INT13-3
2 Oct. 2013

Collective mass parameters in Skyrme EDF

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Key ingredients for spontaneous fission in nuclear EDF

Collective Hamiltonian describing the fission dynamics

$$\mathcal{H} = \frac{1}{2}\sum_{kl} M_{kl}(s)\dot{s}_k\dot{s}_l + V_{\rm coll}(s)$$

Dynamical variables $s = (s_1, s_2, \cdots) = (\beta, \gamma, \beta_3, \cdots)$

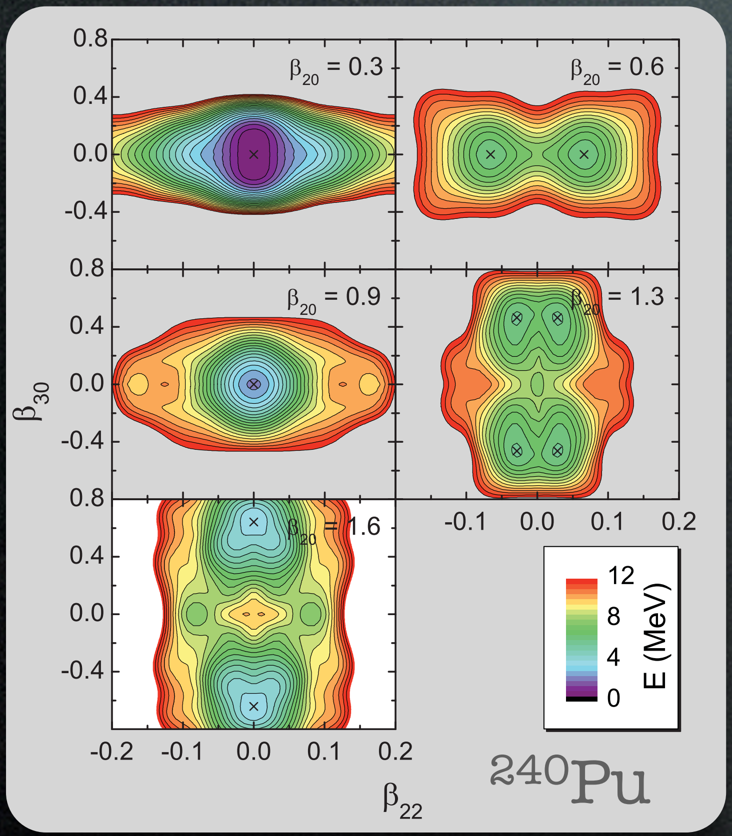
Collective potential $V_{\rm coll}(s)$

Inertia functions for the collective mode $M_{kl}(s)$

Collective potential

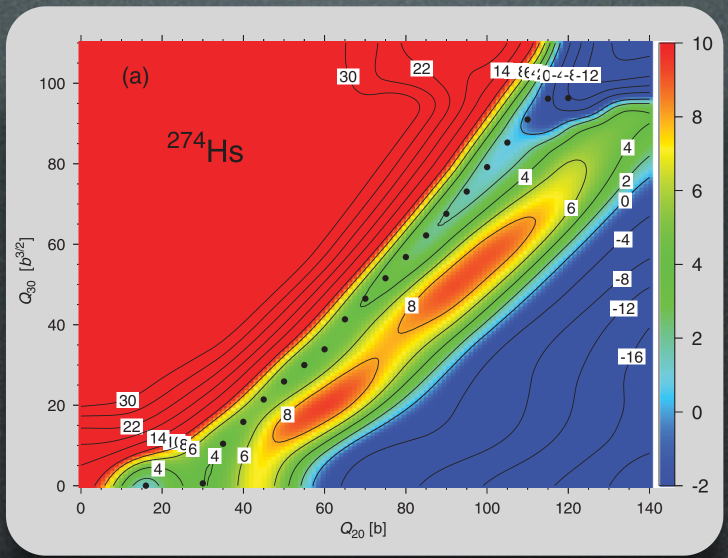
✓potential energy surface in multi-dimensional constrained EDF method

relativistic



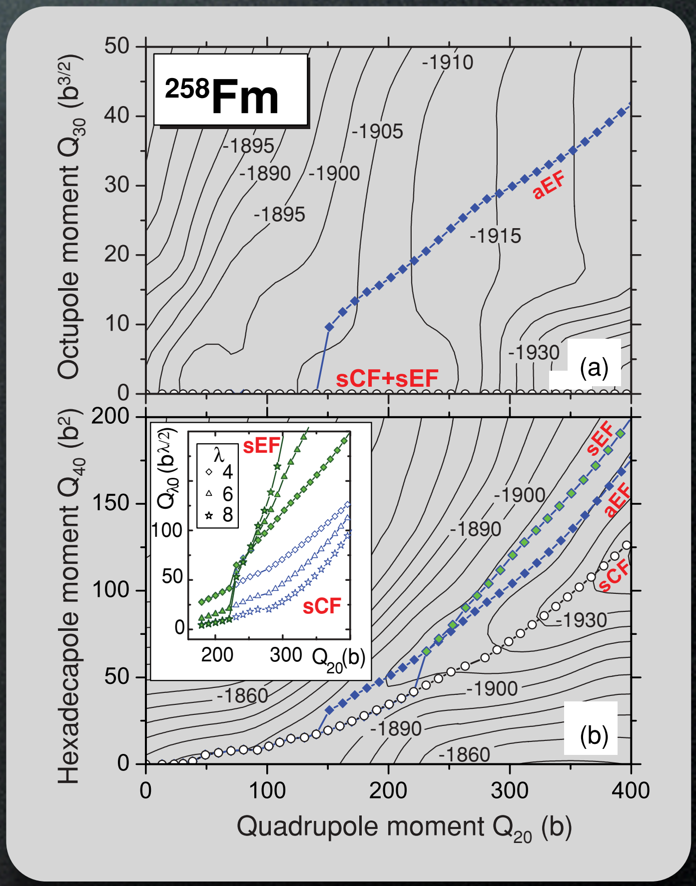
Lu, Zhao, Zhou, PRC85(2012)011301(R)

Gogny



Warda, Egido, PRC86(2012)014322

Skyrme



Staszczak, Baran, Dobaczewski, Nazarewicz, PRC85(2012)024314

✓continuous potential energy surface

toward a class-3 PES (talk by Dubray)

Microscopic collective-mass parameter

- GCM-GOA mass

  exact calculation (talk by Robledo)

- ATDHFB mass

$$\mathcal{M}_{ij} = \frac{i}{2\dot{q}_i\dot{q}_j}\mathrm{Tr}(F^{i*}Z^j - F^i Z^{j*}). \qquad (34)$$

time-odd fields neglected

Cranking approximation

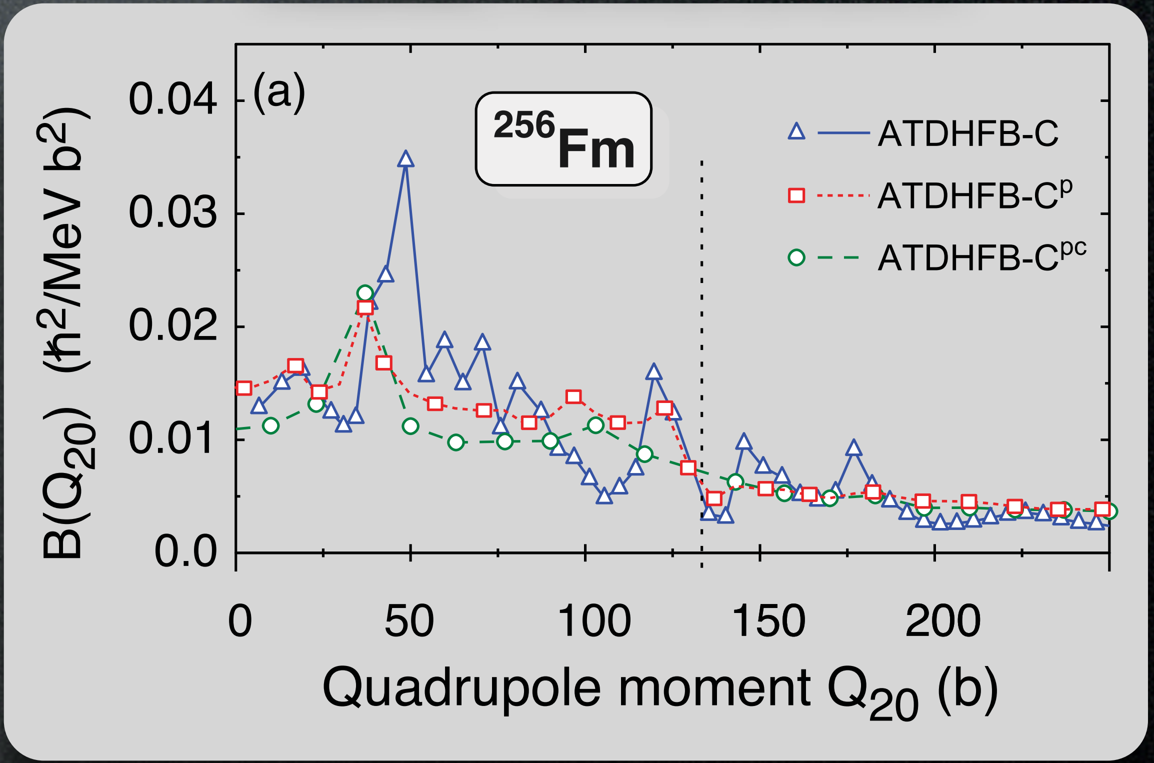
$$\mathcal{M}^C_{ij} = \frac{1}{2\dot{q}_i\dot{q}_j}\sum_{\alpha\beta}\frac{(F^{i*}_{\alpha\beta}F^j_{\alpha\beta} + F^i_{\alpha\beta}F^{j*}_{\alpha\beta})}{E_\alpha + E_\beta}$$

Perturbative cranking

$$\mathcal{M}^{C^p} = \frac{1}{4}[M^{(1)}]^{-1}M^{(3)}[M^{(1)}]^{-1}$$

$$M^{(K)}_{ij} = \sum_{\alpha\beta}\frac{\langle 0|\hat{Q}_i|\alpha\beta\rangle\langle\alpha\beta|\hat{Q}^\dagger_j|0\rangle}{(E_\alpha + E_\beta)^K}$$

Baran, Sheikh, Dobaczewski, Nazarewicz, Staszczak, PRC85(2012)024314



Local QRPA method

Hinohara, Sato, Nakatsukasa, Matsuo, Matsuyanagi, PRC82(2010)064313

CHFB eq.

$$\delta\langle\phi(s)|\hat{H}_{\rm CHFB}|\phi(s)\rangle = 0 \quad \rightarrow \quad |\phi(s)\rangle$$

$$V_{\rm coll}(s) = \langle\phi(s)|\hat{H}_{\rm HFB}|\phi(s)\rangle$$

$$\hat{H}_{\rm CHFB} = \hat{H}_{\rm HFB} - \sum_i \mu_i \hat{s}_i$$

Local harmonic approximation at each state $|\phi(s)\rangle$

$$\delta\langle\phi(s)|[\hat{H}_{\rm CHFB}, \hat{Q}_\mu(s)] - \frac{1}{i}\hat{P}_\mu(s)|\phi(s)\rangle = 0$$

$$\delta\langle\phi(s)|[\hat{H}_{\rm CHFB}, \frac{1}{i}\hat{P}_\mu(s)] - C_\mu(s)\hat{Q}_\mu(s)|\phi(s)\rangle = 0$$

✦collective mode generated self-consistently
✦time-odd effects taken into account

Collective kinetic energy

$$\mathcal{T} = \frac{1}{2}\sum_i (\dot{q}_i)^2$$

$$= \frac{1}{2}\sum_i \sum_{kl} \frac{\partial q_i}{\partial s_k}\frac{\partial q_i}{\partial s_l}\dot{s}_k \dot{s}_l \equiv \frac{1}{2}\sum_{kl} M_{kl}(s)\dot{s}_k\dot{s}_l$$

Note that the infinitesimal displacement of the collective coordinates brings about a corresponding change;

$$ds_k = \sum_i \frac{\partial s_k}{\partial q_i} dq_i$$

derivative w.r.t. the collective coordinate q_i

$$\frac{\partial s_k}{\partial q_i} = \frac{\partial}{\partial q_i}\langle \phi(s)|\hat{s}_k|\phi(s)\rangle$$

$$= \langle \phi(s)| \left[\hat{s}_k, \frac{1}{i}\hat{P}_i(s)\right] |\phi(s)\rangle$$

not in need of numerical derivative

Numerical implementation with use of Skyrme EDF

KY, Hinohara, PRC83(2011)061302(R)

Skyrme + pairing EDF: $E[\varrho(\boldsymbol{r}), \tilde{\varrho}(\boldsymbol{r})]$

CHFB eq. in cylindrical coordinates assuming the axial, reflection symmetries

$\boldsymbol{r} = (\rho, z, \phi)$

$$\begin{pmatrix} h(\boldsymbol{r}\sigma) - \lambda & \tilde{h}(\boldsymbol{r}\sigma) \\ \tilde{h}(\boldsymbol{r}\sigma) & -h(\boldsymbol{r}\sigma) + \lambda \end{pmatrix} \begin{pmatrix} \varphi_{1,\alpha}(\boldsymbol{r}\sigma) \\ \varphi_{2,\alpha}(\boldsymbol{r}\sigma) \end{pmatrix} = E_\alpha \begin{pmatrix} \varphi_{1,\alpha}(\boldsymbol{r}\sigma) \\ \varphi_{2,\alpha}(\boldsymbol{r}\sigma) \end{pmatrix}$$

Mean field (ph) and pair field (pp): β constraint

$$h = \frac{\delta E}{\delta \varrho} - \mu q_{20}, \qquad \tilde{h} = \frac{\delta E}{\delta \tilde{\varrho}}$$

LQRPA eq. in the matrix form (P-Q representation)

$$(A - B) Q_\mu = \frac{1}{i} P_\mu$$

$$(A + B) \frac{1}{i} P_\mu = \omega_\mu^2 Q_\mu$$

→

$$(A + B)(A - B) Q_\mu = \omega_\mu^2 Q_\mu$$

applicable to the situation where the eigen-frequencies of the local normal modes are imaginary

Quadrupole collective mass $M_{\beta\beta}(\beta)$ in the LQRPA

- choose "the most collective mode" out of numerous eigenmodes

  practically, the mode possessing the smallest quadrupole mass
  in the low-frequency region of $\omega_i^2 < 15 \ \mathrm{MeV}^2$

- calculate the quadrupole collective mass

$$
\begin{aligned}
M_{Q_{20}Q_{20}}(\beta) &= \left(\frac{dq_i}{dQ_{20}}\right)^2 \\
&= \left|\langle\phi(\beta)|[\hat{Q}_{20}, \frac{1}{i}\hat{P}_i(\beta)|\phi(\beta)\rangle\right|^{-2} \\
&= \left[\frac{2}{i}\sum_{\alpha\alpha'} q_{20,\alpha\alpha'} P_{i,\alpha\alpha'}(\beta)\right]^{-2} \\
&= \left[\sum_{\alpha\alpha'} B_{\alpha\alpha'}(\beta)\right]^{-2}
\end{aligned}
$$

Note:

$$M_{\beta\beta}(\beta) = \frac{1}{\eta^2} M_{Q_{20}Q_{20}}(\beta)$$

$$\eta = \sqrt{\frac{\pi}{5}}\frac{1}{\langle r^2\rangle}$$

$B_{\alpha\alpha'}(\beta)$ Microscopic structure of the collective mass

CHFB calculation: MPI parallelization

use of N processors

neutrons | protons

proc. 1, proc. 2, proc. N/2, proc. N/2+1, proc. N

$\Omega^\pi = 1/2^+$ $1/2^-$ $(N-2)/4^-$ $1/2^+$ $(N-2)/4^-$

diagonalization w/ lapack: dgeev

↓

proc. 1 — densities, hamiltonians

↓

proc. 1, proc. 2, proc. N/2, proc. N/2+1, proc. N

↓

iterations: Broyden

Baran et al., PRC78(2008)014318

QRPA calculation on parallel computer: MPI and BLACS

QRPA: use of N processors

matrix elements of the QRPA eq.: $A_{\alpha\beta\gamma\delta}$ $B_{\alpha\beta\gamma\delta}$

ScaLAPACK

2D-block cyclic distribution for load balancing

function: indxl2g for distribution
subroutine: pdsyev for diagonalization

Ex. dim. : 50,000 for K=0 in ^{240}Pu

	w/ 512 cores	1024 cores	2048 cores
matrix element:	14,000 secs	7,000 secs	3,600 secs
diagonalization:	1,400 secs	740 secs	680 secs
inversion :	21 secs	15 secs	13 secs

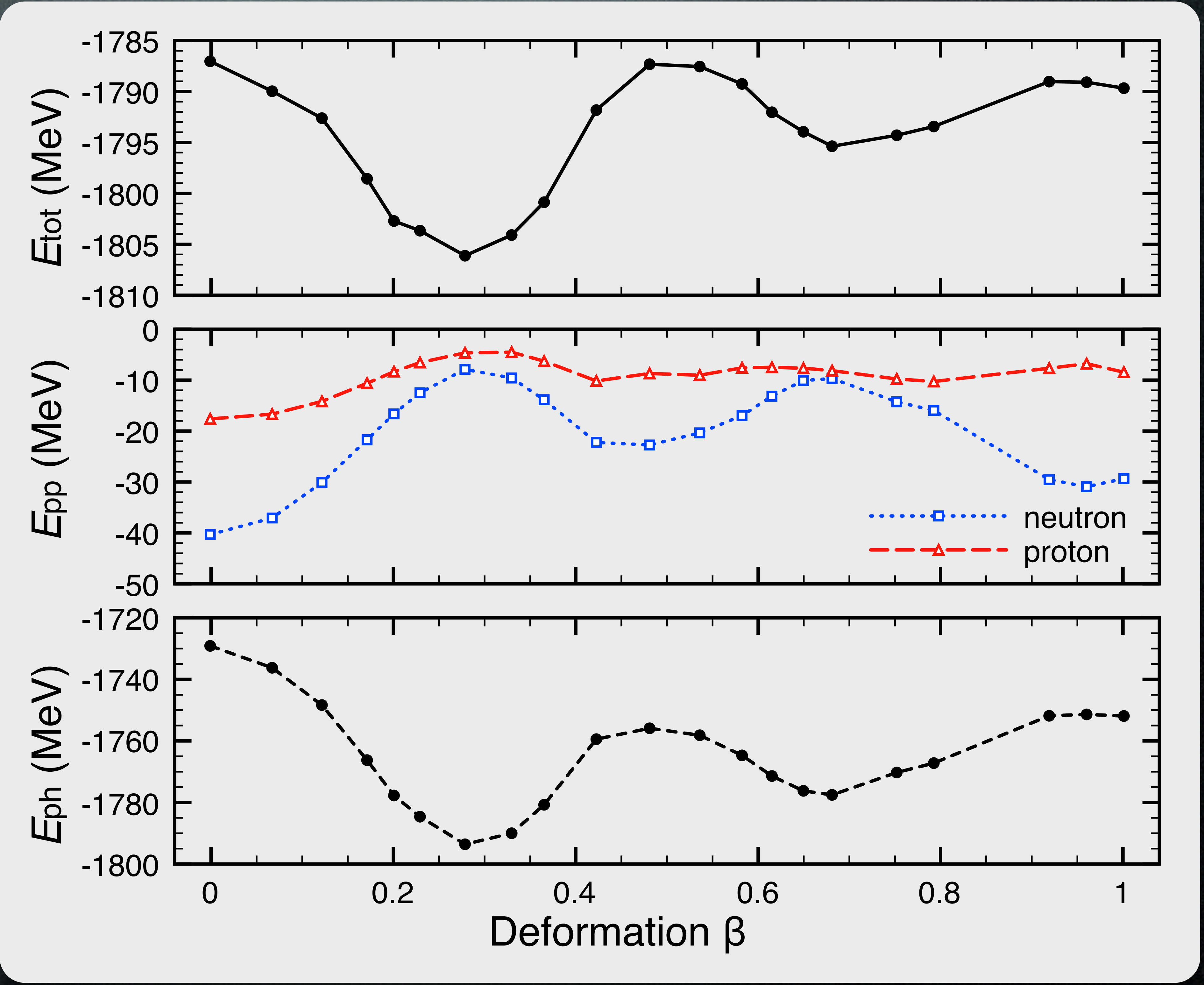
Numerical results for ^{240}Pu: Potential energy

SkM* +

pairing EDF

Yamagami, Shimizu, Nakatsukasa, PRC80(2009)064301

adjusted to pairing properties of well-deformed nuclei

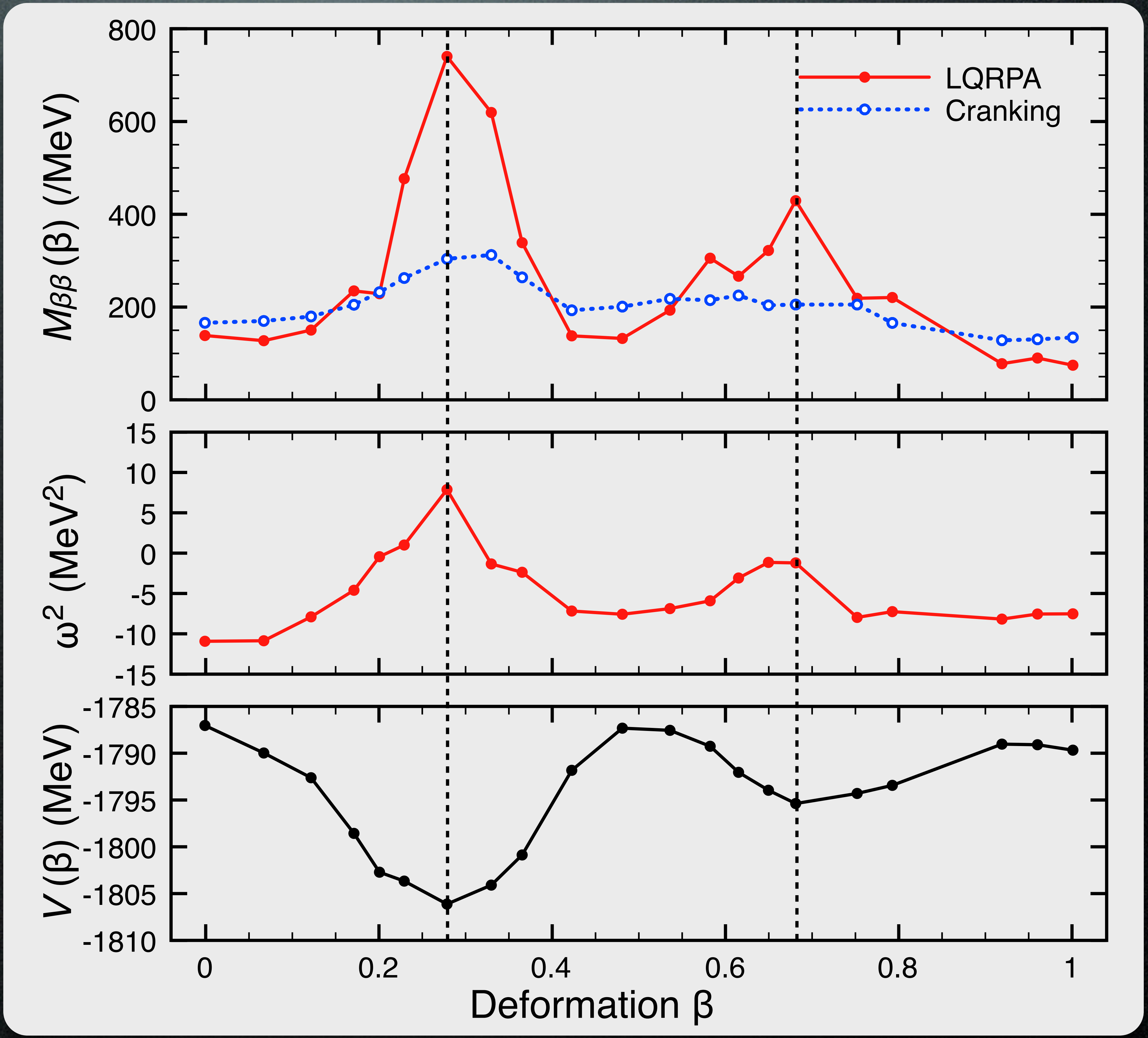


Quadrupole mass parameter in ^{240}Pu

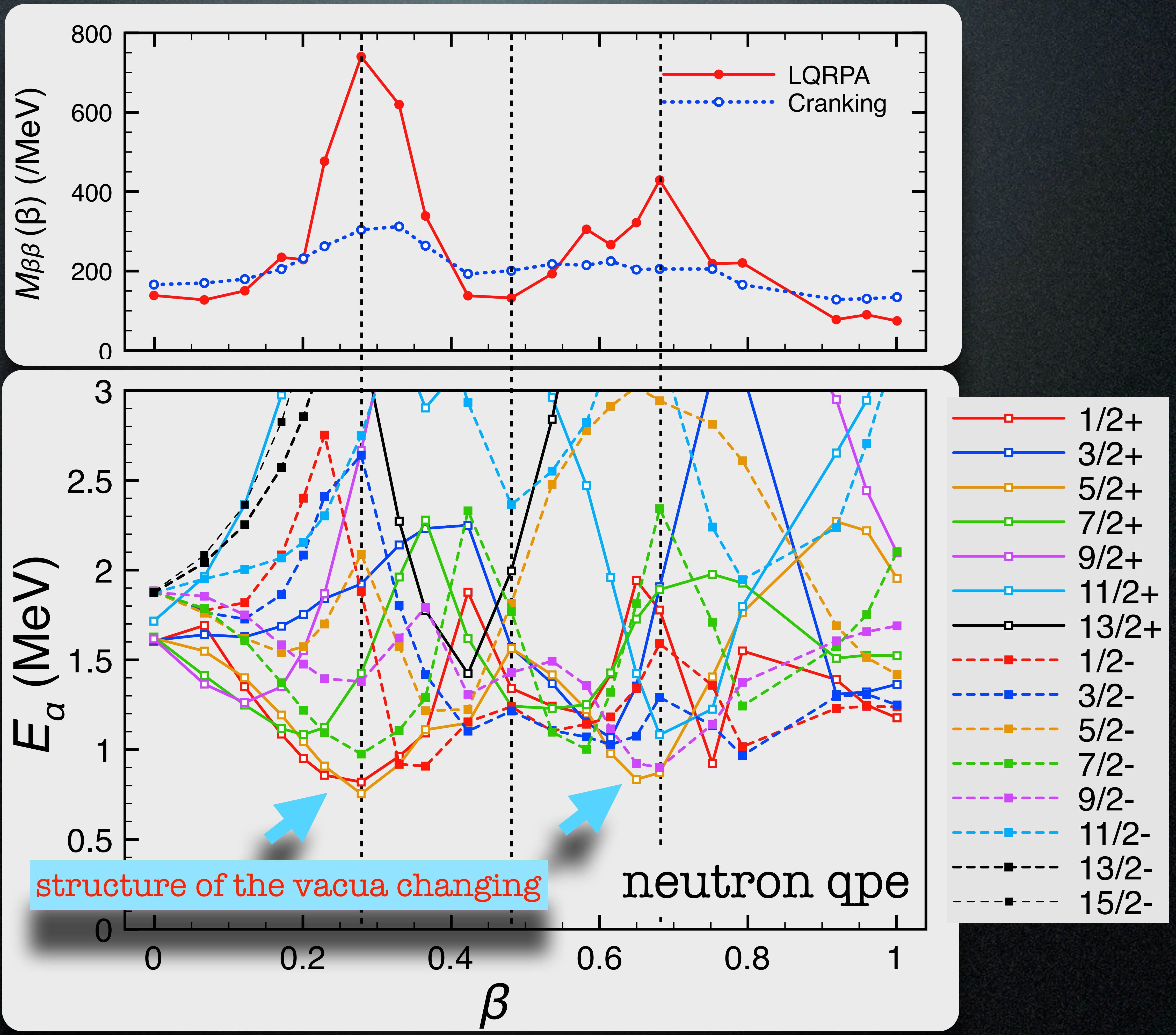
strong dependence on the shell structure/ configuration

curvature of the collective potential

$$C_i(\beta) = \omega_i^2(\beta)$$

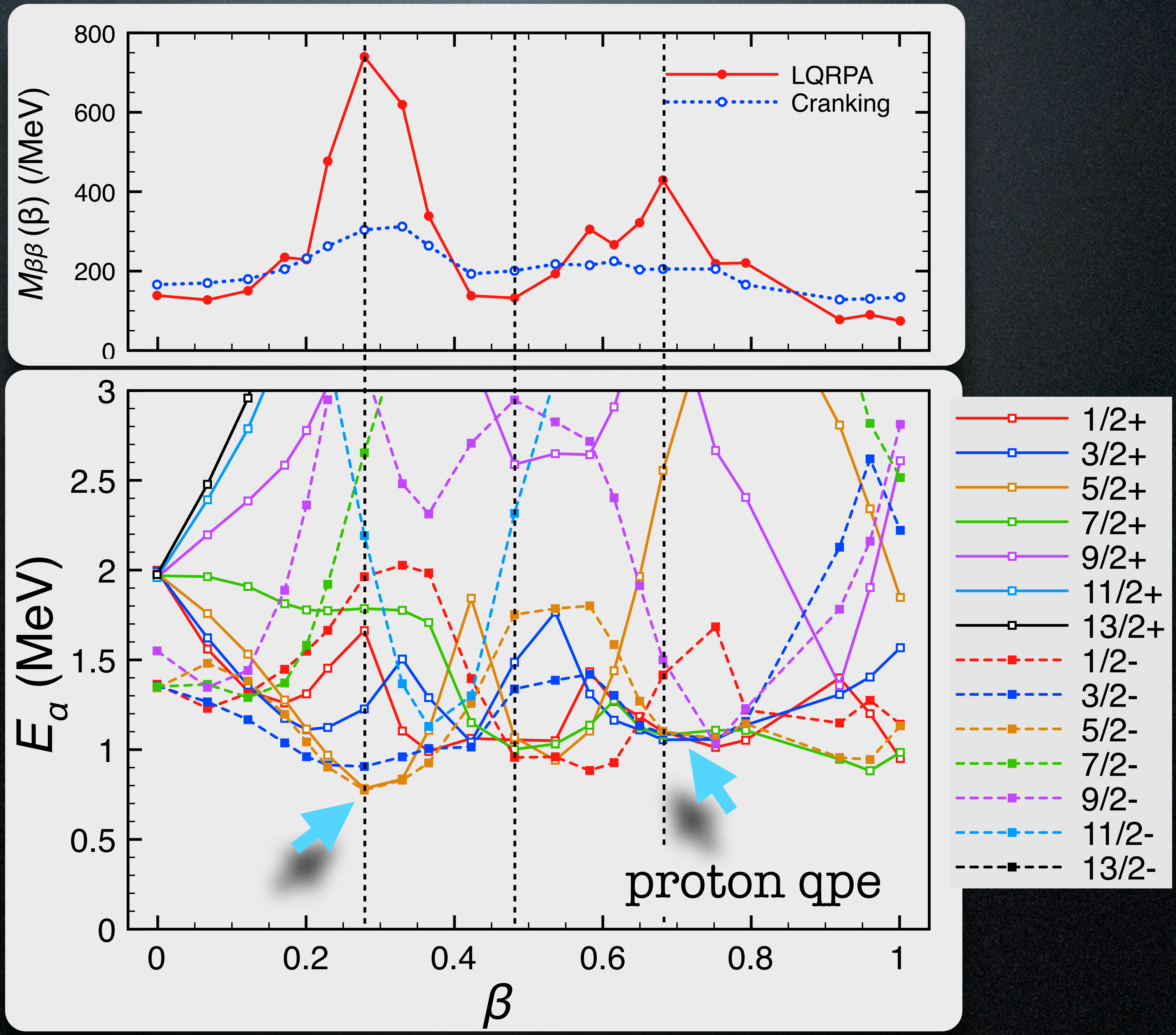


lowest qpe's



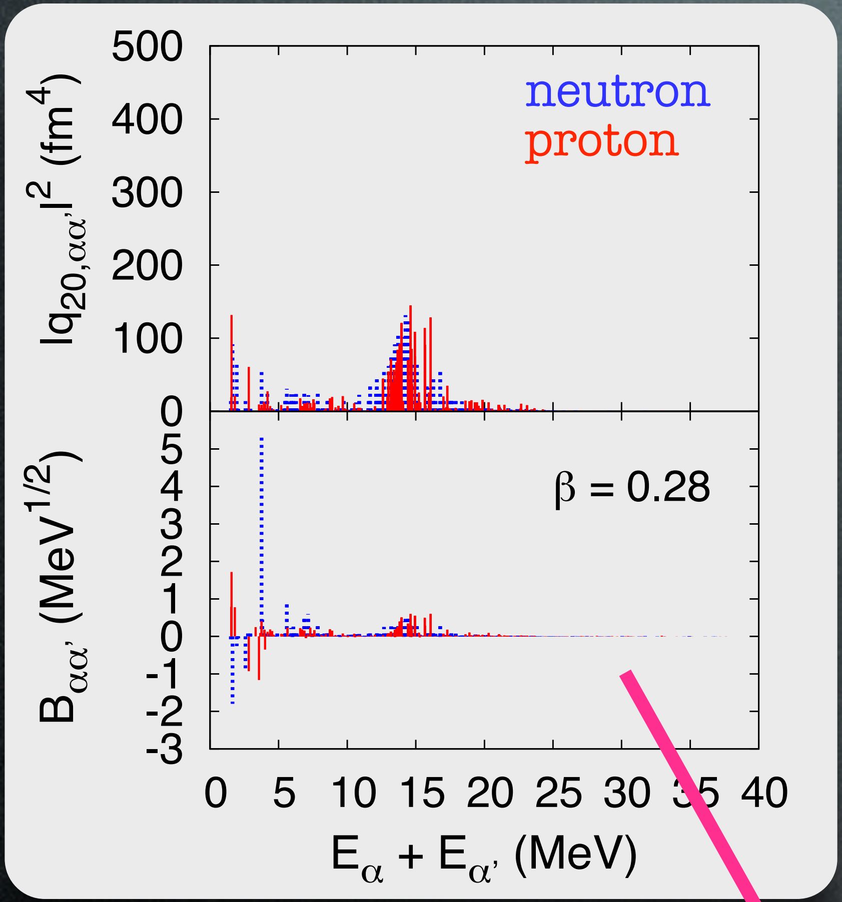
800
600
400
200
0
$M_{\beta\beta}$ (β) (/MeV)
LQRPA
Cranking
3
2.5
2
1.5
1
0.5
0
E_α (MeV)
0
0.2
0.4
0.6
0.8
1
β
1/2+
3/2+
5/2+
7/2+
9/2+
11/2+
13/2+
1/2-
3/2-
5/2-
7/2-
9/2-
11/2-
13/2-
15/2-
structure of the vacua changing
neutron qpe

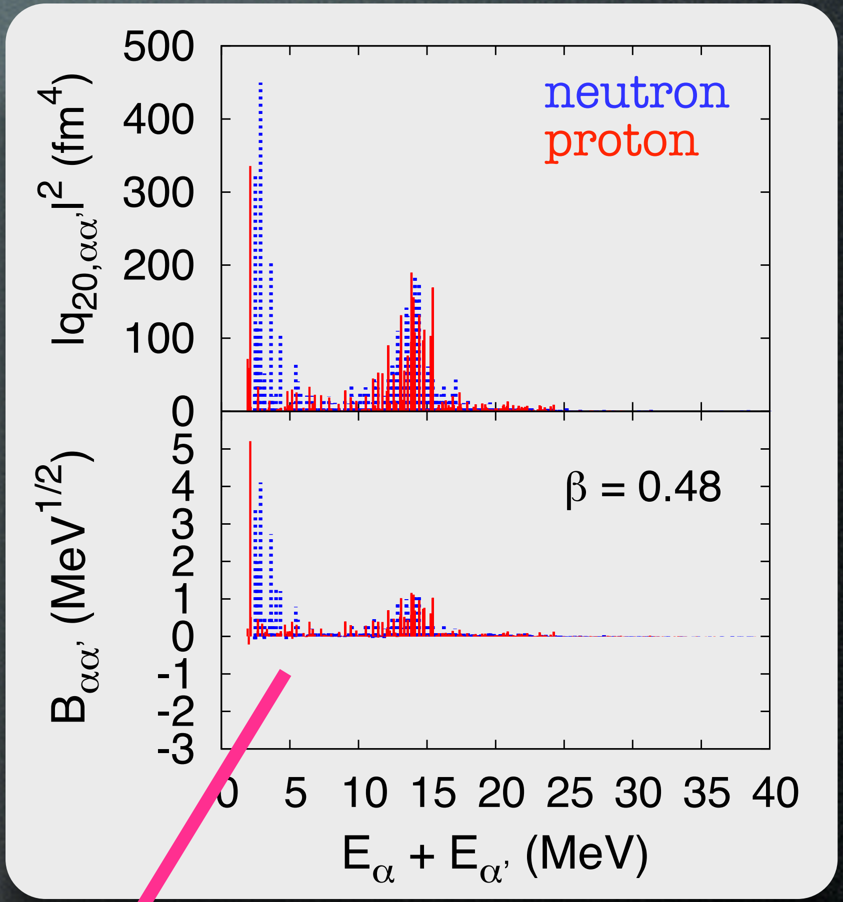
lowest qpe's



LQRPA
Cranking
$M_{\beta\beta}(\beta)$ (/MeV)
E_α (MeV)
β
1/2+
3/2+
5/2+
7/2+
9/2+
11/2+
13/2+
1/2-
3/2-
5/2-
7/2-
9/2-
11/2-
13/2-
proton qpe

Microscopic structure of collective mass in ^{240}Pu



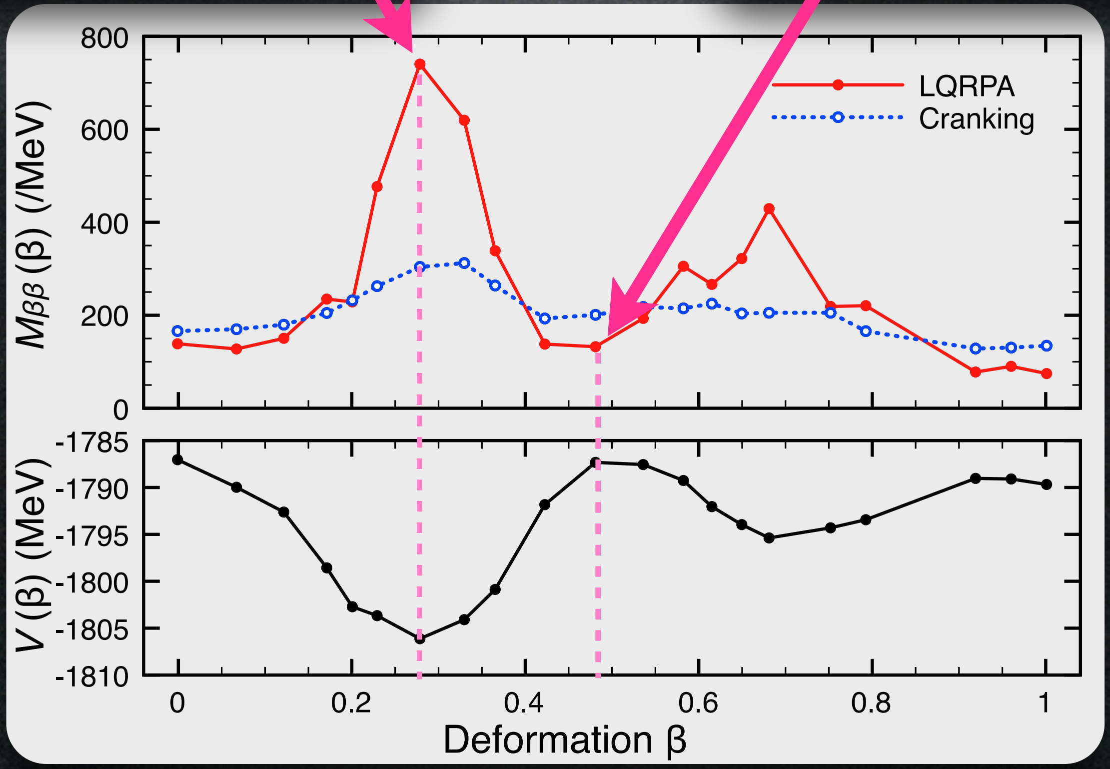


difference seen in the low-energy 2qp excitations

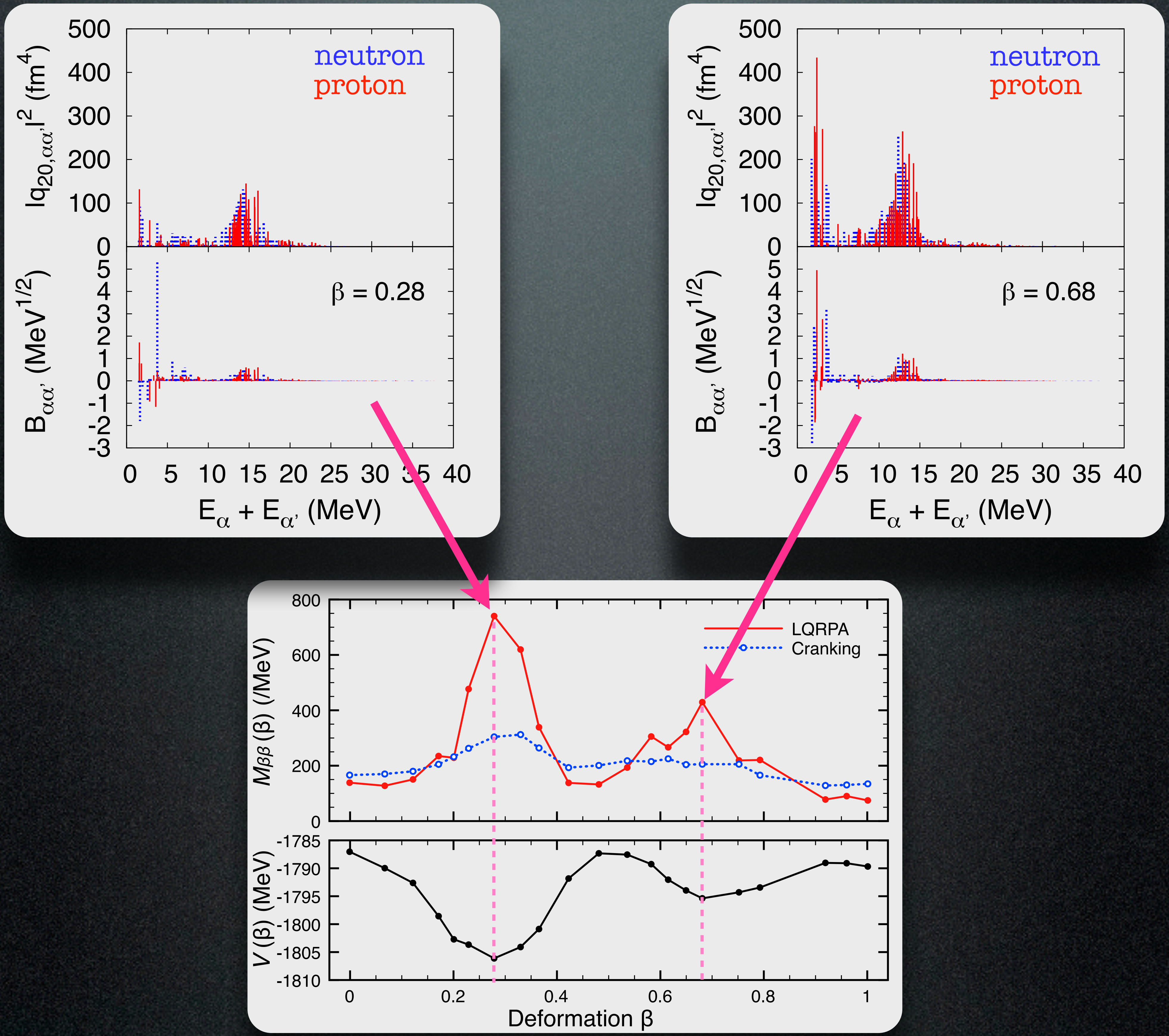
Cranking mass (perturbation)

$$M^{\rm cr}_{Q_{20}Q_{20}}(\beta) = \frac{1}{2}[S^{(-1)}]^{-1} S^{(3)} [S^{(-1)}]^{-1}$$

$$S^{(K)} = \sum_{\alpha\alpha'} \frac{|q_{20,\alpha\alpha'}|^2}{(E_\alpha + E_{\alpha'})^K}$$

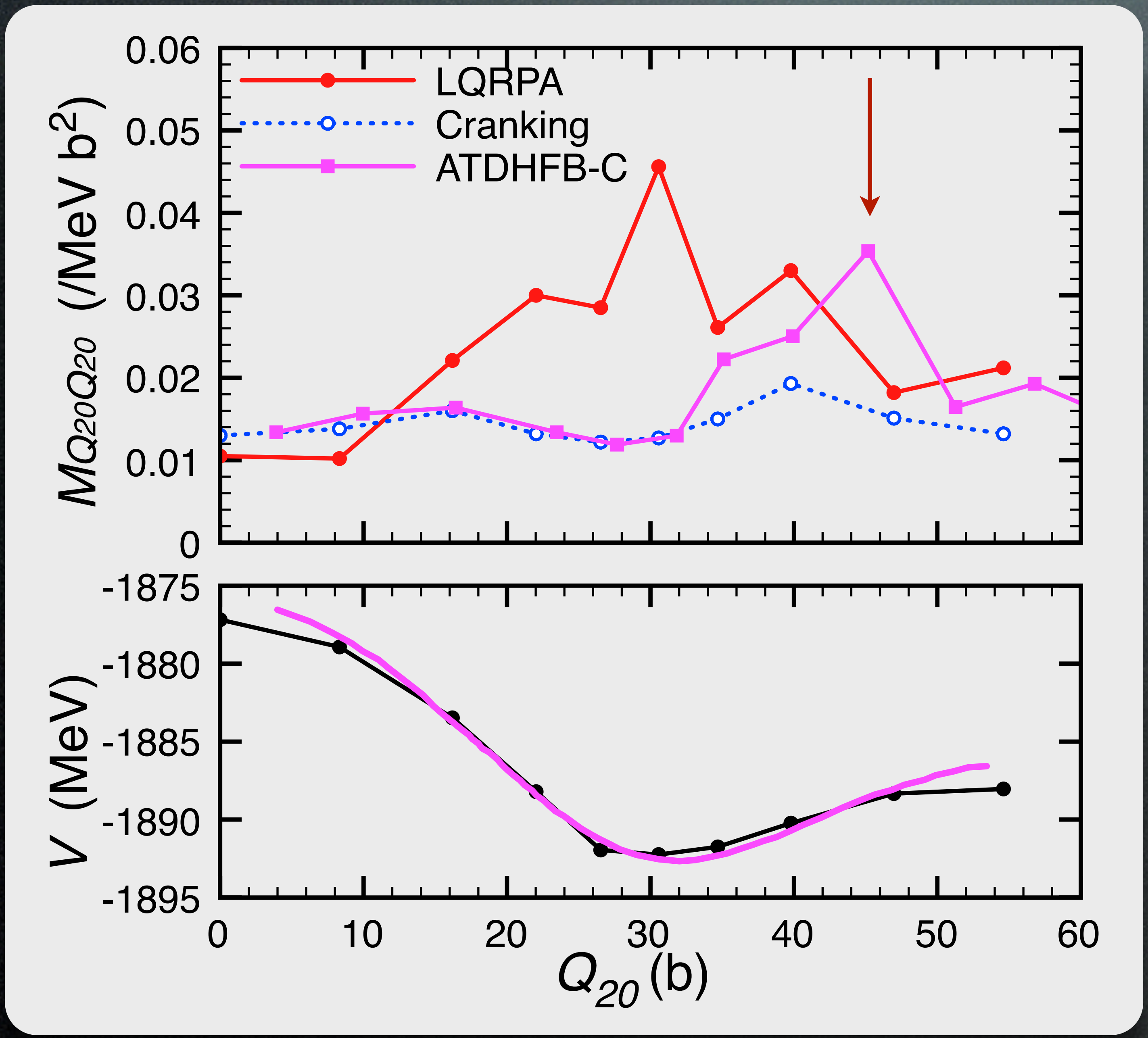


Enhanced collective mass



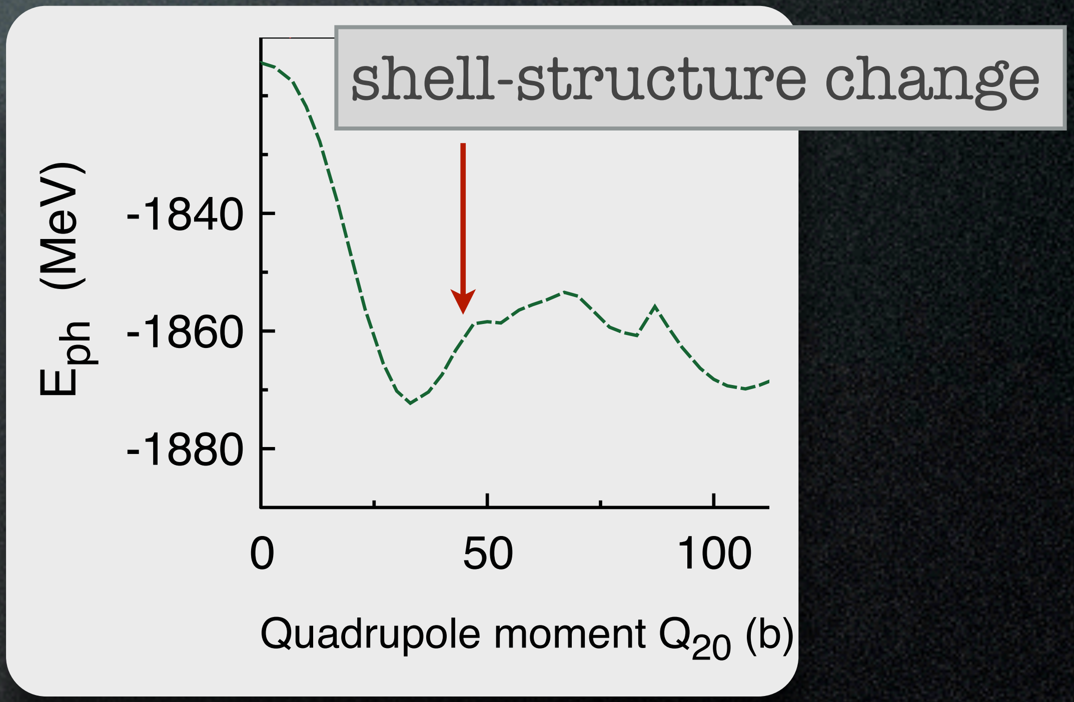
LQRPA and ATDHFB-Cranking masses in ^{256}Fm

SkM* + mixed-type pairing



ATDHFB:
Baran, Sheikh, Dobaczewski, Nazarewicz, Staszczak, PRC85(2012)024314

using HFODD



Summary

Collective mass parameters for the quadrupole vib.

- calculated by use of the LQPRA method w/Skyrme EDF

Time-odd components are included

- strongly dependent on the structure of the vacua
  - $0\hbar\omega$ 2qp excitation sensitive to the shell structure
  - more than twice at most as large as the perturbative-cranking mass

Perspective

Deeper understanding of the mass parameter microscopically

in terms of the quasiparticle excitation

Benchmark is needed

among the LQRPA, ATDHFB(-Cranking), GCM-GOA masses

Quadrupole mass parameters on the symmetric path way

Application to spontaneous fission dynamics

LQRPA on top of the triaxial and octupole deformed states

3D-QRPA code is needed

HFODD + parallelized m-FAM may be a practical way for it(?)

m-FAM:
Avogadro, Nakatsukasa, PRC87(2013)014331