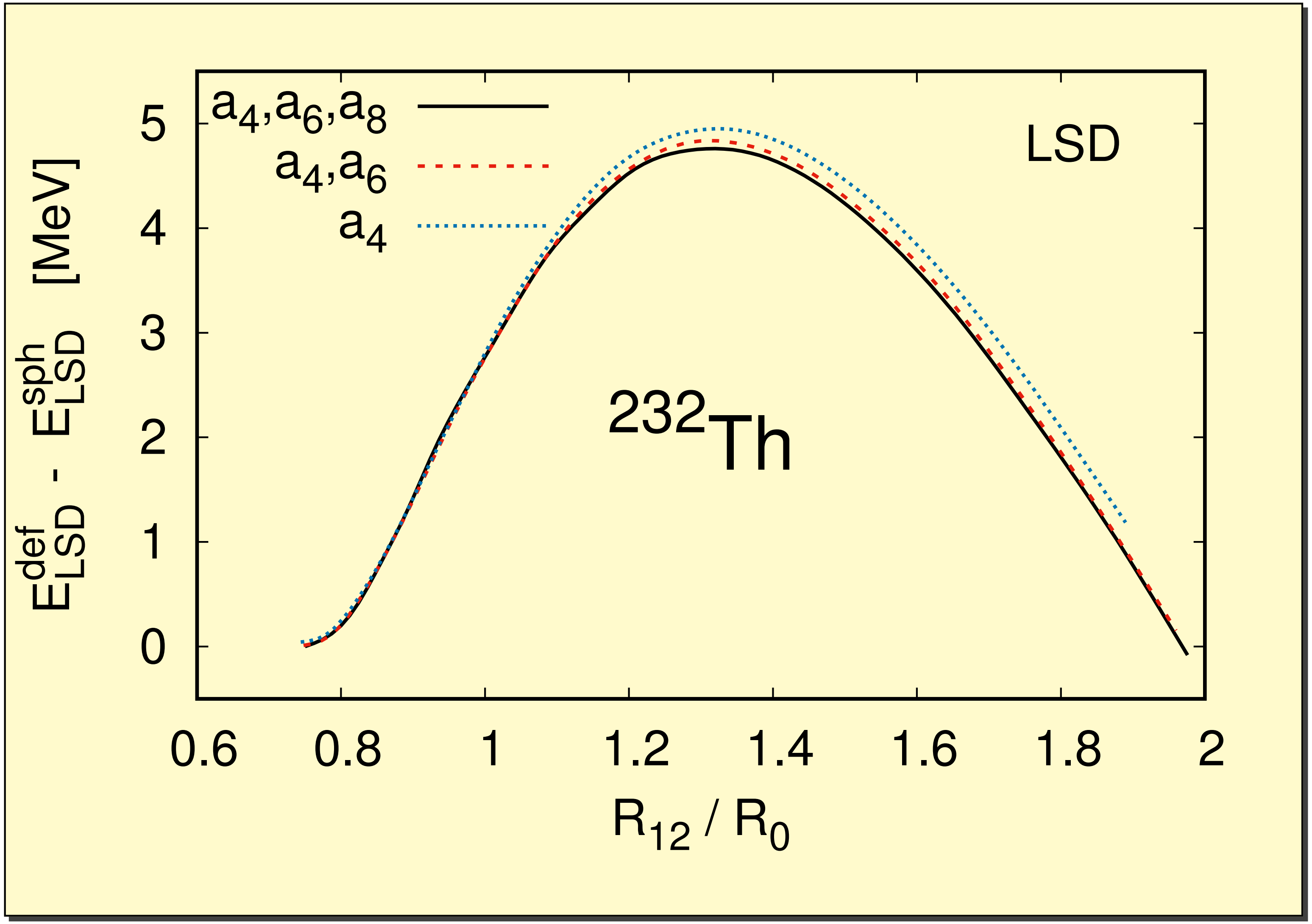
$$\rho_s^2(z) = a(z)b(z)$$

$$\frac{\rho_s^2(z)}{R_0^2} = \sum_{n=1}^{\infty} \left[a_{2n} \cos\left(\frac{(2n-1)\pi}{2} \frac{z - z_{sh}}{z_0} \right) + a_{2n+1} \sin\left(\frac{2n\pi}{2} \frac{z - z_{sh}}{z_0} \right) \right] ,$$

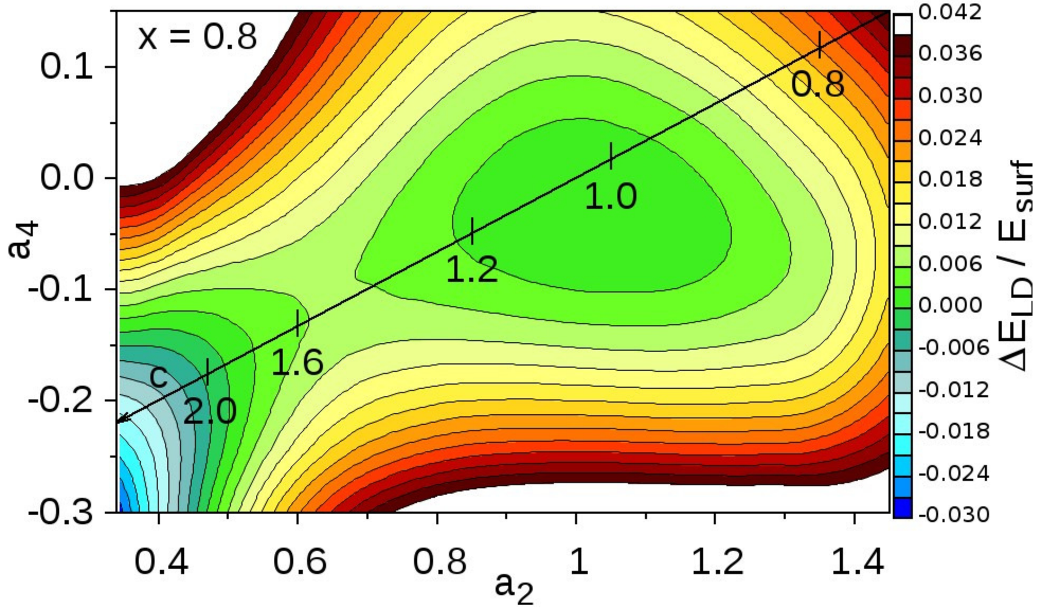
Here R_0 is radius of spherical nucleus, while $2z_0$ is the length of the deformed nucleus.

*K. Pomorski, B. Nerlo-Pomorska, J. Bartel, and C. Schmitt Acta Phys. Pol. B Supl. **8** (2015) 667,
C. Schmitt, K. Pomorski, B. Nerlo-Pomorska, and J. Bartel, Phys. Rev. C **95** (2017) 034612.

Convergence of the Fourier expansion



Potential energy surface in the (a_2, a_4) plane



Optimal coordinates:

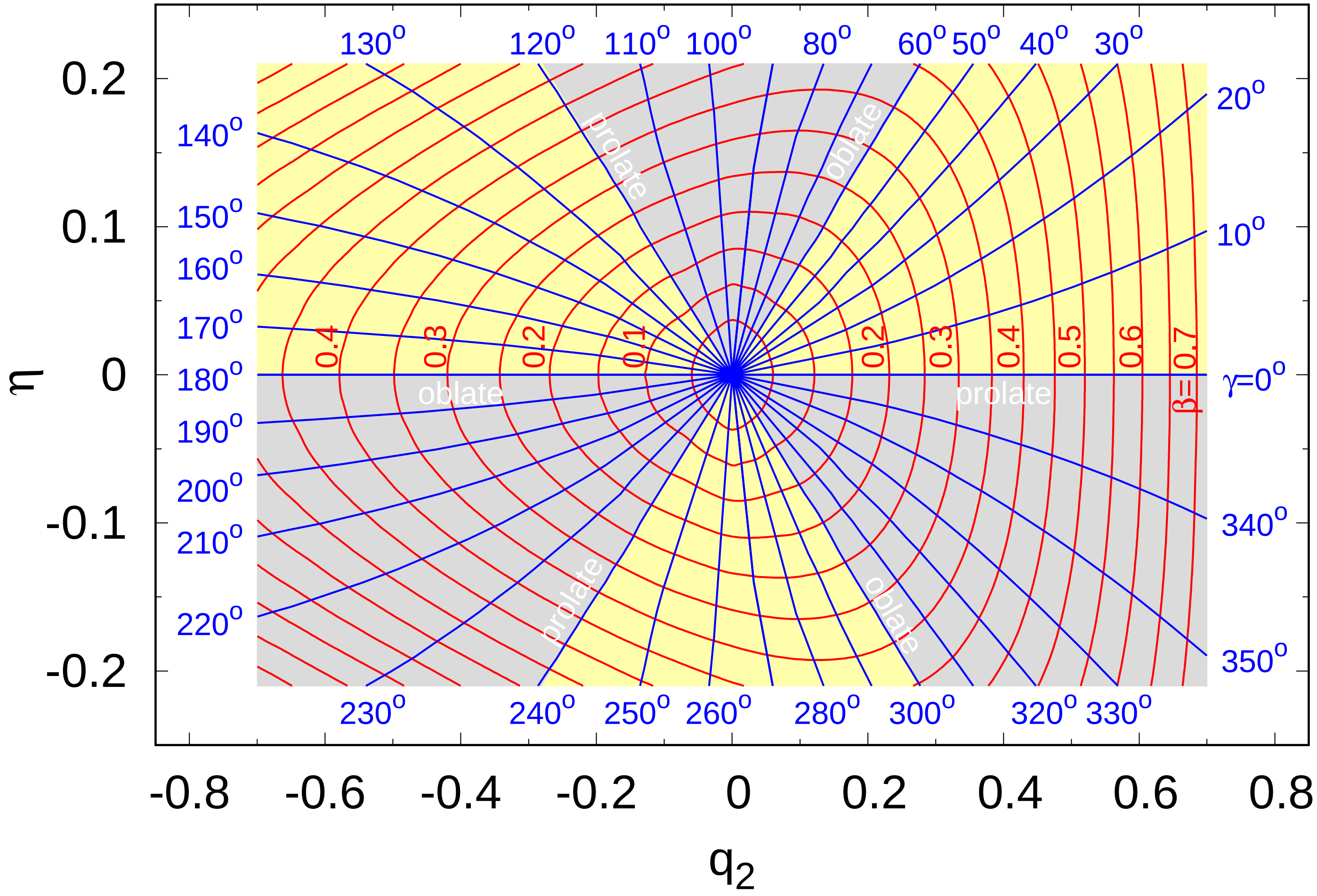
$$q_2 = a_2^{(0)}/a_2 - a_2/a_2^{(0)} \ ,$$
$$q_3 = a_3 \ ,$$
$$q_4 = a_4 + \sqrt{(q_2/9)^2 + (a_4^{(0)})^2} \ ,$$
$$q_5 = a_5 - (q_2 - 2)a_3/10 \ ,$$
$$q_6 = a_6 - \sqrt{(q_2/100)^2 + (a_6^{(0)})^2} \ .$$

Here $a_2^{(0)} = 1.03205$, $a_4^{(0)} = -0.03822$, and $a_6^{(0)} = 0.00826$ are the Fourier expansion coefficients of a sphere. q_2 describes the elongation of a nucleus, q_3 its left-right asymmetry, and q_4 formation of the neck.

See also an alternative expansion around a spheroid:

K. Pomorski, B. Nerlo-Pomorska, J. Bartel, Phys. Scr. **92** (2017) 064006.

Relation between (q_2, η) and (β, γ)



$$\beta = \frac{\sqrt{5\pi}}{3r_0^2 A^{5/3}} \sqrt{Q_{20}^2 + Q_{22}^2}$$

$$\gamma = \arctan\left(\frac{Q_{22}}{Q_{20}}\right)$$

$$Q_{20} = < 2z^2 - x^2 - y^2 >$$

$$Q_{22} = \sqrt{3} < y^2 - x^2 >$$

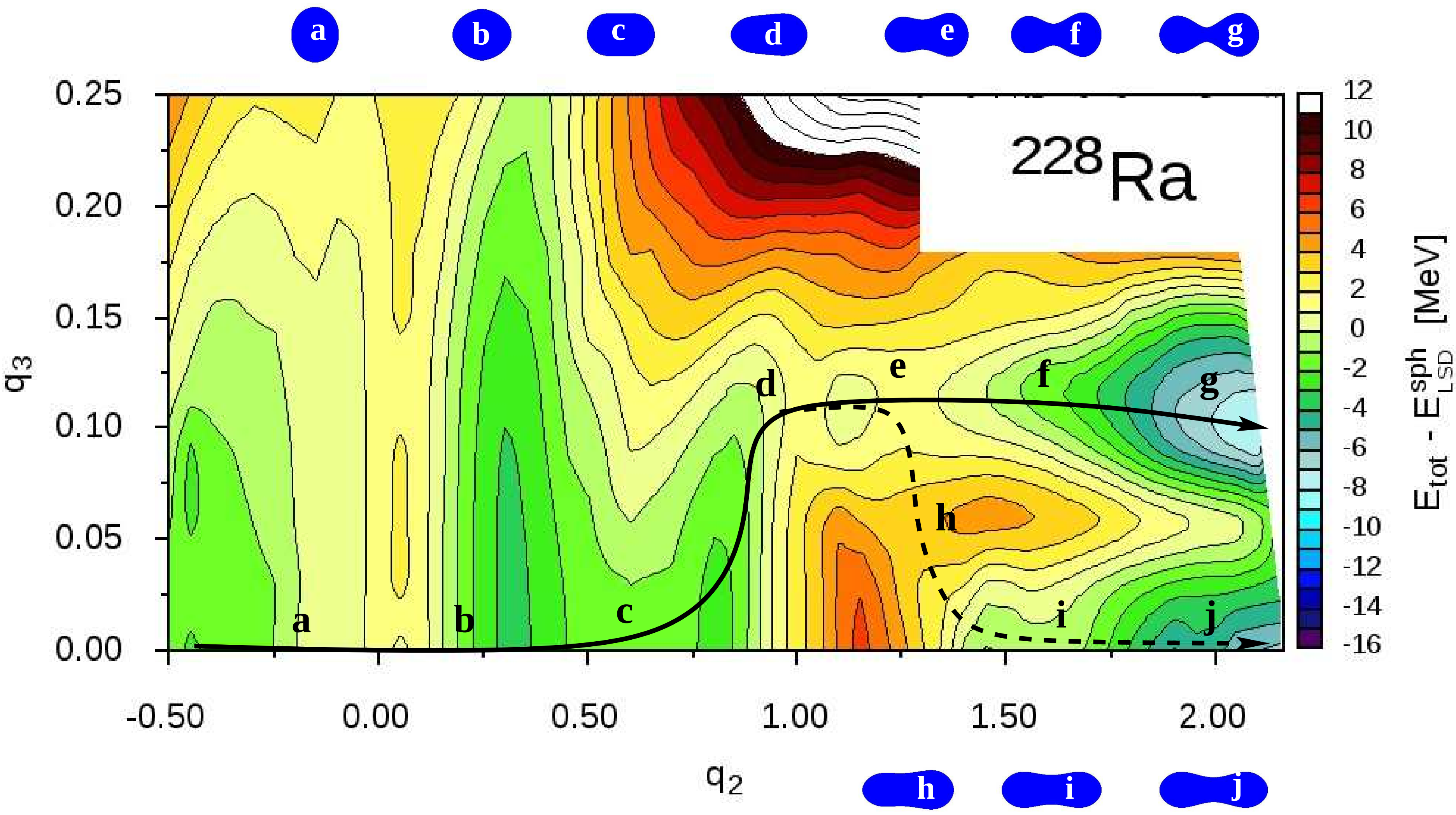
Main ingredients of our model:

- Macroscopic-microscopic approximation of nuclear energy,
- Lublin-Strasbourg-Drop for the macroscopic part of energy,
- Yukawa-folded single-particle potential,
- Strutinsky shell-correction method,
- BCS with the monopole pairing force and the GCM+GOA projection,
- Fourier parametrisation of nuclear shapes,

Calculations are already preformed for 324 even-even isotopes from ^{226}U to ^{324}126. The results for odd-Z or/and odd-N nuclei are in preparation.

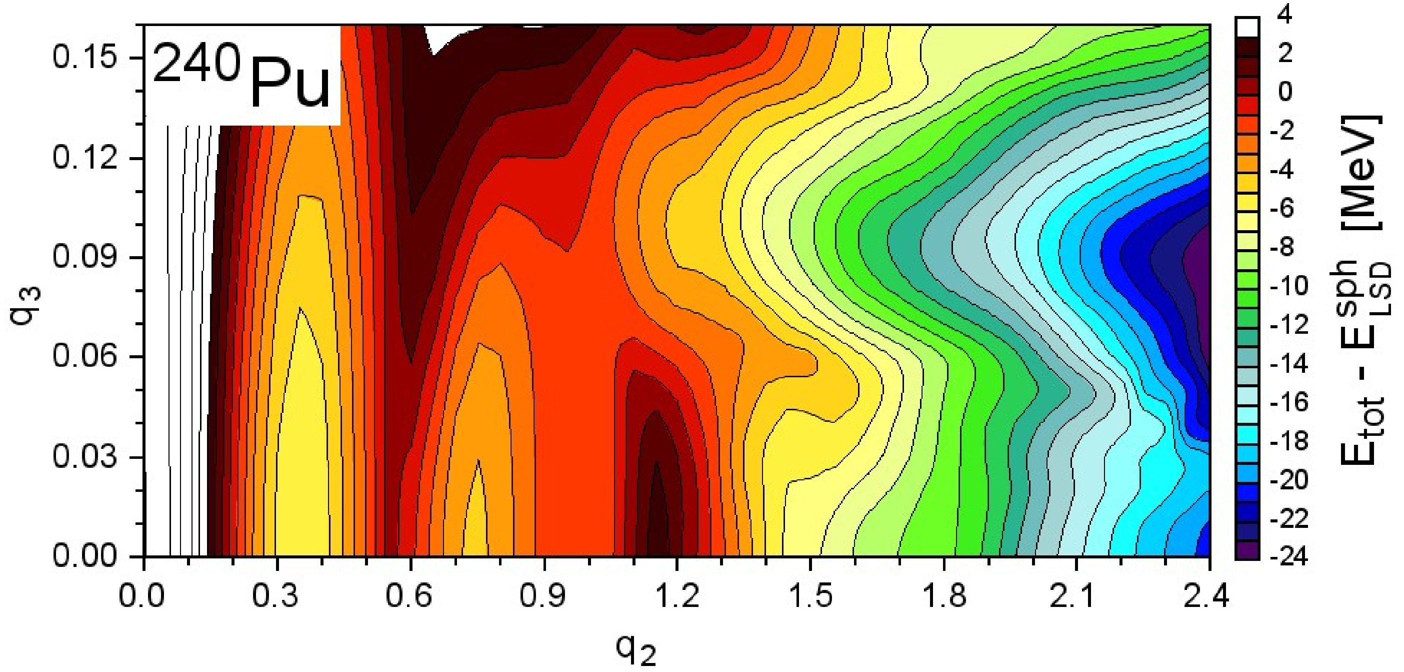
All parameters of the calculation are standard. None of them is specially fitted to the considered nuclei.

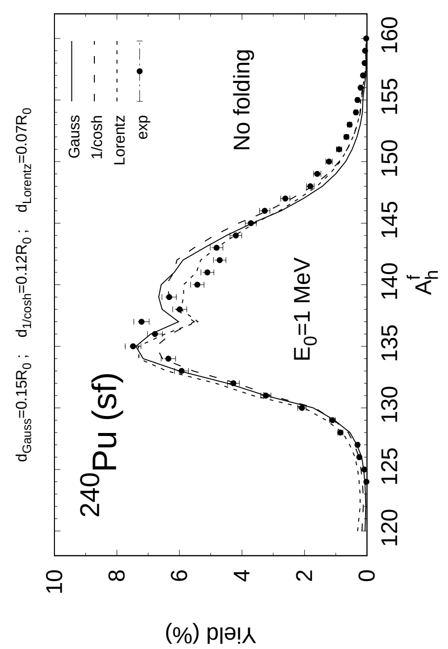
Potential energy surface of ^{228}Ra on the (q_2, q_3) plane*



*C. Schmitt, K. Pomorski, B. Nerlo-Pomorska, and J. Bartel, Phys. Rev. C **95** (2017) 034612.

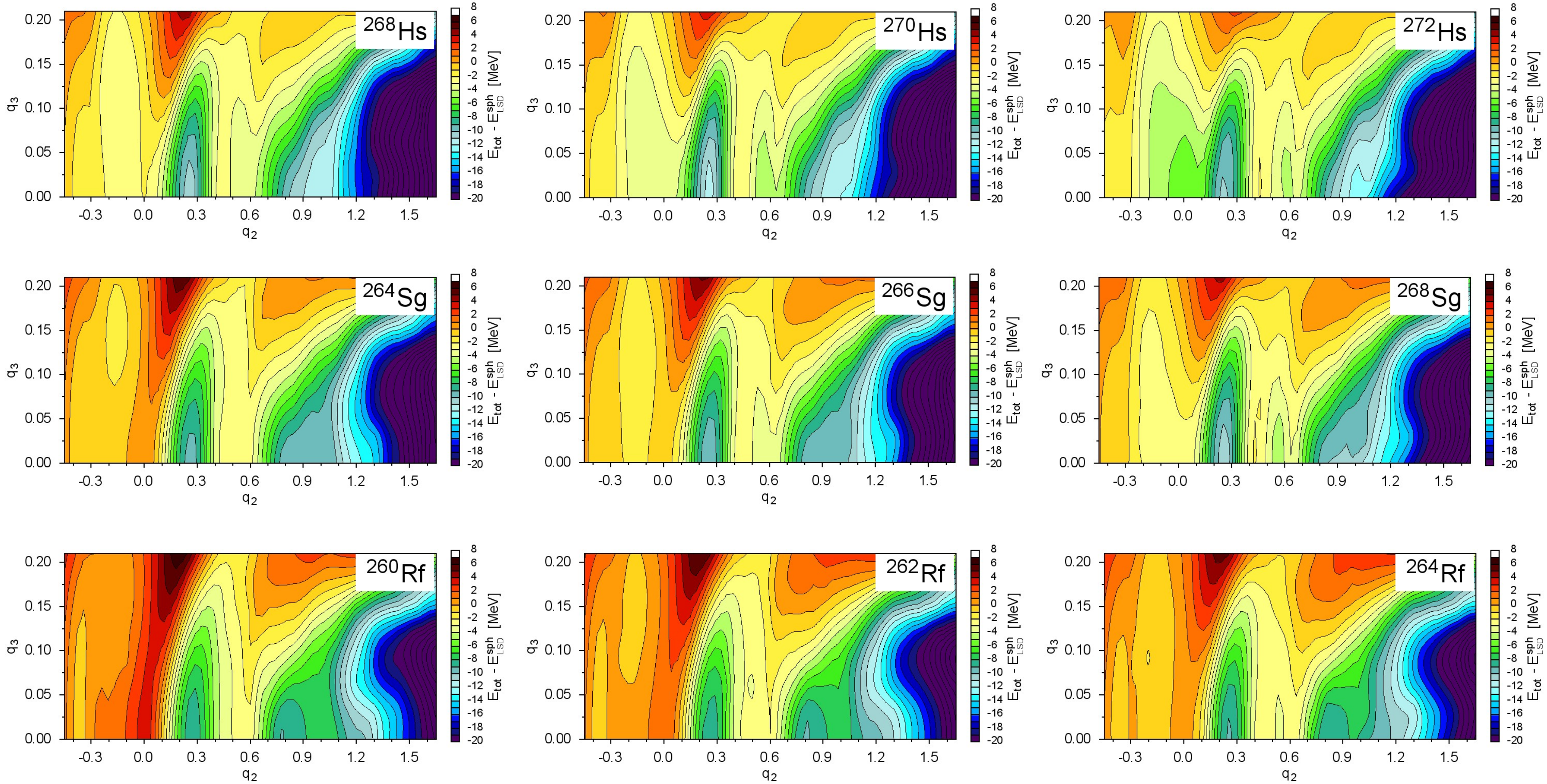
Potential energy surface of ^{236}Pu on the (q_2, q_3) plane*



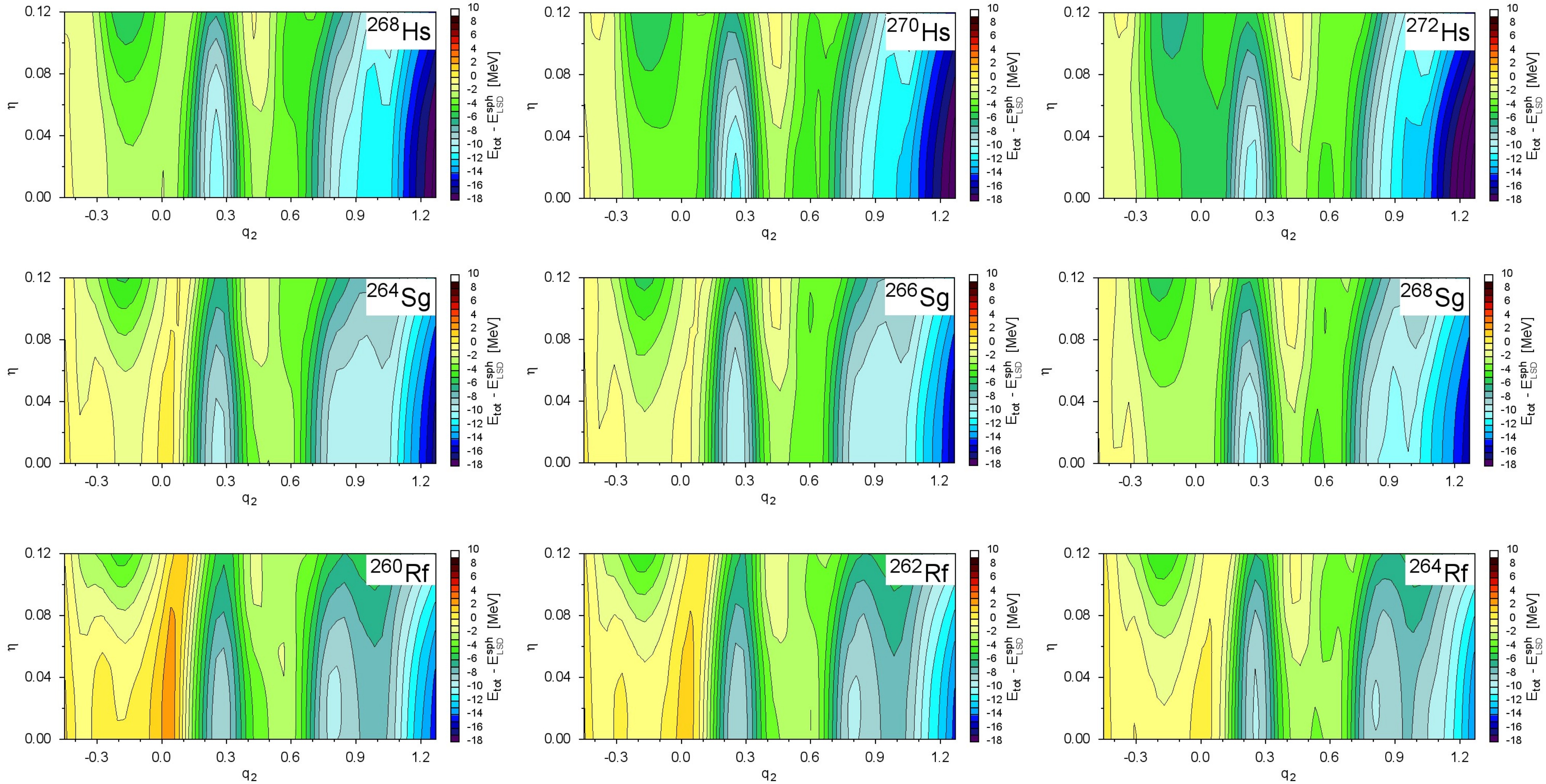


*K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt, Eur. Phys. Journ. Conf. Proc., accepted for publication (Theory-4 Workshop, Varna, June 2017, Editor F.-J. Hambsch EC JRC, Geel, Belgium)

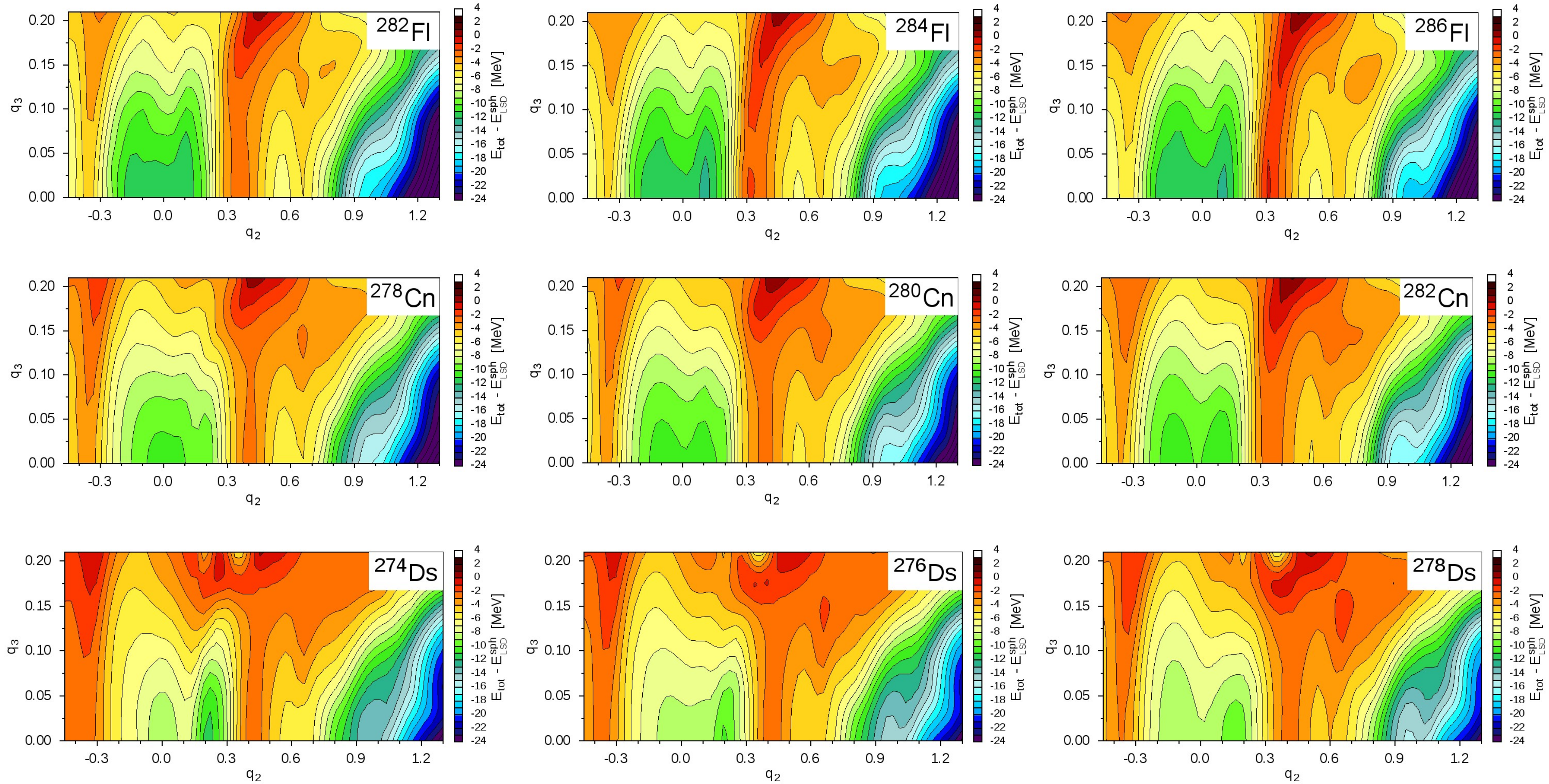
PES of ^{266}Sg and neighbouring nuclei on the (q_2, q_3) plane



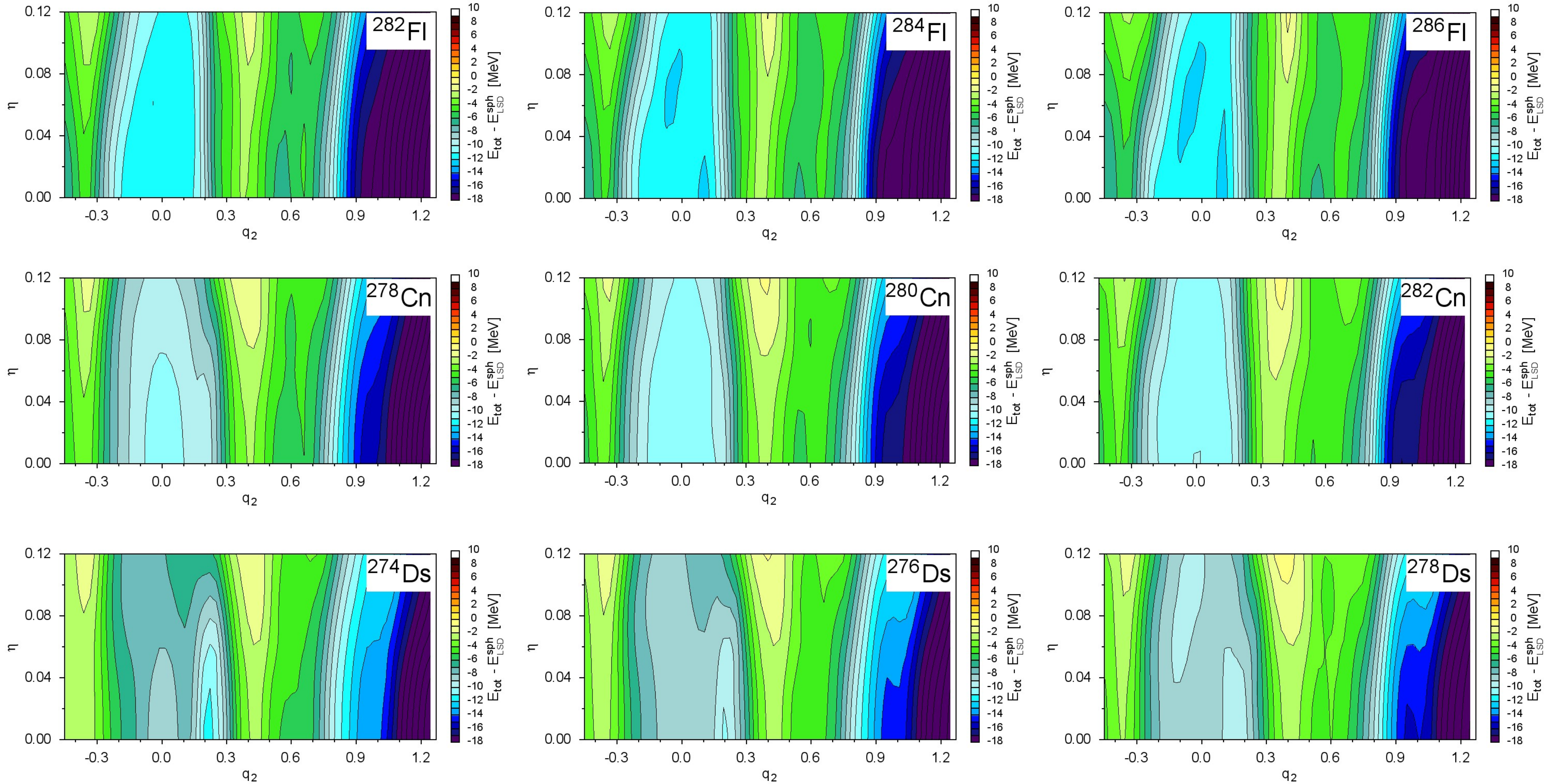
PES of ^{266}Sg and neighbouring nuclei on the (q_2, η) plane



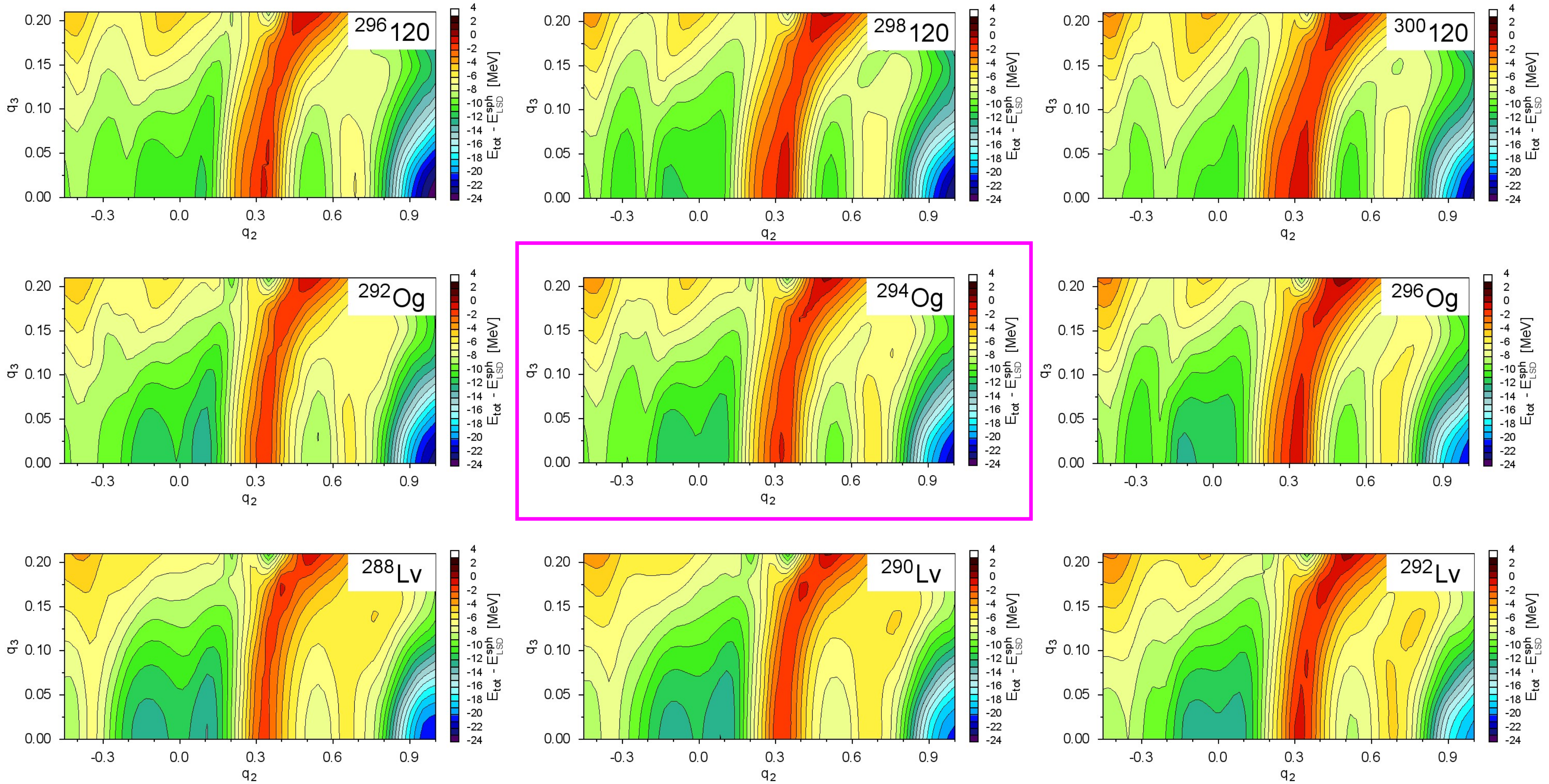
PES of ^{280}Cn and neighbouring nuclei on the (q_2, q_3) plane



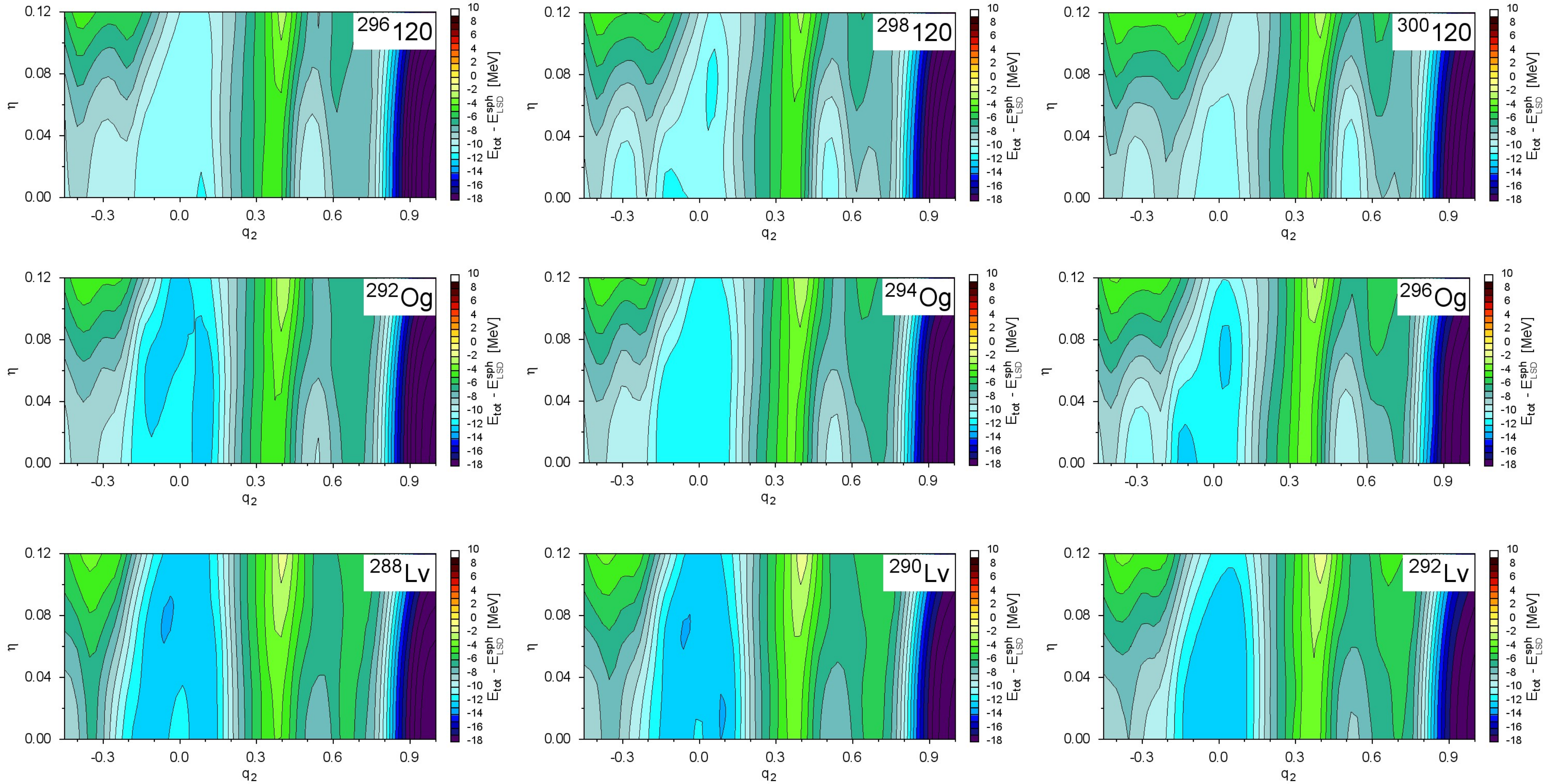
PES of ^{280}Cn and neighbouring nuclei on the (q_2, η) plane



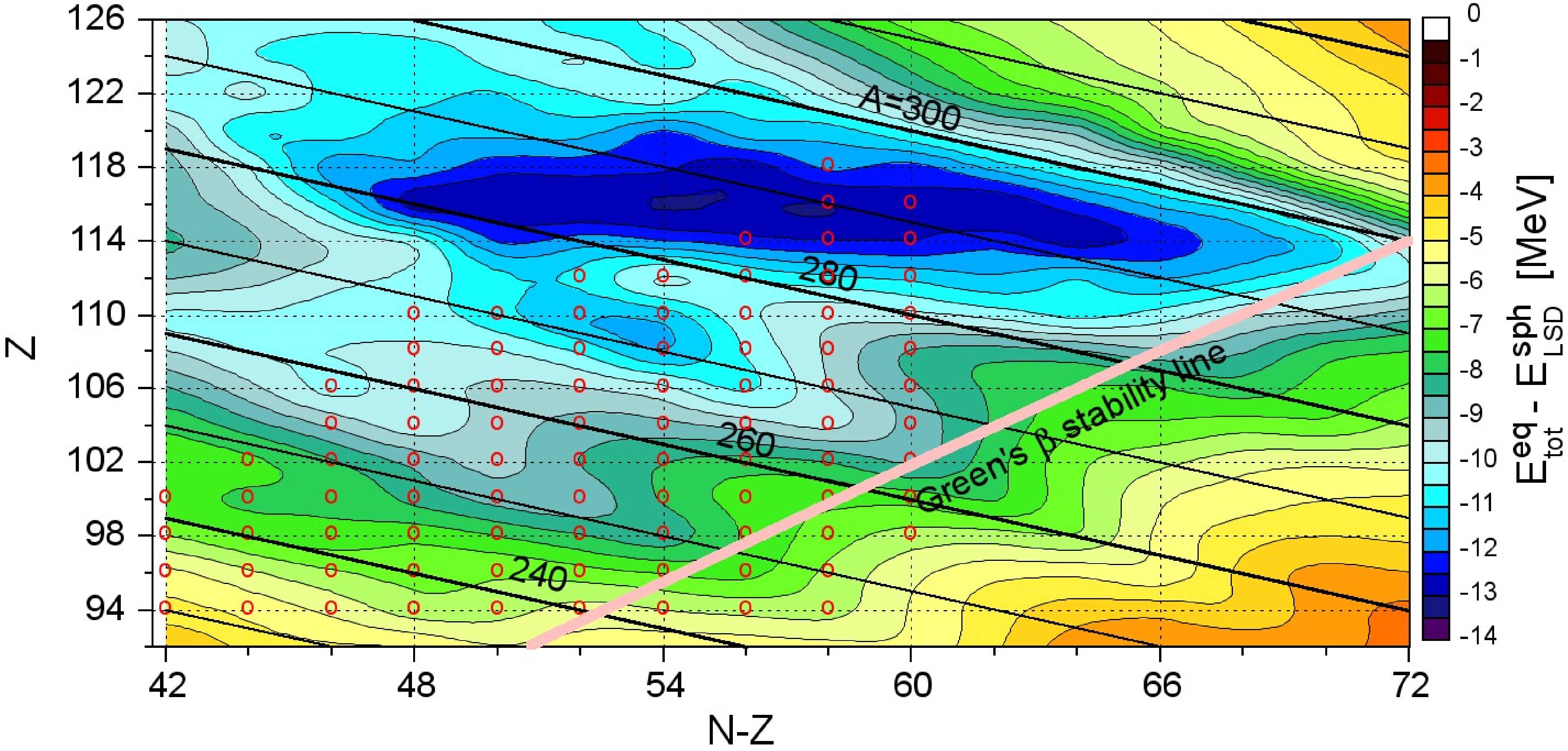
PES of ^{294}Og and neighbouring nuclei on the (q_2, q_3) plane



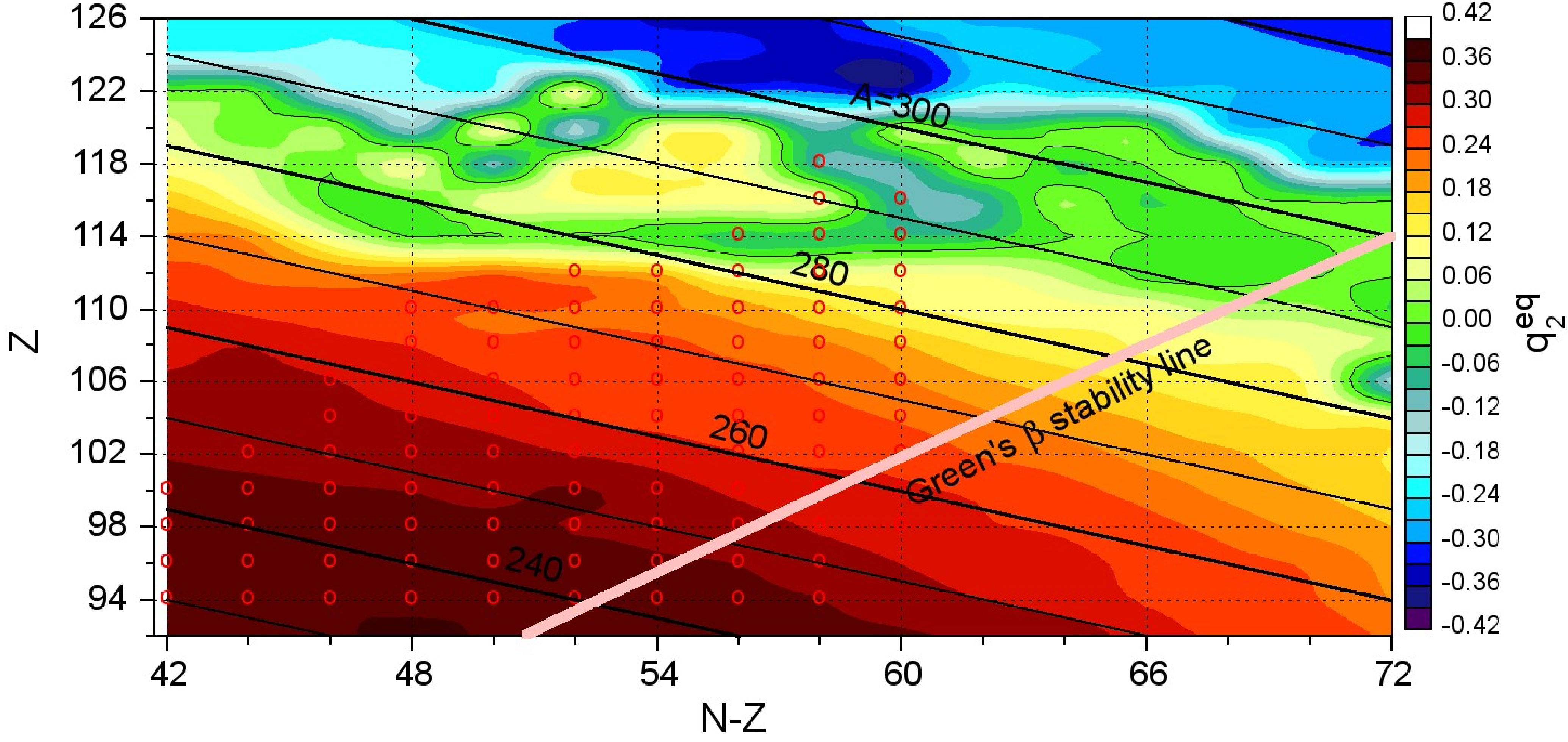
PES of ^{294}Og and neighbouring nuclei on the (q_2, η) plane



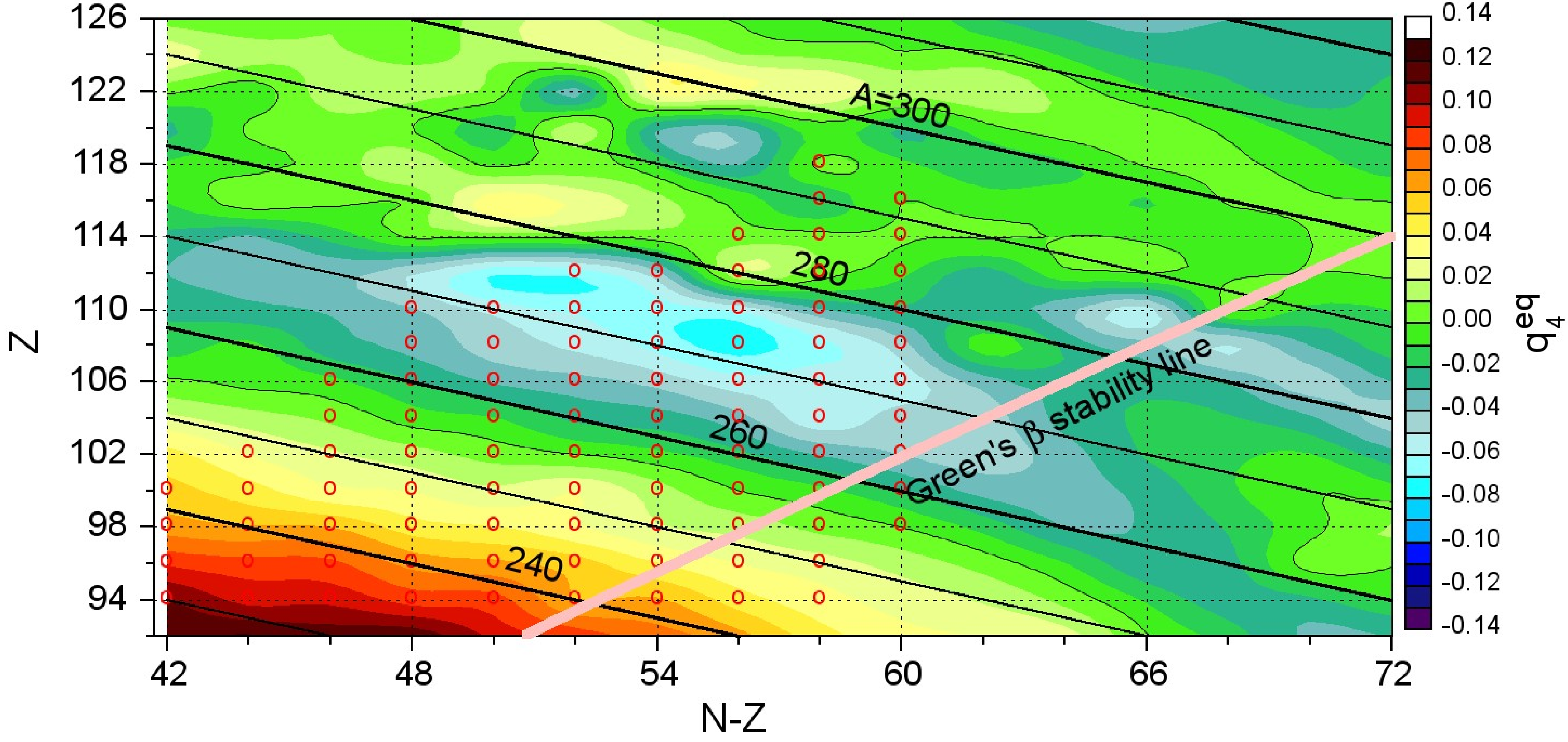
Microscopic energy correction: $E^{gs}_{micr} = E^{gs}_{tot} - E^{sph}_{LSD}$



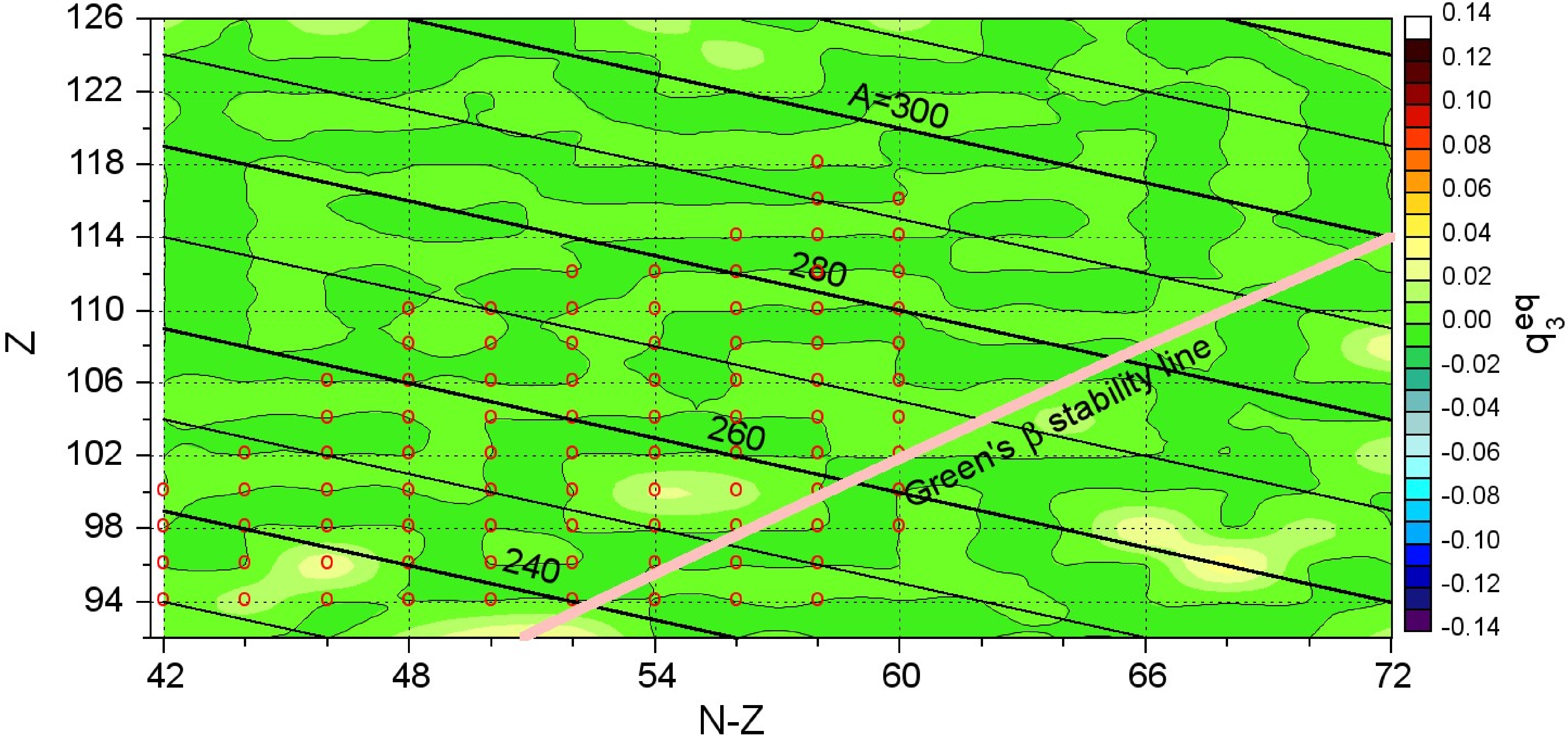
Ground state *quadrupole* deformation



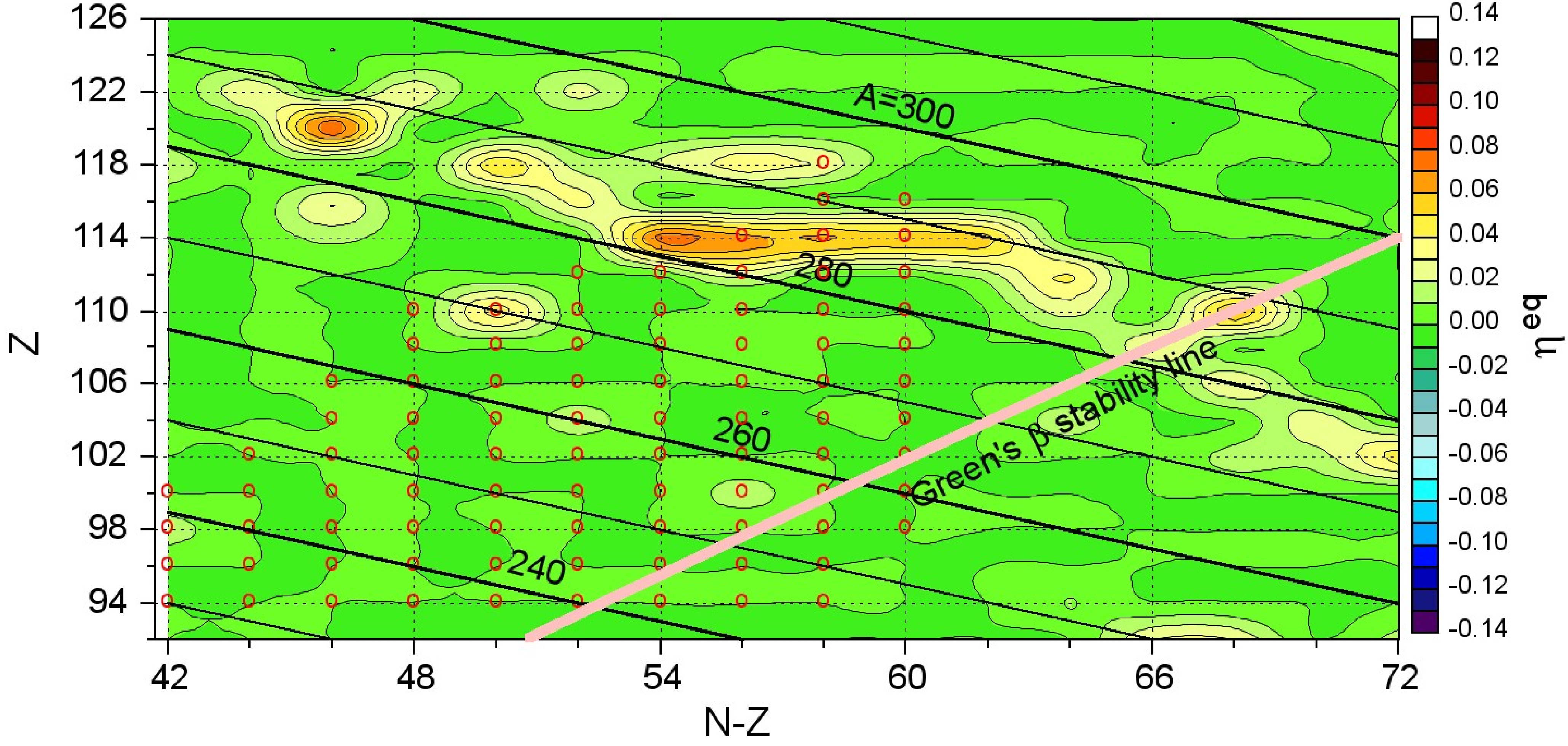
Ground state *hexadecapole* deformation



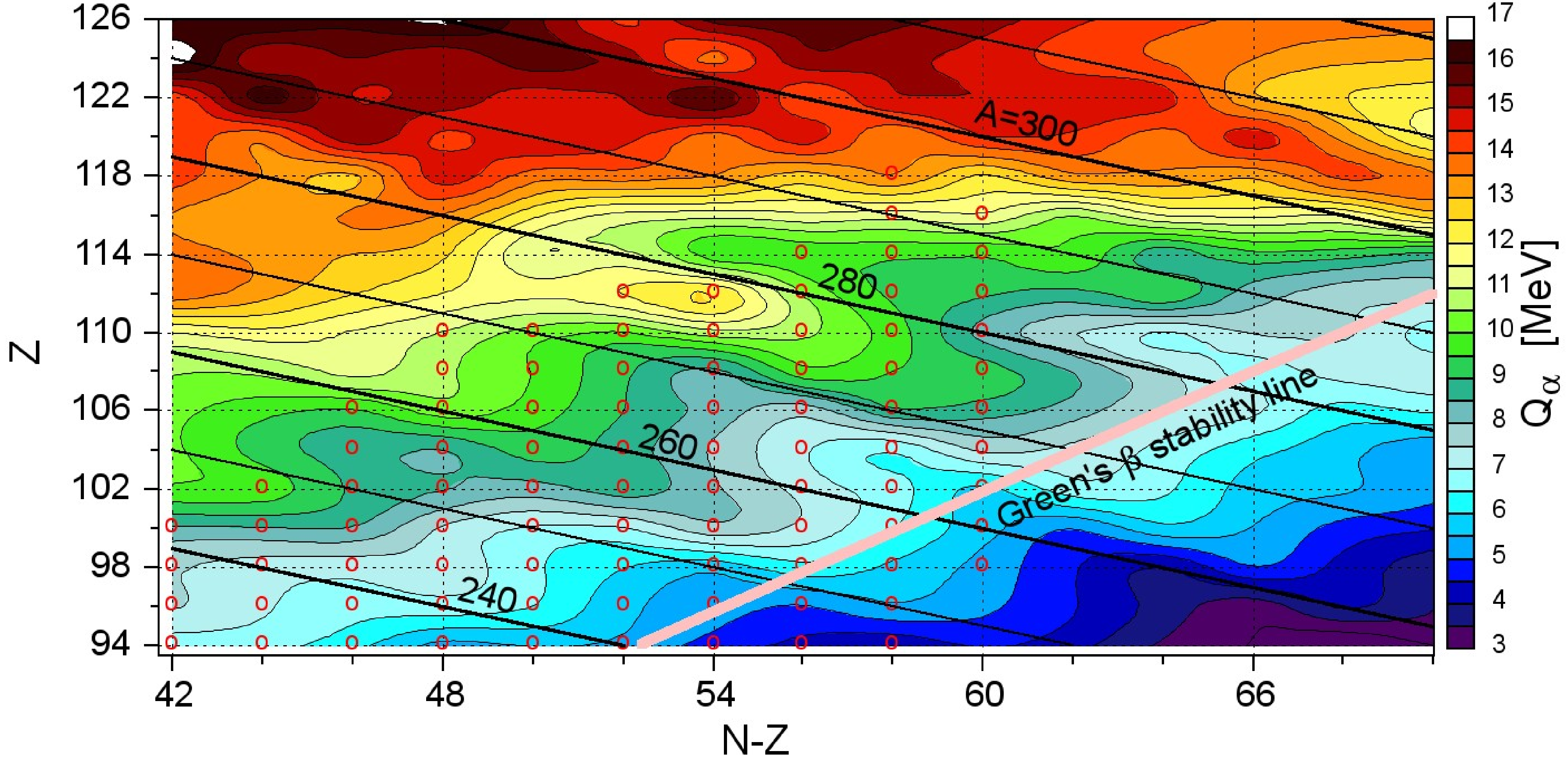
Ground state *octupole* deformation



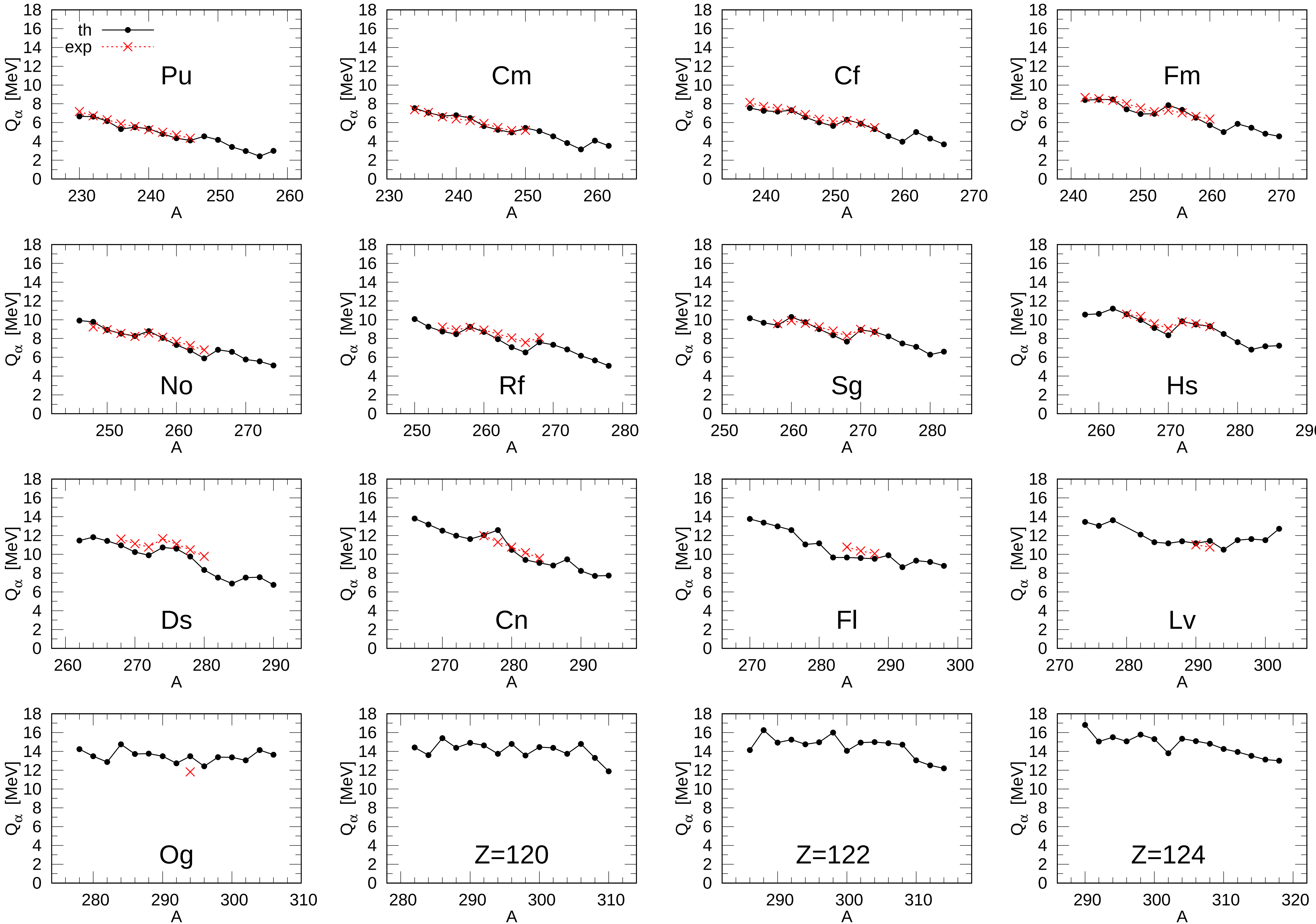
Ground state nonaxial deformation



Alpha particle energy Q_α

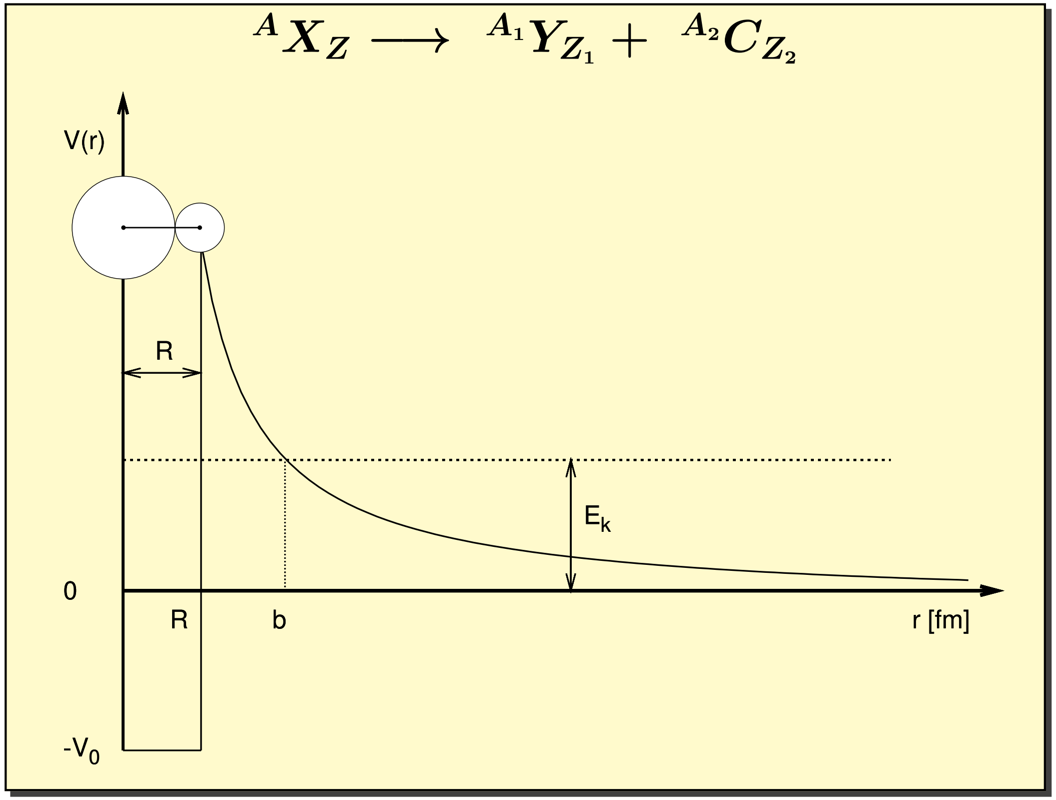


The r.m.s. deviation of Q_α for Z$\geq$ 94 is 0.51 MeV only.



th
exp
Pu
Cm
Cf
Fm
No
Rf
Sg
Hs
Ds
Cn
Fl
Lv
Og
Z=120
Z=122
Z=124
Q_α [MeV]
A

Gamow like model of the alpha decay and cluster radioactivity*



The half-life of a decaying nuclei is given by:

$$T_{1/2} = \frac{\ln 2}{\lambda} \cdot 10^h$$

Here h is a hindrance factor for o-o or o-e nuclei ($h = 0$ for e-e) and $\lambda = \nu P$, where ν is the number of assaults against the barrier.
Within the WKB theory the probability of the barrier penetration P is equal to:

$$P = \exp\left[-\frac{2}{\hbar}\int_R^b \sqrt{2\mu(V(r) - E_{\mathrm{k}})}\, dr\right] .$$

Here μ is the reduced mass of emitted particle.
The exit point from the barrier b corresponds to point, where the Coulomb potential is equal to the kinetic energy (E_{k}).

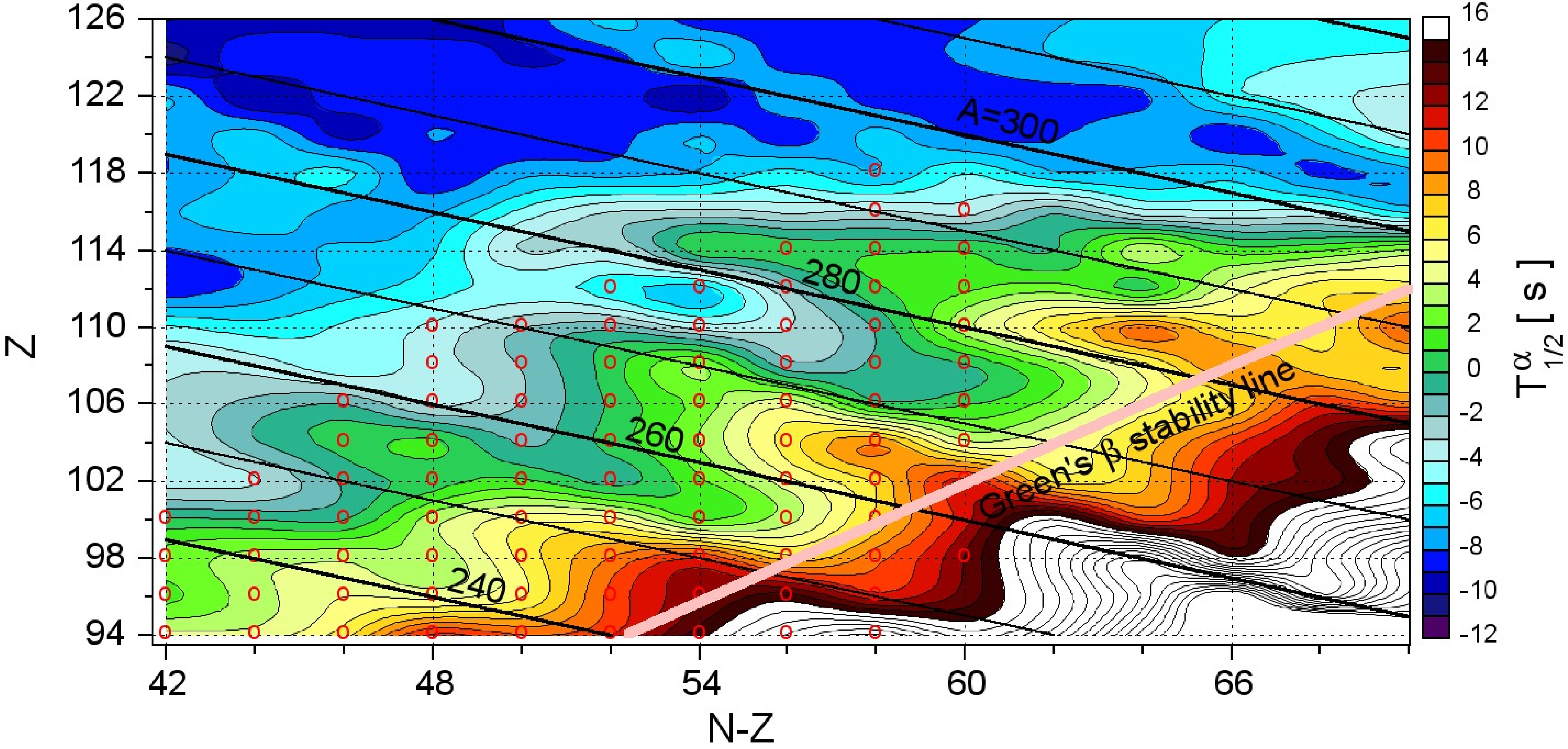
The probability of tunnelling of the above barrier is given by:

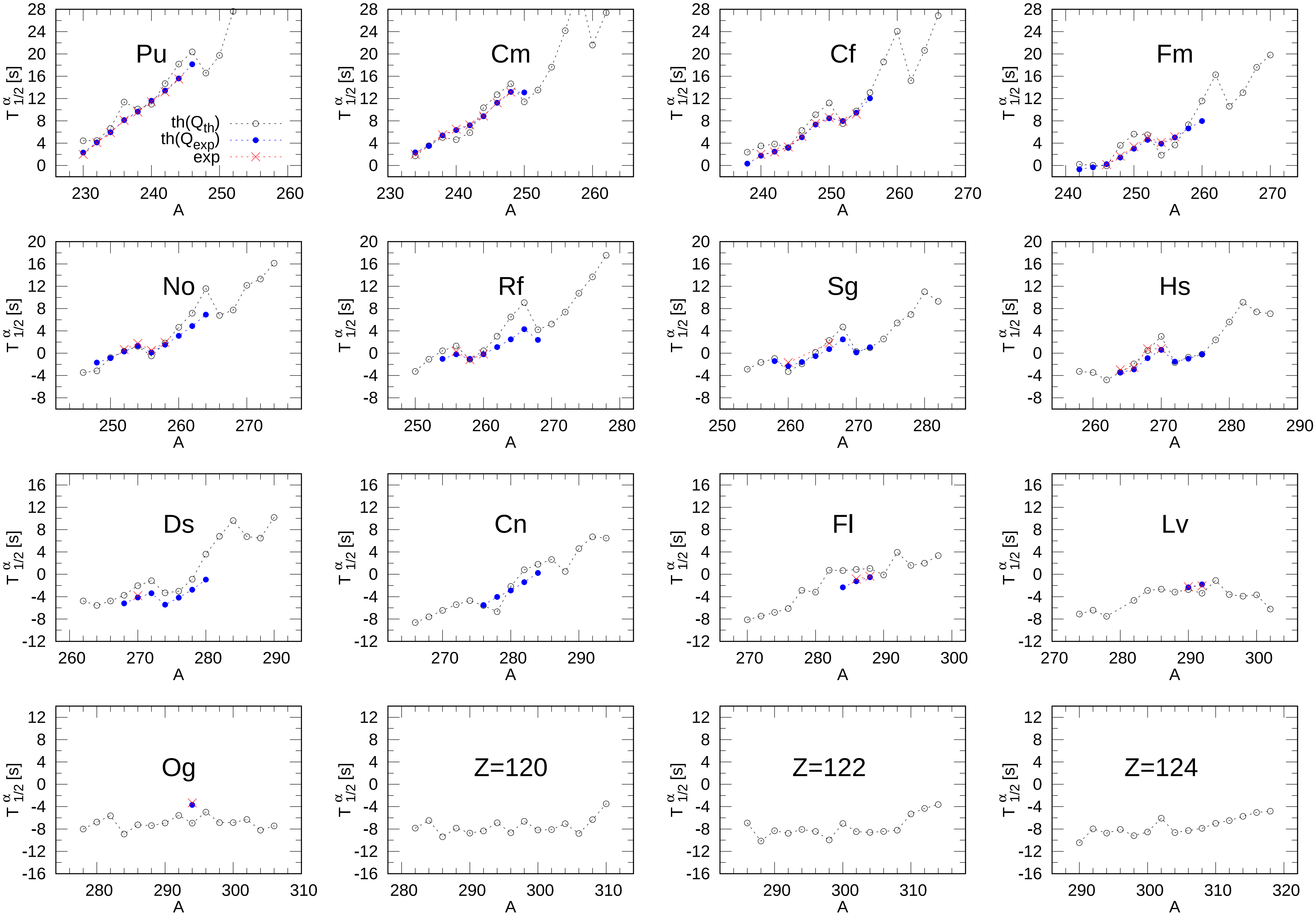
$$P = \exp\left\{-\frac{2}{\hbar}\sqrt{2\mu Z_1 Z_2 e^2 b}\left[\arccos\sqrt{\frac{R}{b}} - \sqrt{\frac{R}{b} - \left(\frac{R}{b}\right)^2}\right]\right\}$$

Here $R = r_0(A_1^{1/3} + A_2^{1/3})$. In the g.s. of a square well potential one has $\nu = \frac{\pi\hbar}{2\mu R^2}$.

* A. Zdeb, M. Warda, and K. Pomorski, Phys. Rev. C **87**, 024308 (2013).

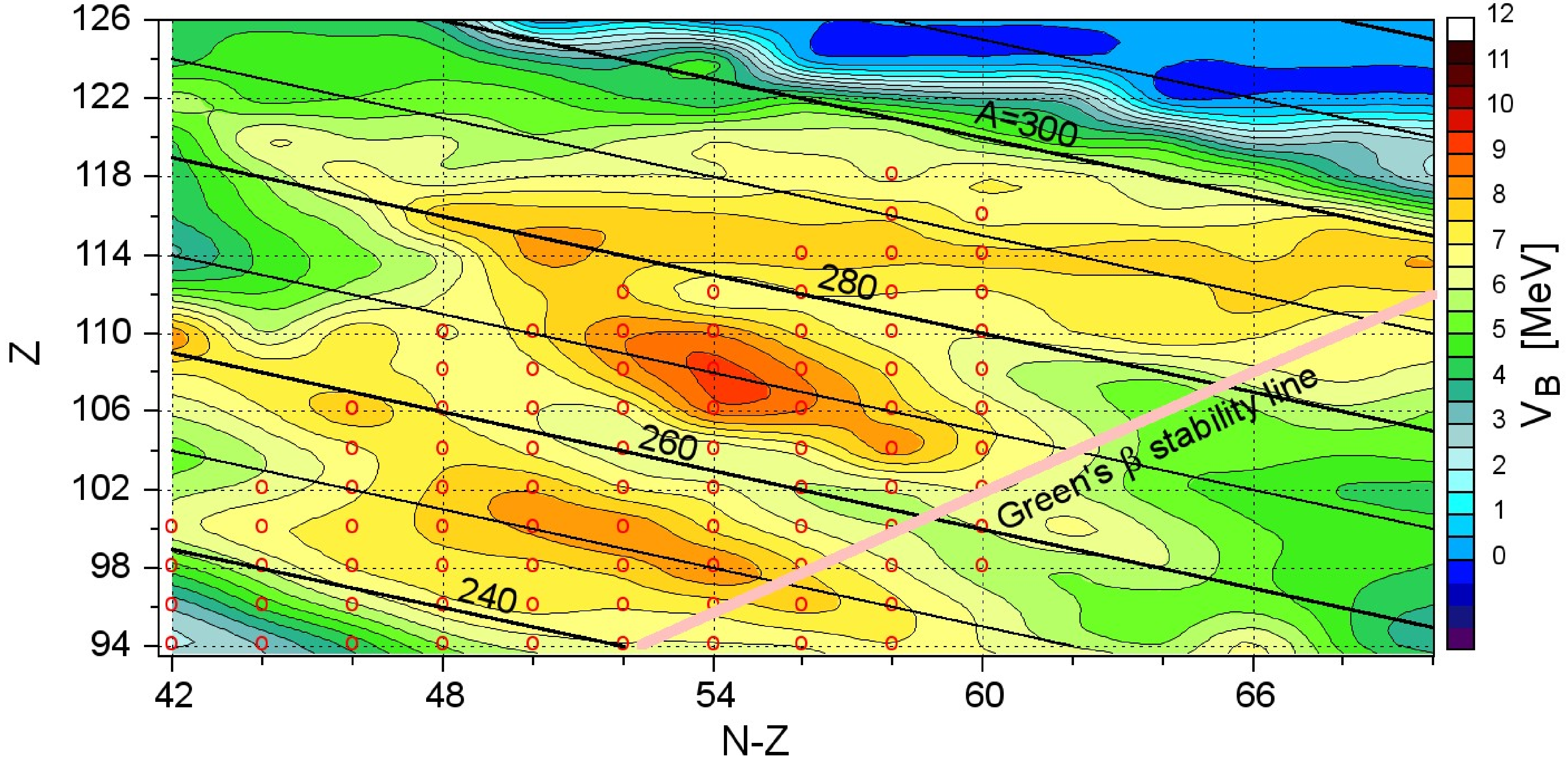
Prediction of the α-decay half-lives

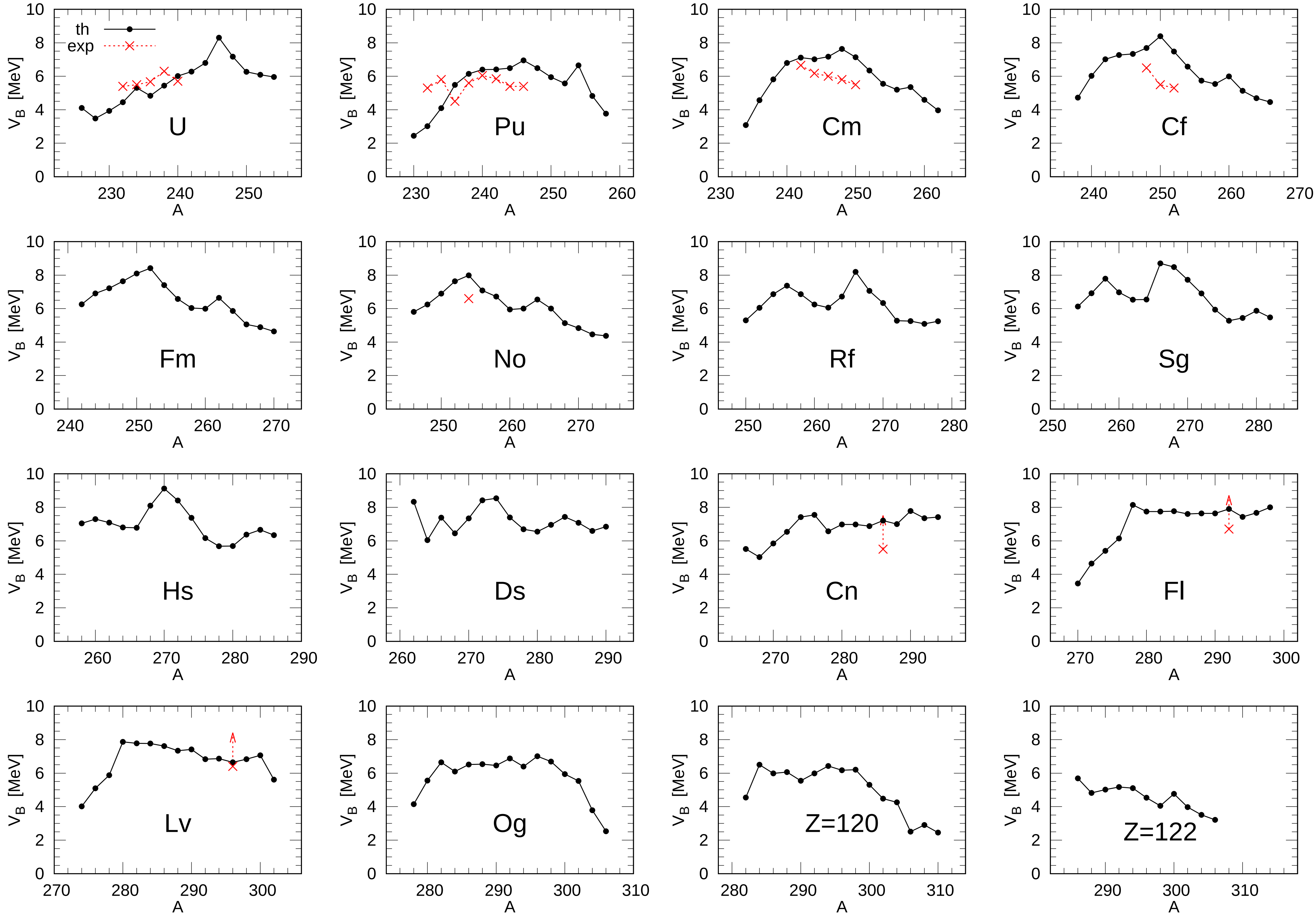




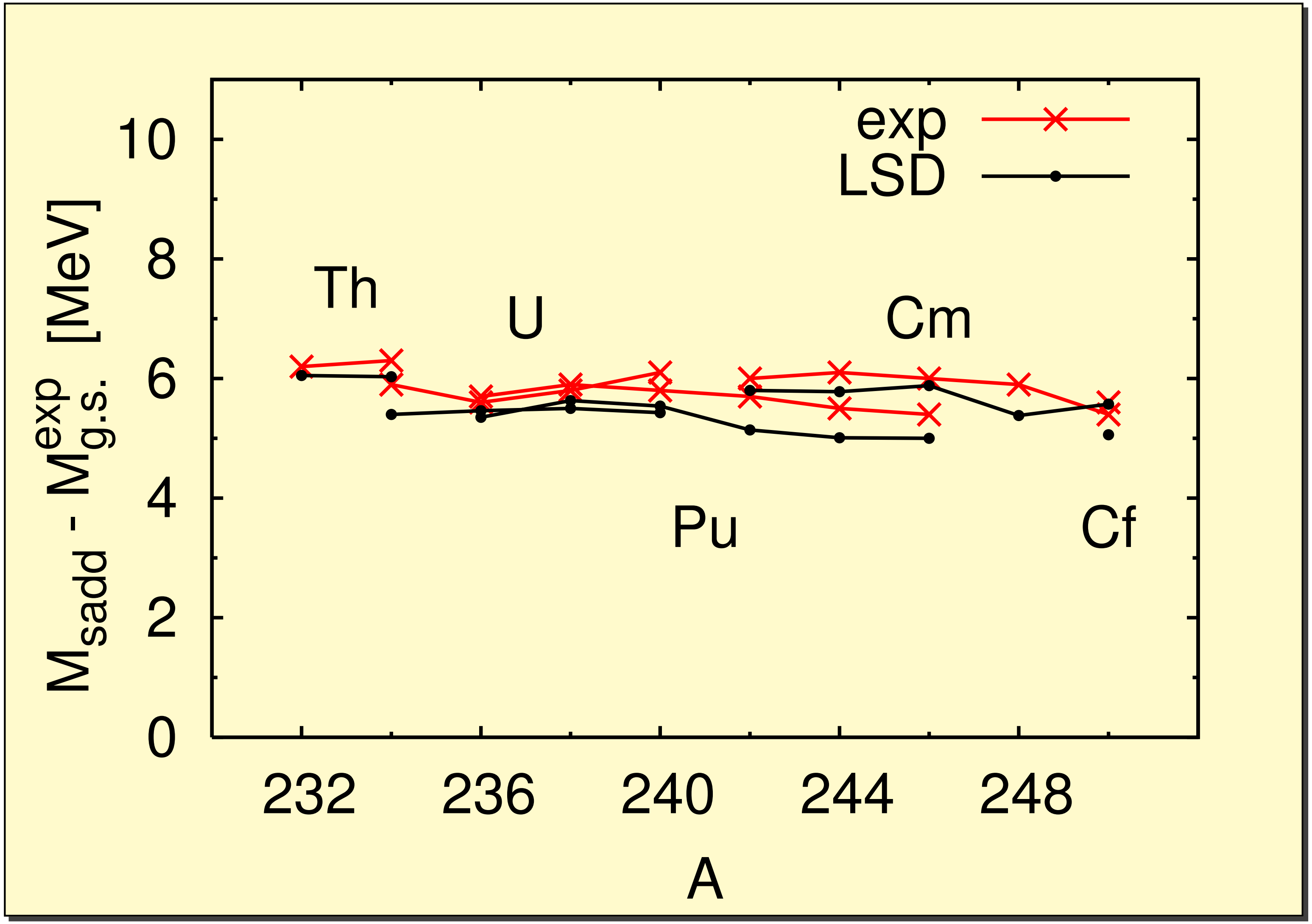
Pu
Cm
Cf
Fm
No
Rf
Sg
Hs
Ds
Cn
Fl
Lv
Og
Z=120
Z=122
Z=124
th(Q_th)
th(Q_exp)
exp
T^α_1/2 [s]
A

Fission barrier heights




th
exp
U
Pu
Cm
Cf
Fm
No
Rf
Sg
Hs
Ds
Cn
Fl
Lv
Og
Z=120
Z=122
V_B [MeV]
A

Nuclear fission and Świątecki topographical theorem



$$V_B = M^{\mathrm{exp}}_{\mathrm{sadd}} - M^{\mathrm{exp}}_{gs}$$

$$M^{\mathrm{exp}}_{\mathrm{sadd}} \approx M^{\mathrm{mac}}_{\mathrm{sadd}}$$

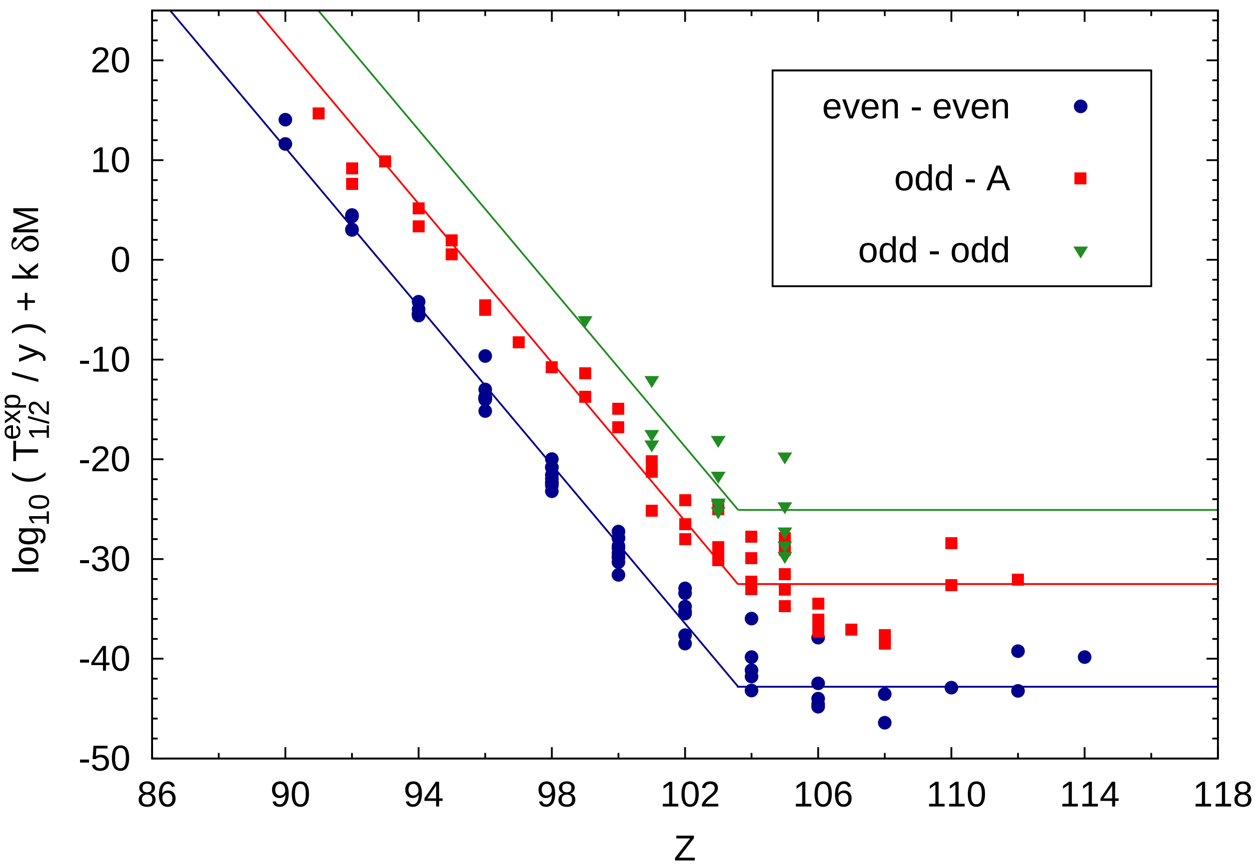
The agreement of the macroscopic saddle point masses with the data is striking. The average difference is only 310 keV ....

Władek Świątecki email from 9 Nov. 2006.

W. D. Myers, W.J. Świątecki, Nucl.Phys. **A612** (1997) 249. ← Topographical theorem

A. Dobrowolski, B. Nerlo-Pomorska, K. Pomorski, Acta Phys. Pol. **B40**, 705 (2009).

Spontaneous fission half-lives systematics *

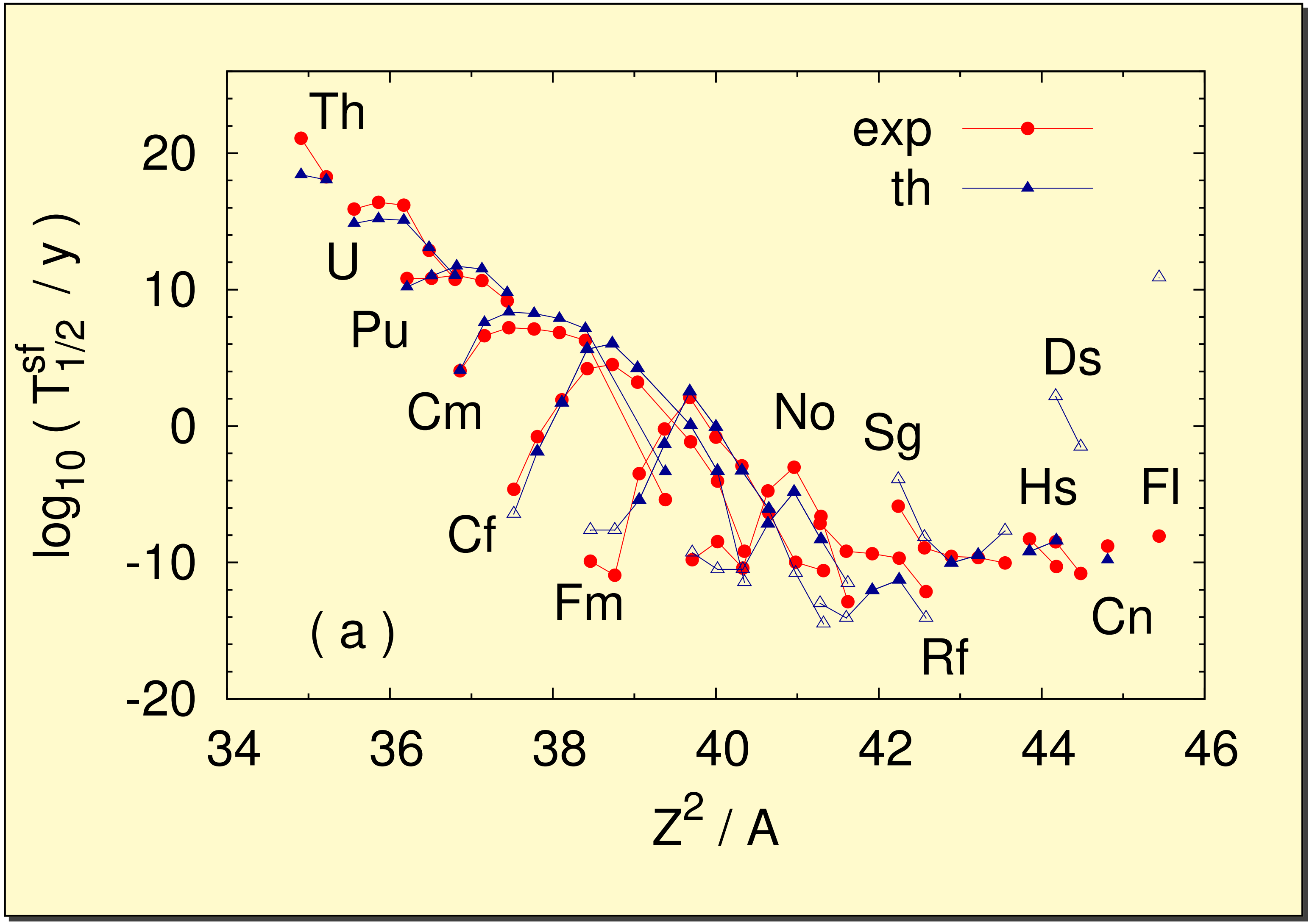


$\log T^{\rm sf}_{1/2} + 7.7 * \delta M(Z,A) = -4.1 \cdot \min(Z, 103) + 308.2$, where $\delta M = M_{\rm exp} - M_{\rm LSD}$.

Confer also: W.J. Świątecki, Phys. Rev. **100**, 937 (1955). $\to \log T^{\rm sf}_{1/2} = f(Z^2/A) - k\delta M(Z,A)$

*K. Pomorski, M. Warda and A. Zdeb, Acta Phys. Polon. **46**(2015) 4233.

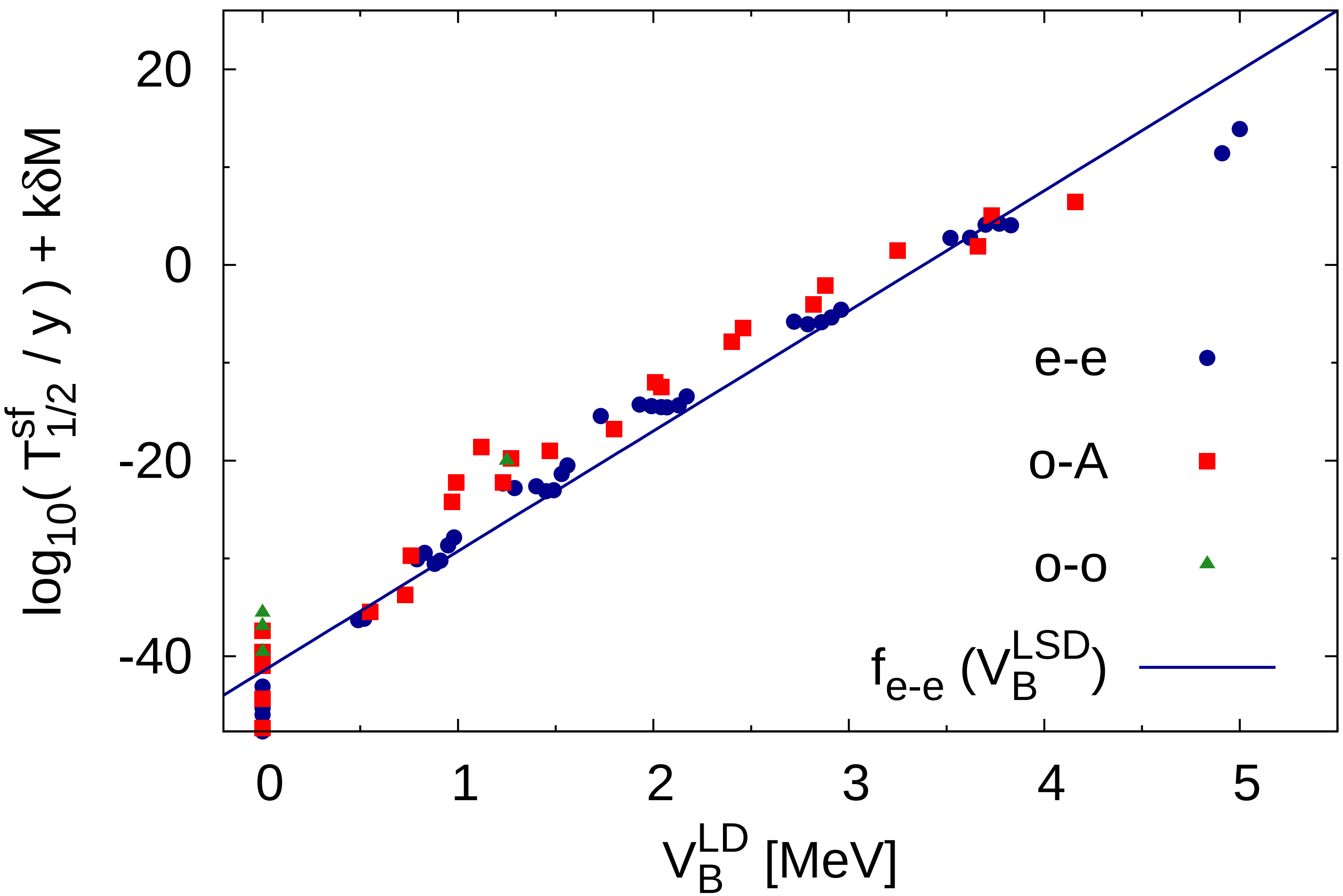
Spontaneous fission half-lives of e-e isotopes*



$$\log T^{\rm sf}_{1/2} = -4.1 \cdot \min(Z, 103) + 308.2 - 7.7 * (M_{\rm exp} - M_{\rm LSD}).$$

*K. Pomorski, M. Warda and A. Zdeb, Phys. Scr. **90** (2015) 114013.

Spontaneous fission half-lives and the LSD barrier heights*



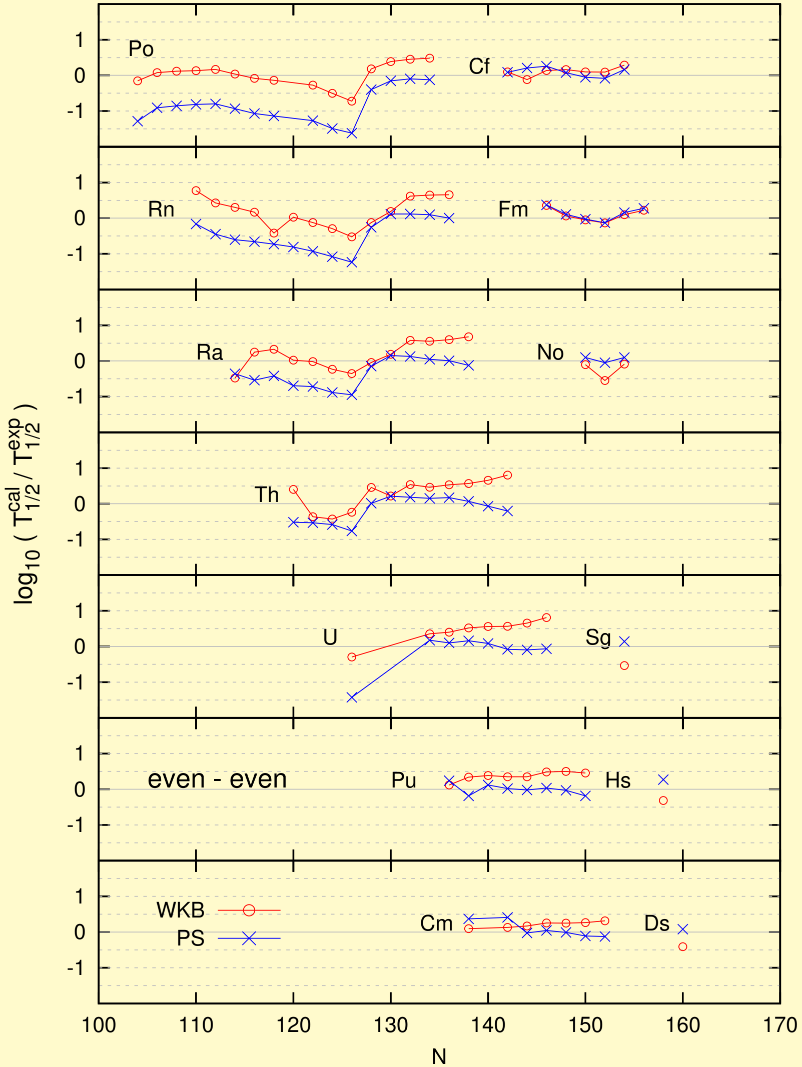
*K. Pomorski, M. Warda and A. Zdeb, Phys. Scr. **90** (2015) 114013.

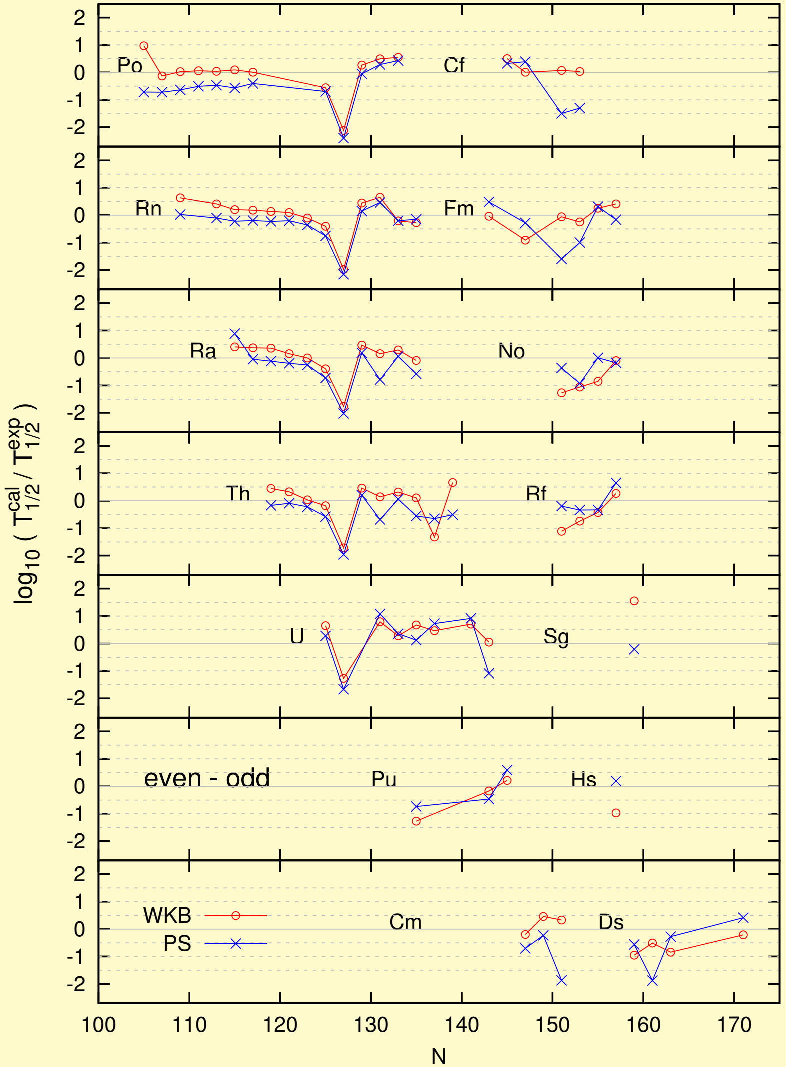
Conclusions:

- Fourier expansion offers a very effective way of describing the shapes of fissioning nuclei.
- Macroscopic-microscopic model basing on the LSD energy and the Yukawa-Folded s.p. potential describes well global properties of the heavy and super-heavy nuclei.
- Simple WKB model with only one adjustable parameter describes well the probabilities of proton, alpha and cluster emission.
- The ground-state shell and pairing effects determine the fission barrier heights. The role of those at the saddle is almost negligible.
- The spontaneous fission life-times of nuclei are mostly determined by the microscopic energy correction in the ground-state and the macroscopic fission barrier.

Thank you for your attention!

Deviations from the data of $\log(T_{1/2})$ for even-even nuclei

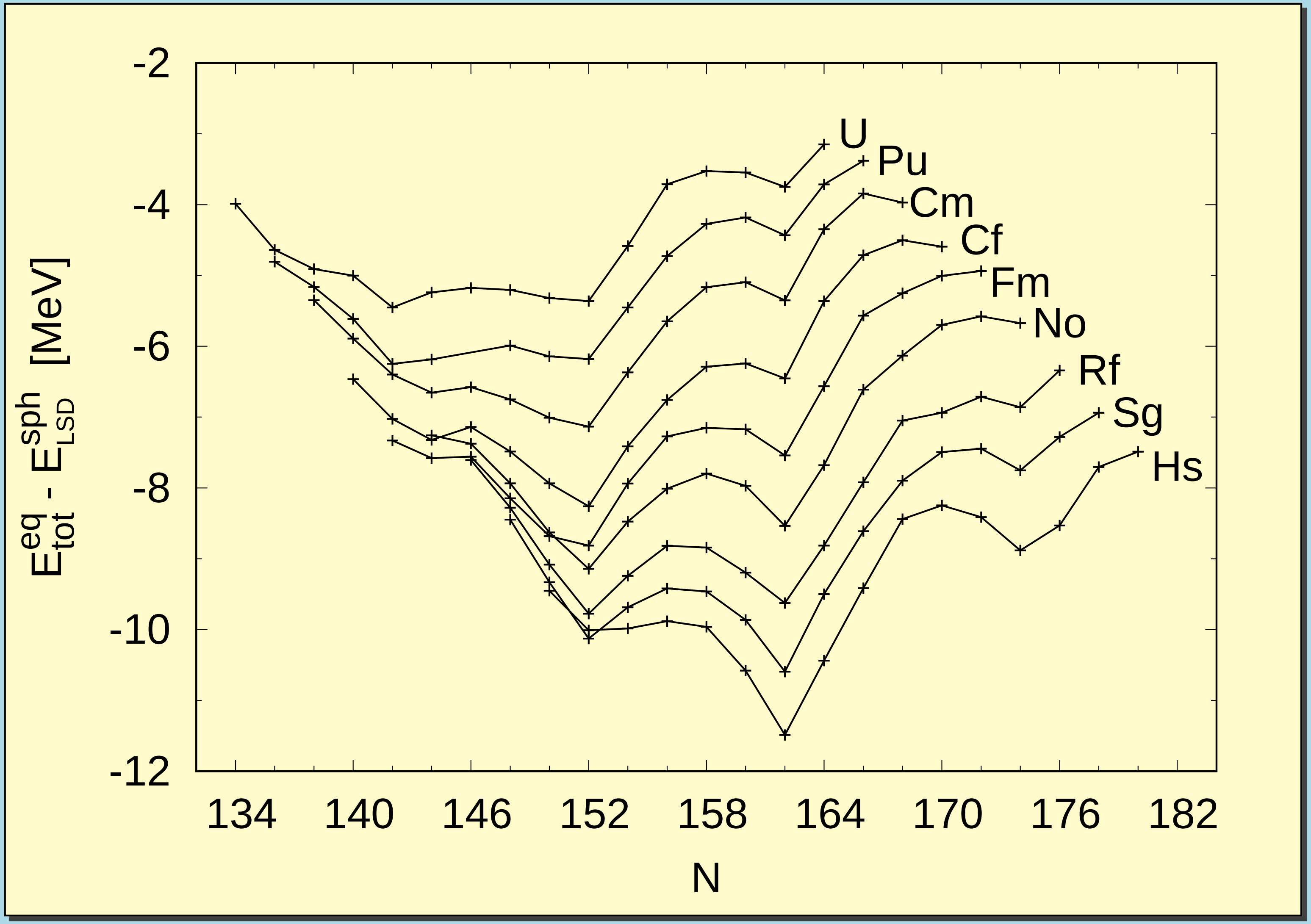




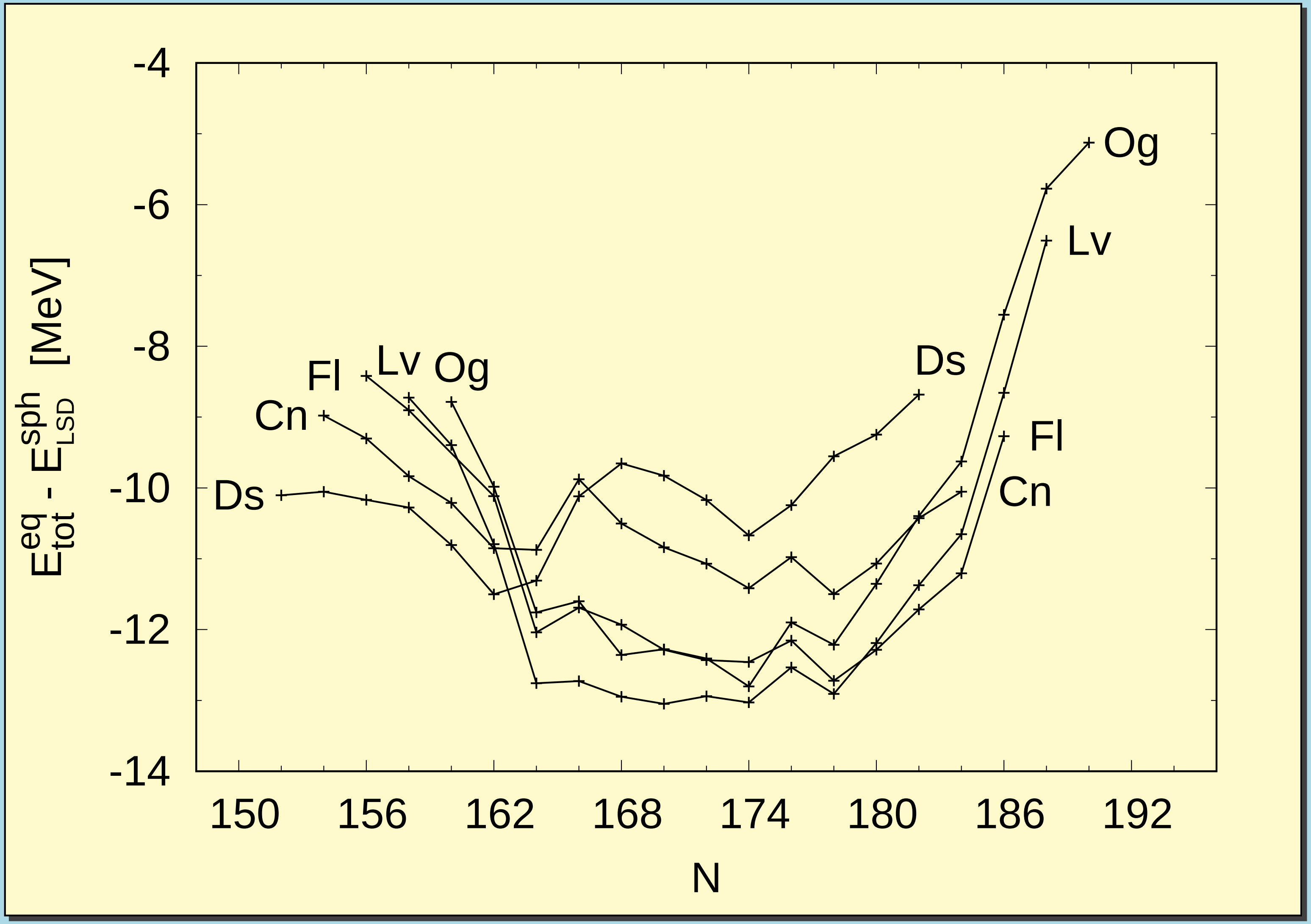
PS: A. Parkhomenko and A. Sobiczewski, Acta Phys. Polon. B **36**, 3095 (2005) $\longrightarrow$ 4 parameters,

WKB: A. Zdeb, M. Warda, K.P., Phys. Rev. C **87**, 024308 (2013) $\longrightarrow$ 1 parameter: r_0=1.21 fm.

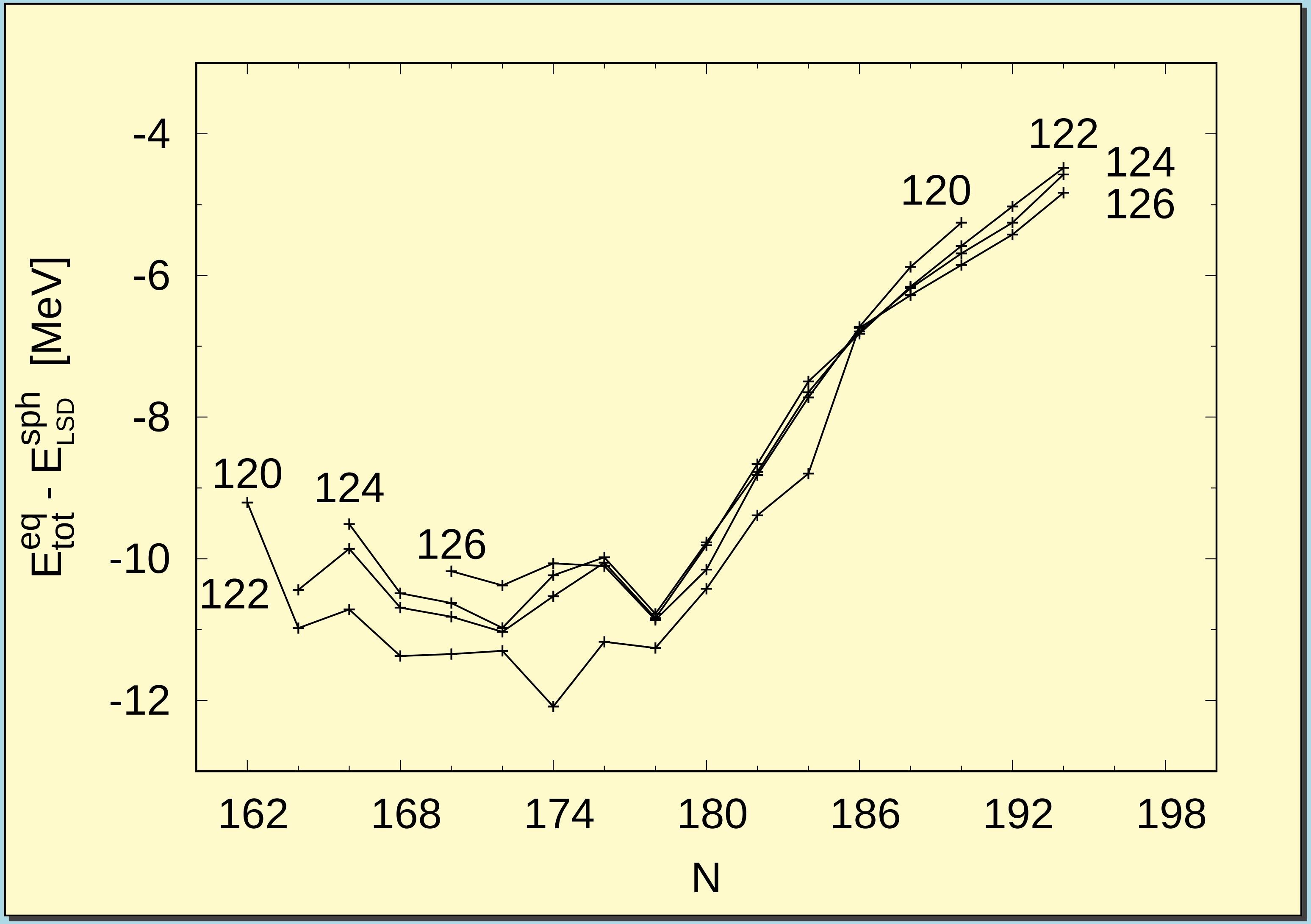
Microscopic energy correction to the LSD energy for spherical nucleus



Microscopic energy correction to the LSD energy for spherical nucleus

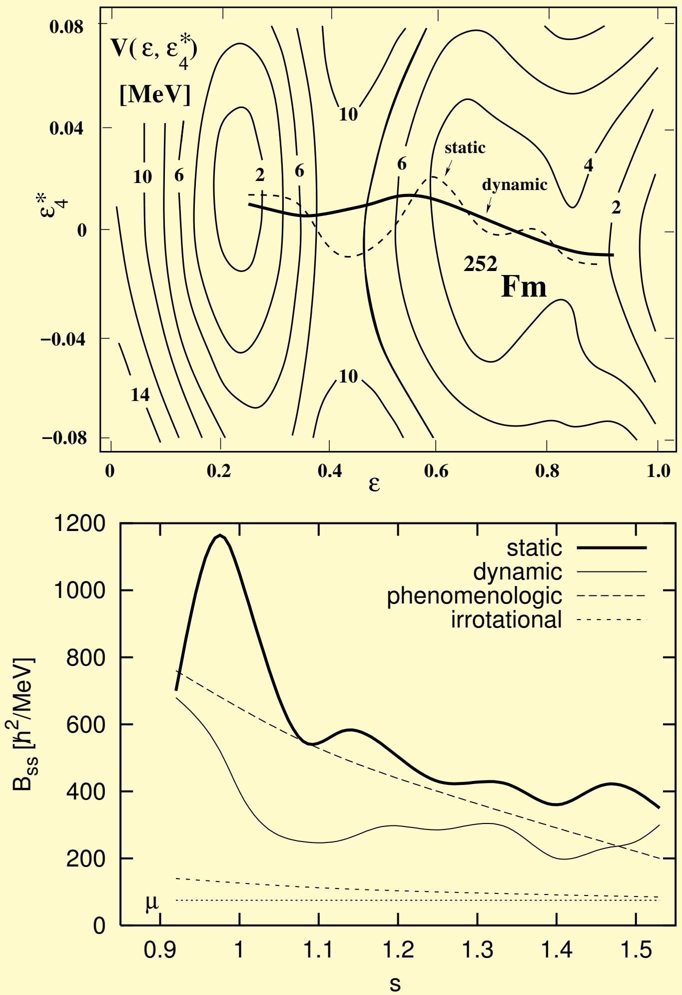


Microscopic energy correction to the LSD energy for spherical nucleus



Simple model for spontaneous fission probability *

A. Baran, K. Pomorski, A. Łukasiak, and A. Sobiczewski, Nucl. Phys. **A361**, 83 (1981).

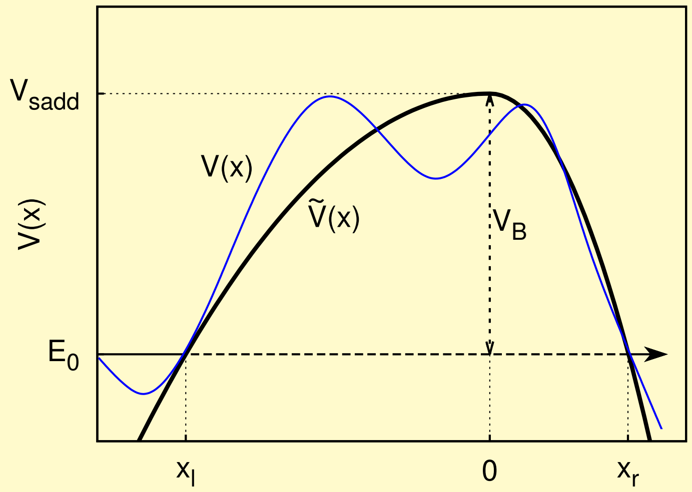


The transformation:

$$x(s) = \int_{s_{\rm sadd}}^{s} \sqrt{\frac{B_{ss}(s')}{m}}\, ds' \;,$$

ensures that $B_{xx} = m$=const.
The potential $V[s(x)]$ in the new coordinate x can be approximated by two (or more) parabolas:

$$\tilde{V}(x) = \begin{cases} V_{\rm sadd} - \frac{1}{2} C_l\, x^2 & \text{for } x < 0 \;, \\ V_{\rm sadd} - \frac{1}{2} C_r\, x^2 & \text{for } x > 0 \;, \end{cases}$$



*K. Pomorski, M. Warda and A. Zdeb, Phys. Scr. **90**, 114013 (2015).

Barrier penetration in the WKB approximation

The spontaneous fission half–life is given by:

$$T^{\rm sf}_{1/2} = \frac{\ln 2}{nP} \;, \quad \text{where} \quad P = \frac{1}{1 + \exp\{2S(L)\}.}$$

The WKB action-integral along the fission path $L(x)$ is given by:

$$S(L) = \int_{s_l}^{s_r} \sqrt{\frac{2}{\hbar^2} B_{ss}[V(s) - E_0]} ds \approx \int_{-x_l}^{x_r} \sqrt{\frac{2m}{\hbar^2}[\widetilde{V}(x) - E_0]}\, dx$$

For the penetration of the two-inverted parabola barrier of the V_B heights it is equal to:

$$S = \frac{\pi}{2\hbar} V_B \left(\sqrt{\frac{m}{C_l}} + \sqrt{\frac{m}{C_r}} \right) = \frac{\pi}{\hbar} V_B \, \frac{\omega_l + \omega_r}{2\,\omega_l\,\omega_r} \equiv \frac{\pi}{\hbar} V_B \, \tilde{\omega}^{-1} \;,$$

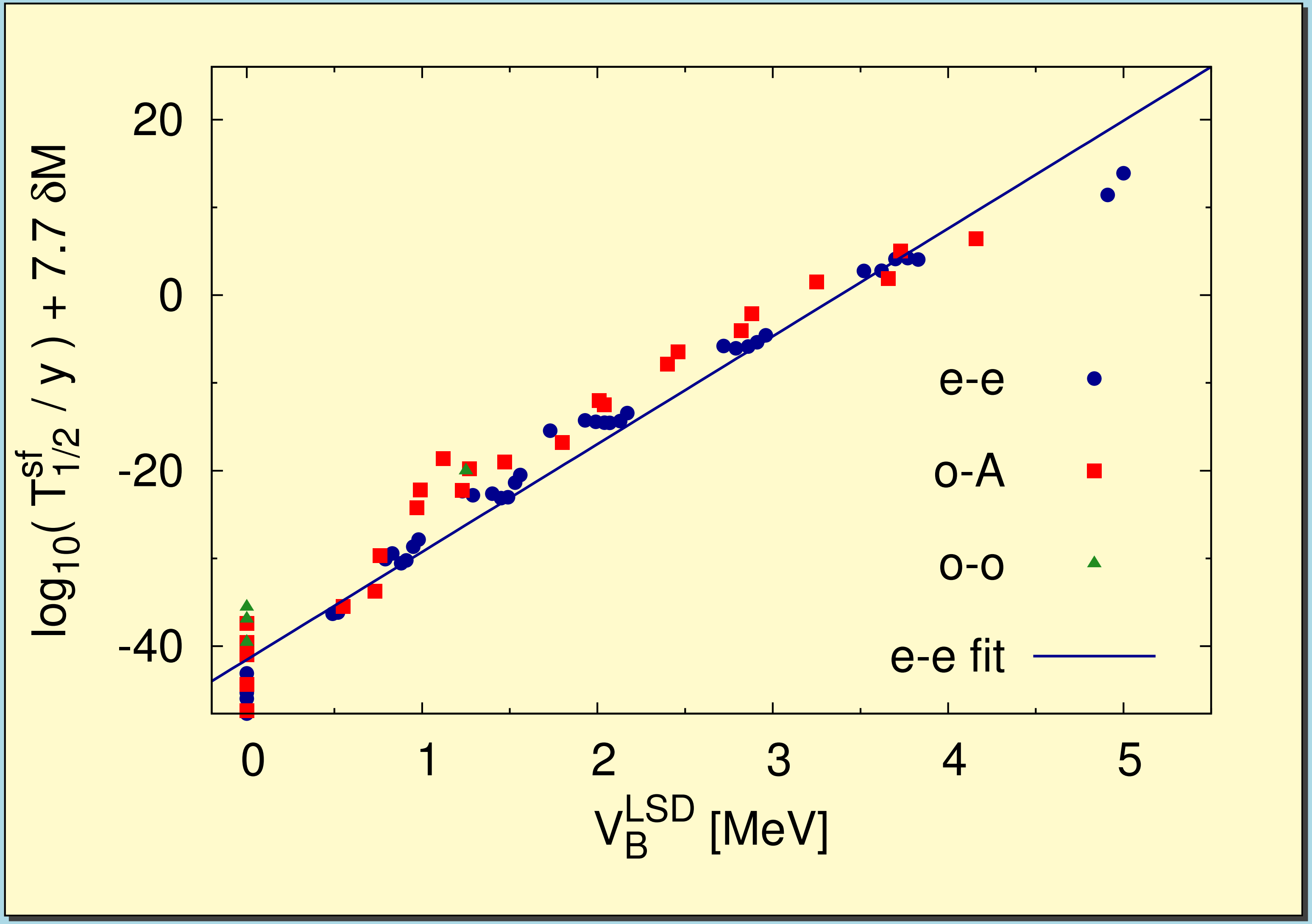
where $\omega_l = \sqrt{C_l/m}$ and $\omega_r = \sqrt{C_r/m}$ are the inverted H.O. frequencies.

For $S \gg 1$ the logarithm of the s.f. half-lives takes the form:

$$\boxed{\log(T^{\rm sf}_{1/2}) = \frac{2\pi}{\hbar\tilde{\omega}} V_B - \log[n \ln 2] \approx \frac{2\pi}{\hbar\tilde{\omega}} (M^{\rm LSD}_{\rm sadd} - M^{\rm exp}_{gs}) - \log[n \ln 2] \;,}$$

where n is the frequency of assaults against the fission barrier.

$$\log(T^{\rm sf}_{1/2}/{\rm y}) + \frac{2\pi\delta M}{\hbar\tilde{\omega}} = \frac{2\pi V_B^{\rm LSD}}{\hbar\tilde{\omega}} - \log(n \ln 2) \; ; \qquad \delta M = M_{\rm exp} - M^{\rm sph}_{\rm LSD}$$



K. Pomorski, M. Warda and A. Zdeb, Phys. Scr. **90** (2015) 114013.