14 Feb. 2013@RIKEN

Skyrme EDF for collective modes of excitation in deformed nuclei with HPC

Kenichi Yoshida

Outline

- Skyrme energy-density functional method for collective dynamics
  - Deformation effects in low-energy and giant dipole excitations
  - Large-amplitude collective motion
    - Shape-phase transition in neutron-rich Cr isotopes
    - Mass parameters of a fissioning nucleus

Skyrme EDF for collective dynamics

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

variation w.r.t densities: $\delta E = 0$

The coordinate-space Kohn-Sham-Bogoliubov eq. for ground states

J. Dobaczewski *et al.*, NPA422(1984)103

$$\begin{pmatrix} h^q(\boldsymbol{r},\sigma) - \lambda^q & \tilde{h}^q(\boldsymbol{r},\sigma) \\ \tilde{h}^q(\boldsymbol{r},\sigma) & -(h^q(\boldsymbol{r},\sigma) - \lambda^q) \end{pmatrix} \begin{pmatrix} \varphi^q_{1,\alpha}(\boldsymbol{r},\sigma) \\ \varphi^q_{2,\alpha}(\boldsymbol{r},\sigma) \end{pmatrix} = E_\alpha \begin{pmatrix} \varphi^q_{1,\alpha}(\boldsymbol{r},\sigma) \\ \varphi^q_{2,\alpha}(\boldsymbol{r},\sigma) \end{pmatrix}$$

$q = \mathrm{n}, \mathrm{p}$

"s.p." hamiltonian and pair potential: $h^q = \dfrac{\delta E}{\delta \varrho^q}, \quad \tilde{h}^q = \dfrac{\delta E}{\delta \tilde{\varrho}^q}$

Skyrme EDF for collective dynamics

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

variation w.r.t densities: $\delta E = 0$

The coordinate-space Kohn-Sham-Bogoliubov eq. for ground states

J. Dobaczewski *et al.*, NPA422(1984)103

Coupling to the continuum is appropriately taken into account.

Deformation is described easily.

$$\begin{pmatrix} h^q(\boldsymbol{r},\sigma) - \lambda^q & \tilde{h}^q(\boldsymbol{r},\sigma) \\ \tilde{h}^q(\boldsymbol{r},\sigma) & -(h^q(\boldsymbol{r},\sigma) - \lambda^q) \end{pmatrix} \begin{pmatrix} \varphi^q_{1,\alpha}(\boldsymbol{r},\sigma) \\ \varphi^q_{2,\alpha}(\boldsymbol{r},\sigma) \end{pmatrix} = E_\alpha \begin{pmatrix} \varphi^q_{1,\alpha}(\boldsymbol{r},\sigma) \\ \varphi^q_{2,\alpha}(\boldsymbol{r},\sigma) \end{pmatrix}$$

$q = \mathrm{n}, \mathrm{p}$

"s.p." hamiltonian and pair potential: $h^q = \dfrac{\delta E}{\delta \varrho^q}, \quad \tilde{h}^q = \dfrac{\delta E}{\delta \tilde{\varrho}^q}$

Skyrme EDF for collective dynamics

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

variation w.r.t densities: $\delta E = 0$

The coordinate-space Kohn-Sham-Bogoliubov eq. for ground states

J. Dobaczewski *et al.*, NPA422(1984)103

$$\begin{pmatrix} h^q(\boldsymbol{r},\sigma) - \lambda^q & \tilde{h}^q(\boldsymbol{r},\sigma) \\ \tilde{h}^q(\boldsymbol{r},\sigma) & -(h^q(\boldsymbol{r},\sigma) - \lambda^q) \end{pmatrix} \begin{pmatrix} \varphi^q_{1,\alpha}(\boldsymbol{r},\sigma) \\ \varphi^q_{2,\alpha}(\boldsymbol{r},\sigma) \end{pmatrix} = E_\alpha \begin{pmatrix} \varphi^q_{1,\alpha}(\boldsymbol{r},\sigma) \\ \varphi^q_{2,\alpha}(\boldsymbol{r},\sigma) \end{pmatrix}$$

$q = \mathrm{n}, \mathrm{p}$

"s.p." hamiltonian and pair potential: $h^q = \dfrac{\delta E}{\delta \varrho^q}, \quad \tilde{h}^q = \dfrac{\delta E}{\delta \tilde{\varrho}^q}$

quasiparticle basis $\alpha, \beta \cdots$

KY, N. V. Giai, PRC78(2008)064316

The quasiparticle RPA eq. for excited states $[\hat{H}, \hat{O}^\dagger_\lambda]|\Psi_\lambda\rangle = \omega_\lambda \hat{O}^\dagger_\lambda |\Psi_\lambda\rangle$

Collective excitation = coherent superposition of 2qp excitations: $\hat{O}^\dagger_\lambda = \sum_{\alpha\beta} \{X^\lambda_{\alpha\beta} \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta - Y^\lambda_{\alpha\beta} \hat{a}_\beta \hat{a}_\alpha\}$

residual interactions: $v^{\mathrm{ph}} = \dfrac{\delta^2 E}{\delta \varrho^2}, \quad v^{\mathrm{pp}} = \dfrac{\delta^2 E}{\delta \tilde{\varrho}^2}$

KSB 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

A. Baran et al., PRC78(2008)014318

QRPA calculation on parallel computer: MPI and BLACS

BLACS:

Basic Linear Algebra Communication Subprograms

↓

- linear algebra oriented message passing interface
- communication layer of ScaLAPACK

Scalable Linear Algebra PACKage

QRPA calculation on parallel computer: MPI and BLACS

QRPA: use of *N* processors

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

Ex.: use of 4 processors

$$\begin{matrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{matrix}$$

QRPA calculation on parallel computer: MPI and BLACS

QRPA: use of *N* processors

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

Ex.: use of 4 processors

block matrix

$$
\begin{array}{cc|cc|c}
a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\
a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\
\hline
a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\
a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\
\hline
a_{51} & a_{52} & a_{53} & a_{54} & a_{55}
\end{array}
$$

QRPA calculation on parallel computer: MPI and BLACS

QRPA: use of *N* processors

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

Ex.: use of 4 processors

a_{11}	a_{12}	a_{15}	a_{13}	a_{14}
a_{21}	a_{22}	a_{25}	a_{23}	a_{24}
a_{51}	a_{52}	a_{55}	a_{53}	a_{54}
a_{31}	a_{32}	a_{35}	a_{33}	a_{34}
a_{41}	a_{42}	a_{45}	a_{43}	a_{44}

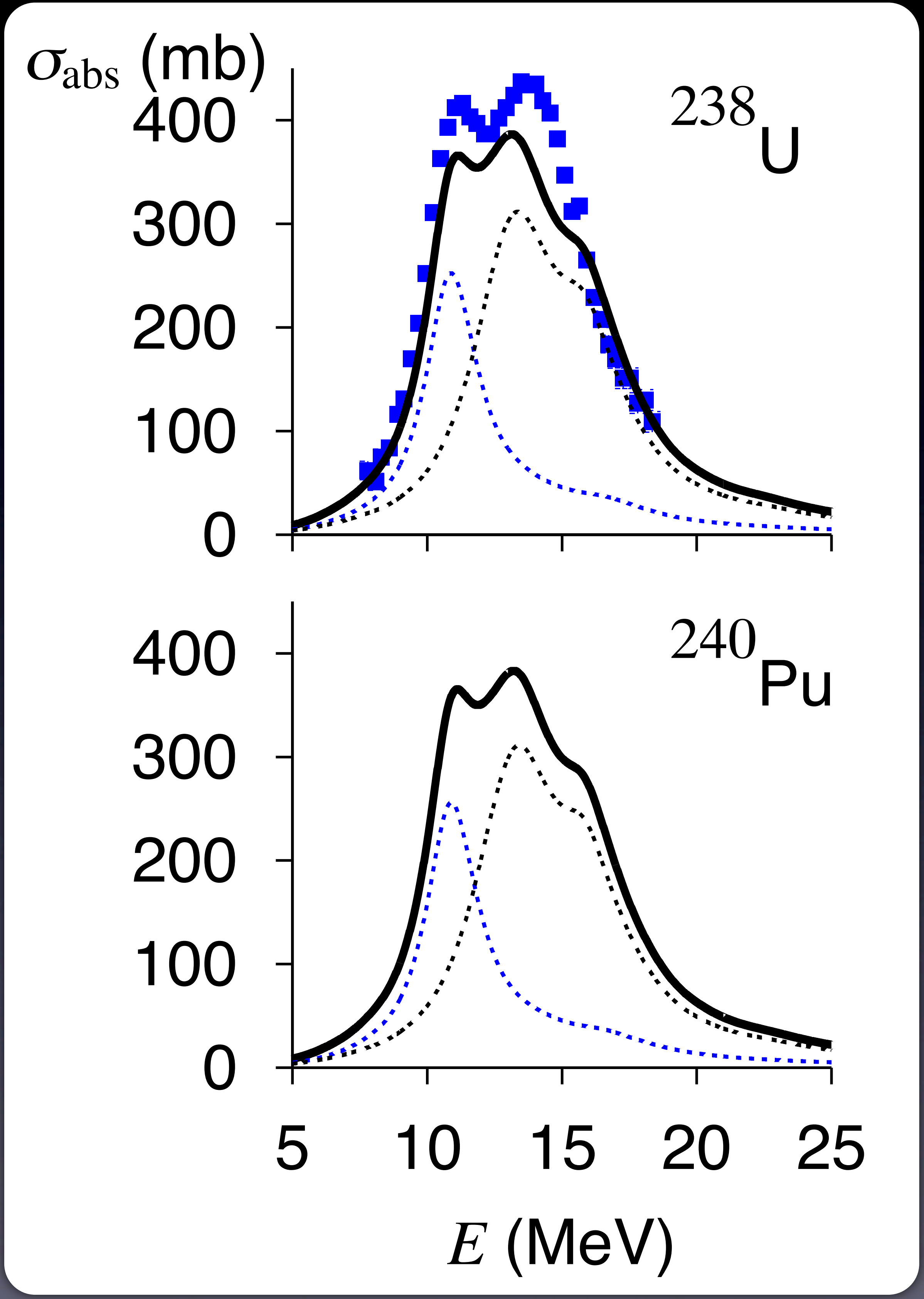
ScaLAPACK

2D-block cyclic distribution for load balancing

function: indxl2g for distribution

subroutine: pdsyev for diagonalization

Giant resonance in a heavy system



HFB cal. (64 CPUs)

Box size: 14.7 fm × 14.4 fm

Cut-off: $\Omega \leqq \frac{31}{2},\ E_\alpha \leqq 60$ MeV

QRPA cal. (512 CPUs)

Cut-off: $E_\alpha + E_\beta \leqq 60$ MeV

For each K^π

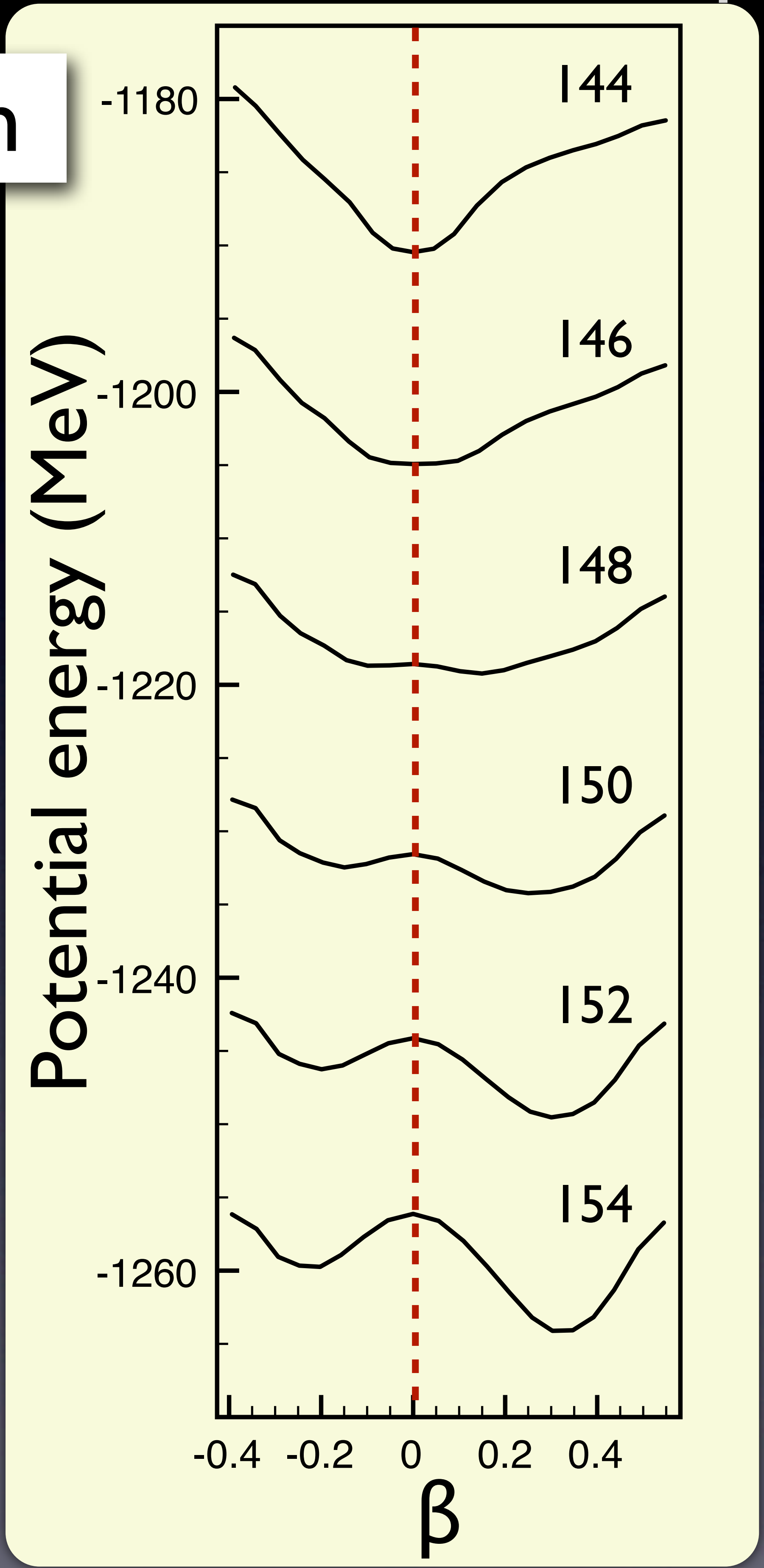
# of 2qp excitation: ~50,000

matrix elements: 590 CPU hours

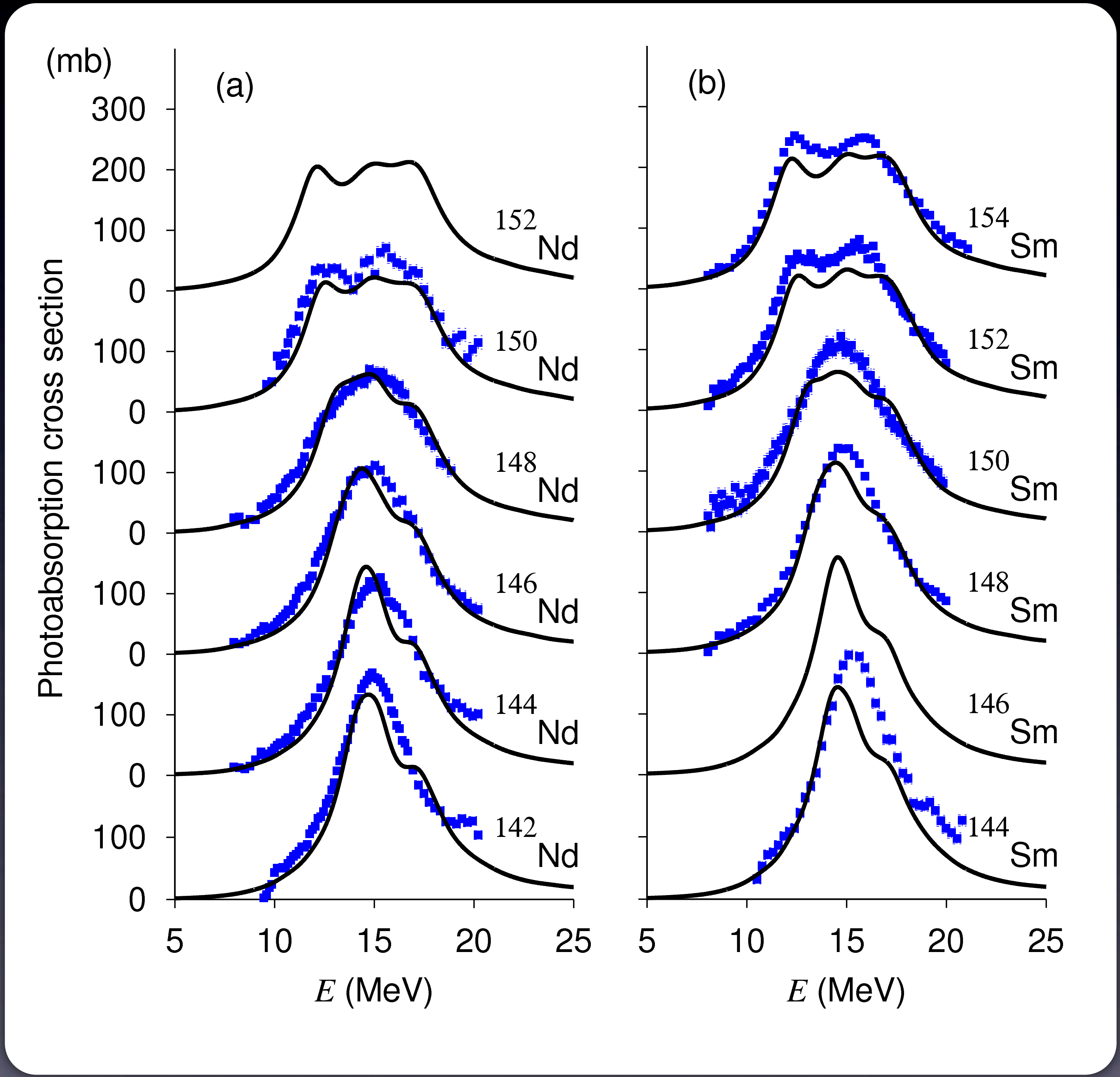
diagonalization: 330 CPU hours

about 200 min for total strengths !

Deformation effect in photo absorption cross sections

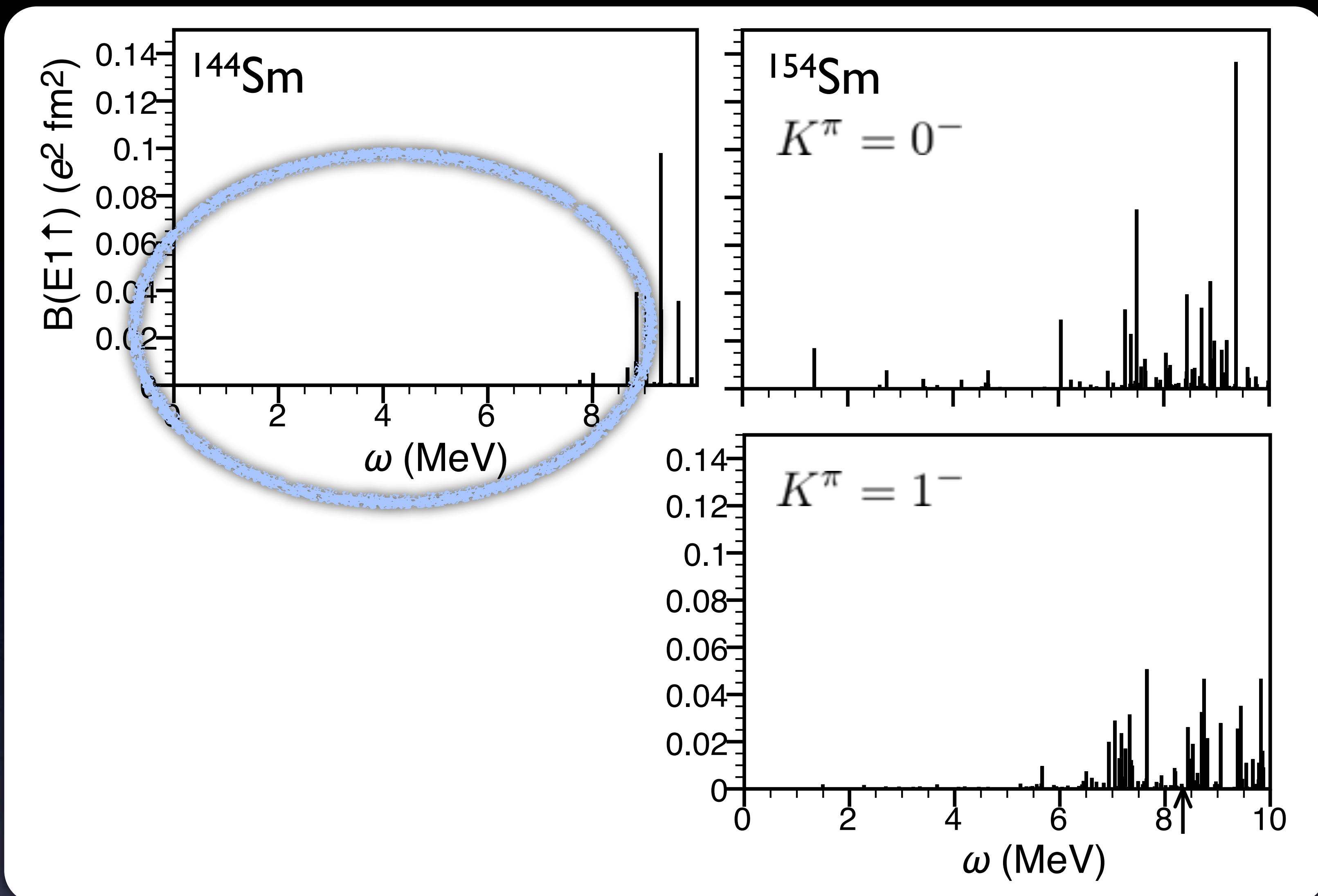


KY, T. Nakatsukasa, PRC83(2011)021304R



Low-lying dipole excitations in Sm

KY, T. Nakatsukasa,
PRC83(2011)021304R



In ^{144}Sm

no strength below 8 MeV

✓consistent with other QRPA cal.

N. Parr et al., PRC67(2003)034312

✓inconsistent with exp.

A. Zilges et al., PLB542(2002)43

$$\sum_{E<10\mathrm{MeV}} B(E1\uparrow) = 0.27\ e^2\mathrm{fm}^2$$

^{144}Sm

↓

$$1.5\ e^2\mathrm{fm}^2$$

^{154}Sm

5% of EWSR

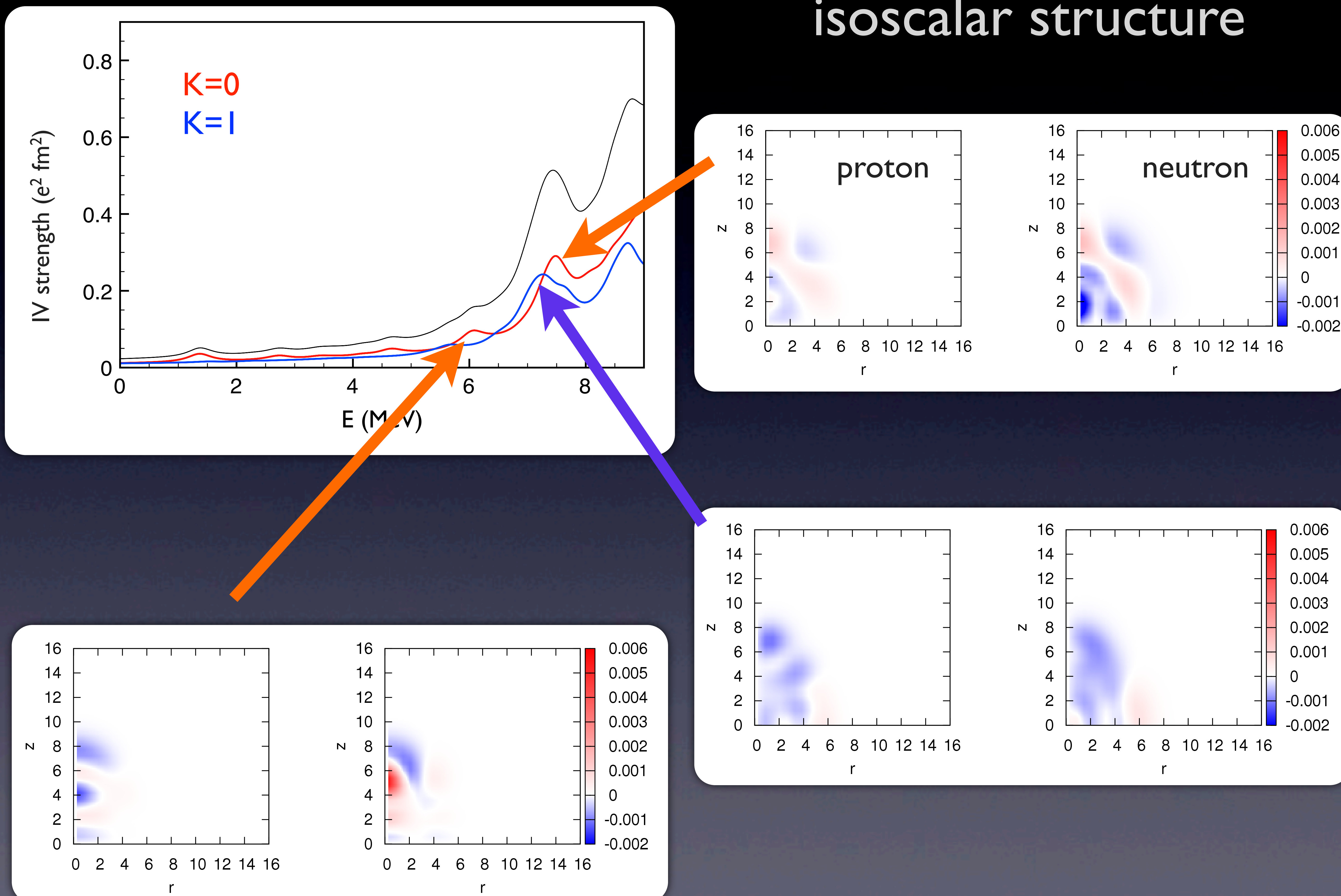
^{154}Sm

enhancement of the low-lying strength

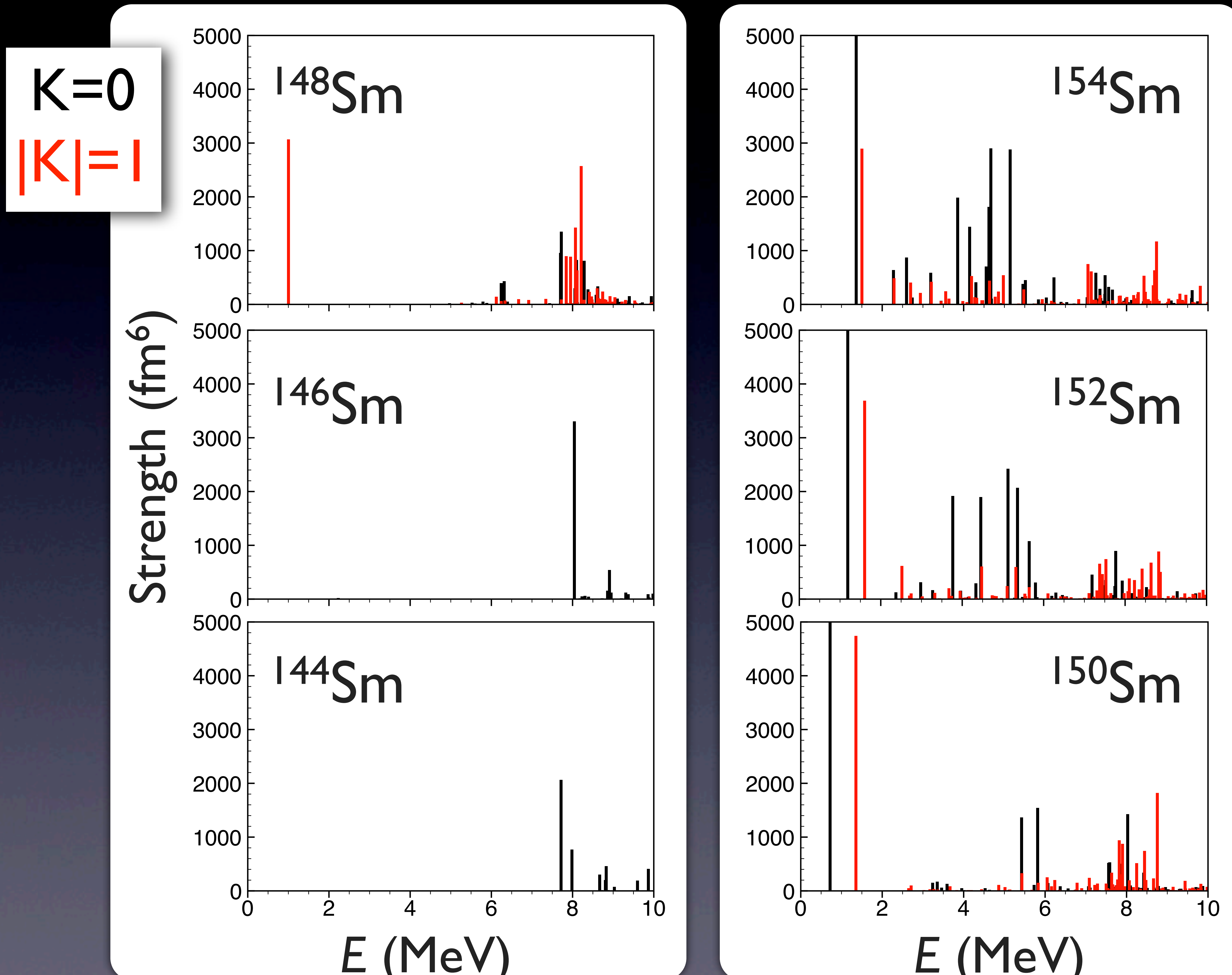
a part of the mode coupling effects is in the deformed QRPA

Transition densities in ^{154}Sm

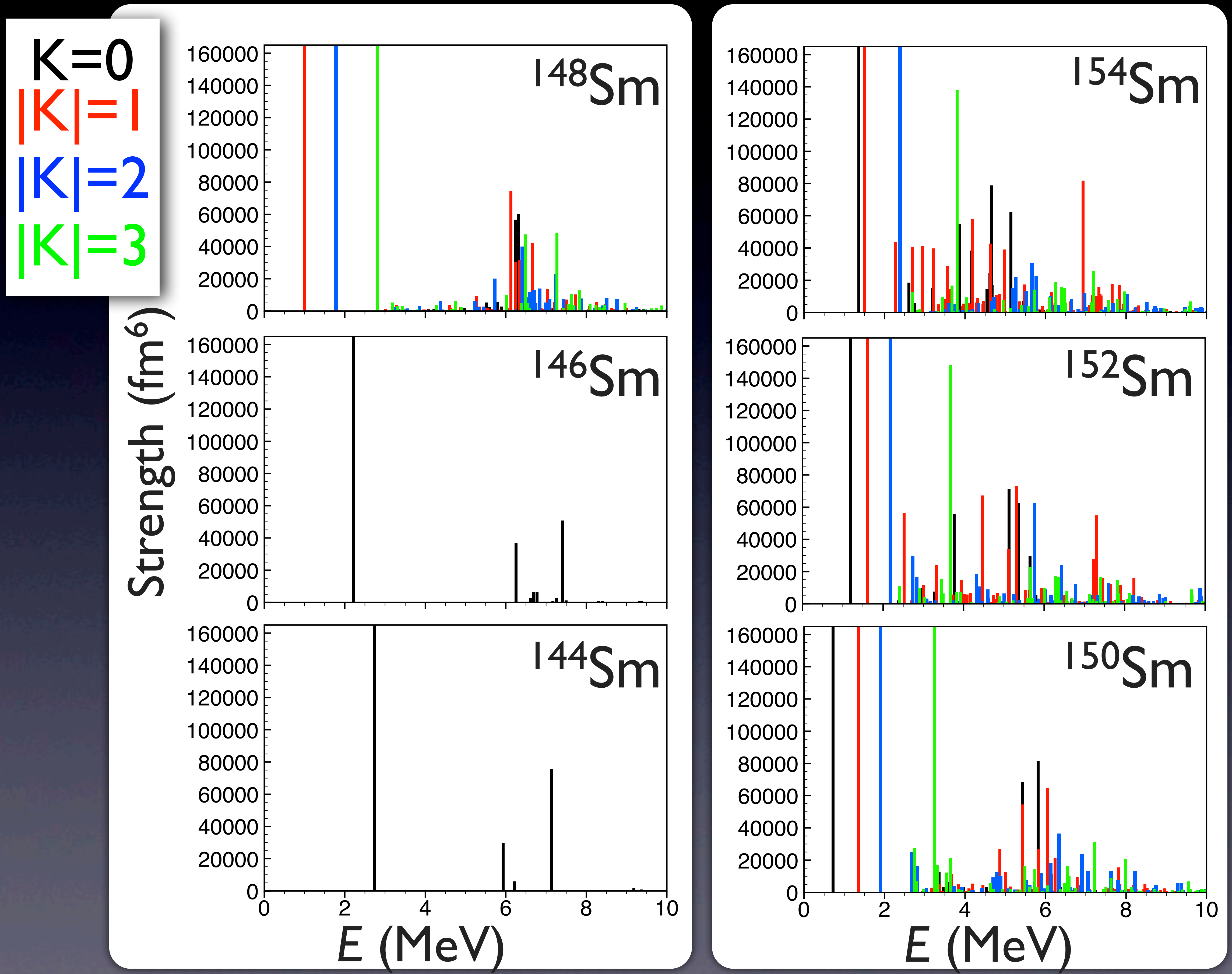
isoscalar structure



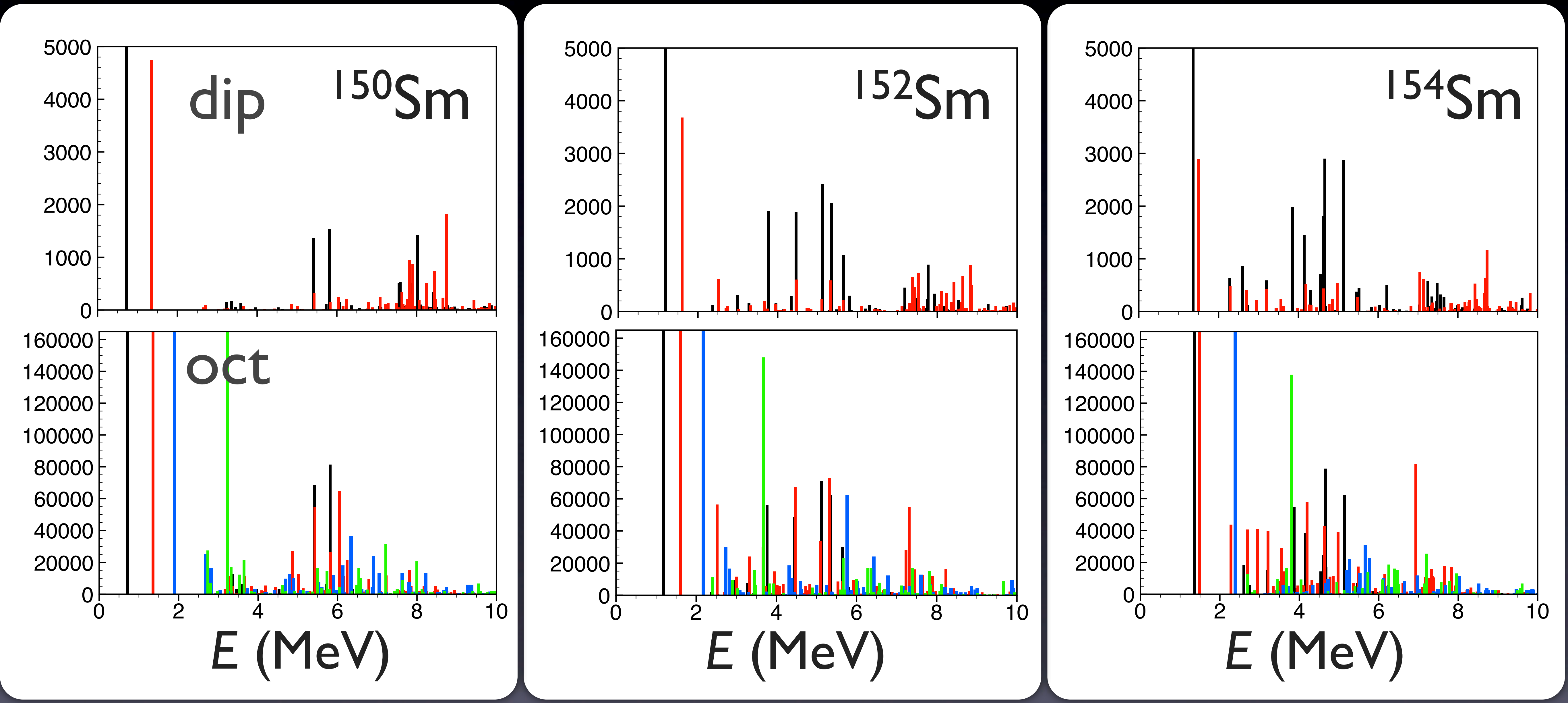
Deformation effect in IS dipole excitation



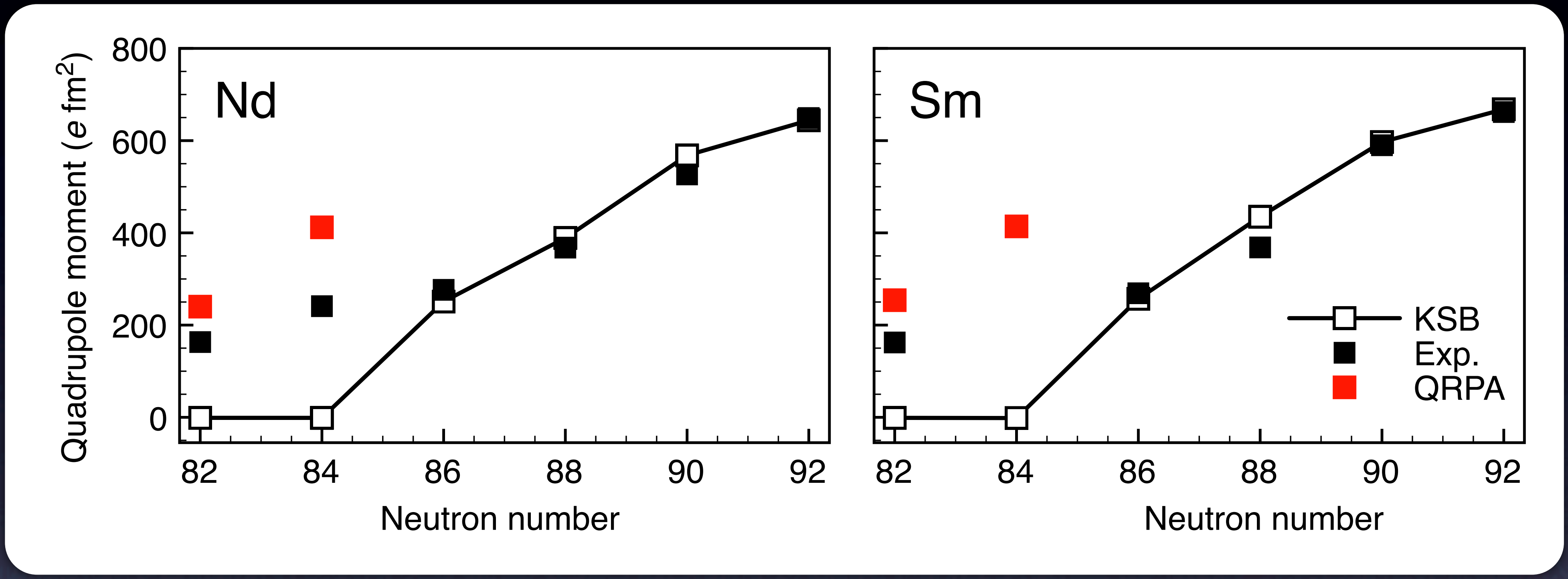
Deformation effect in IS octupole excitation

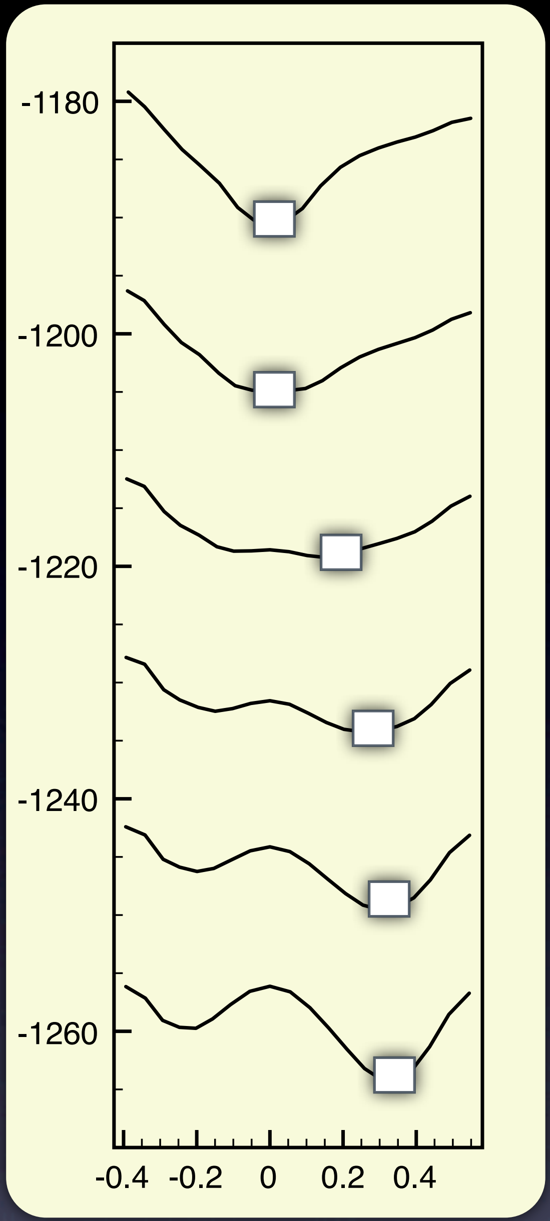


Deformation effect: coupling between IS dipole and LEOR



Indication of the shape fluctuation around N=84





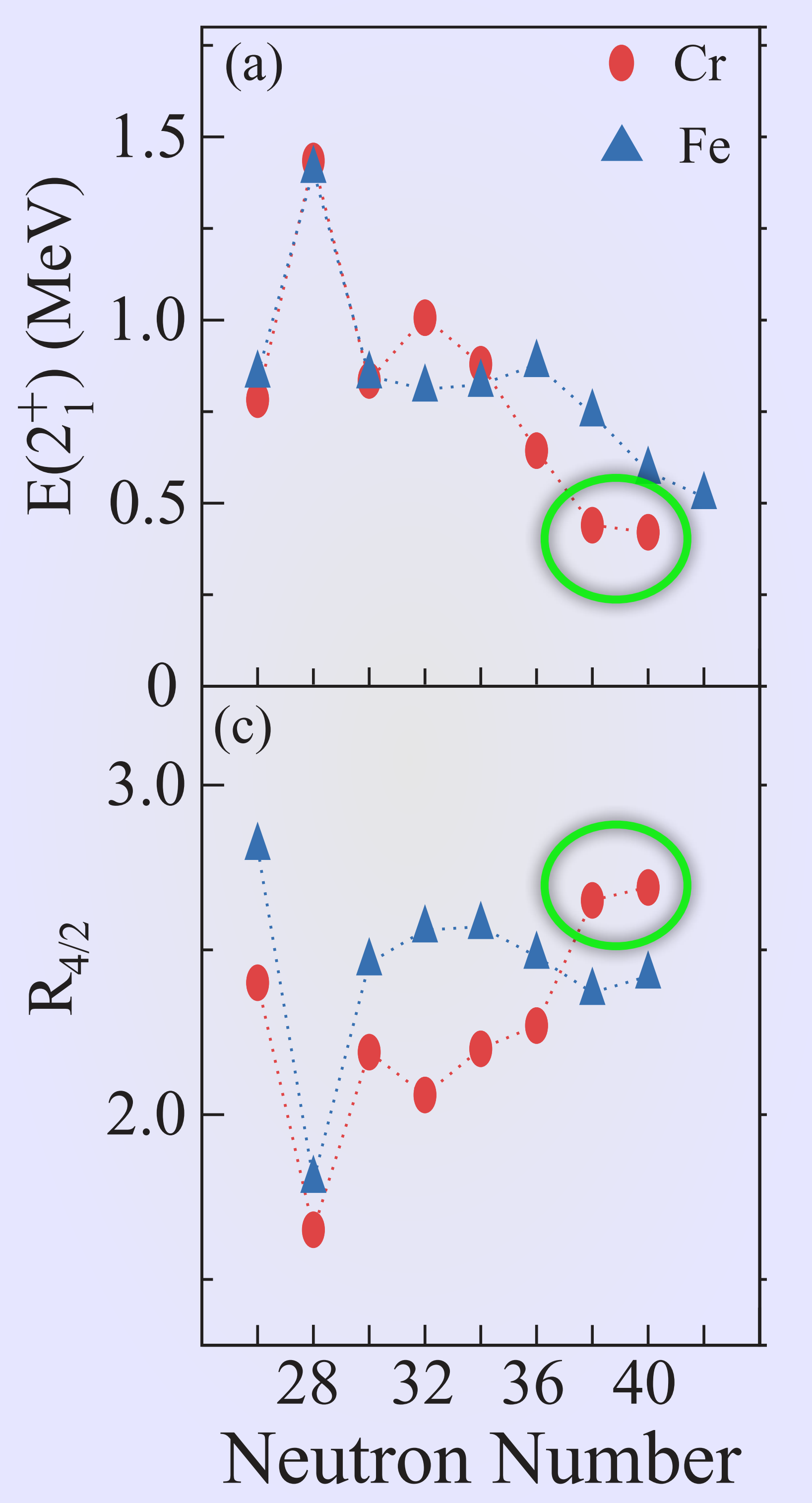
Overestimation of the quadrupole transition strength w/ QRPA

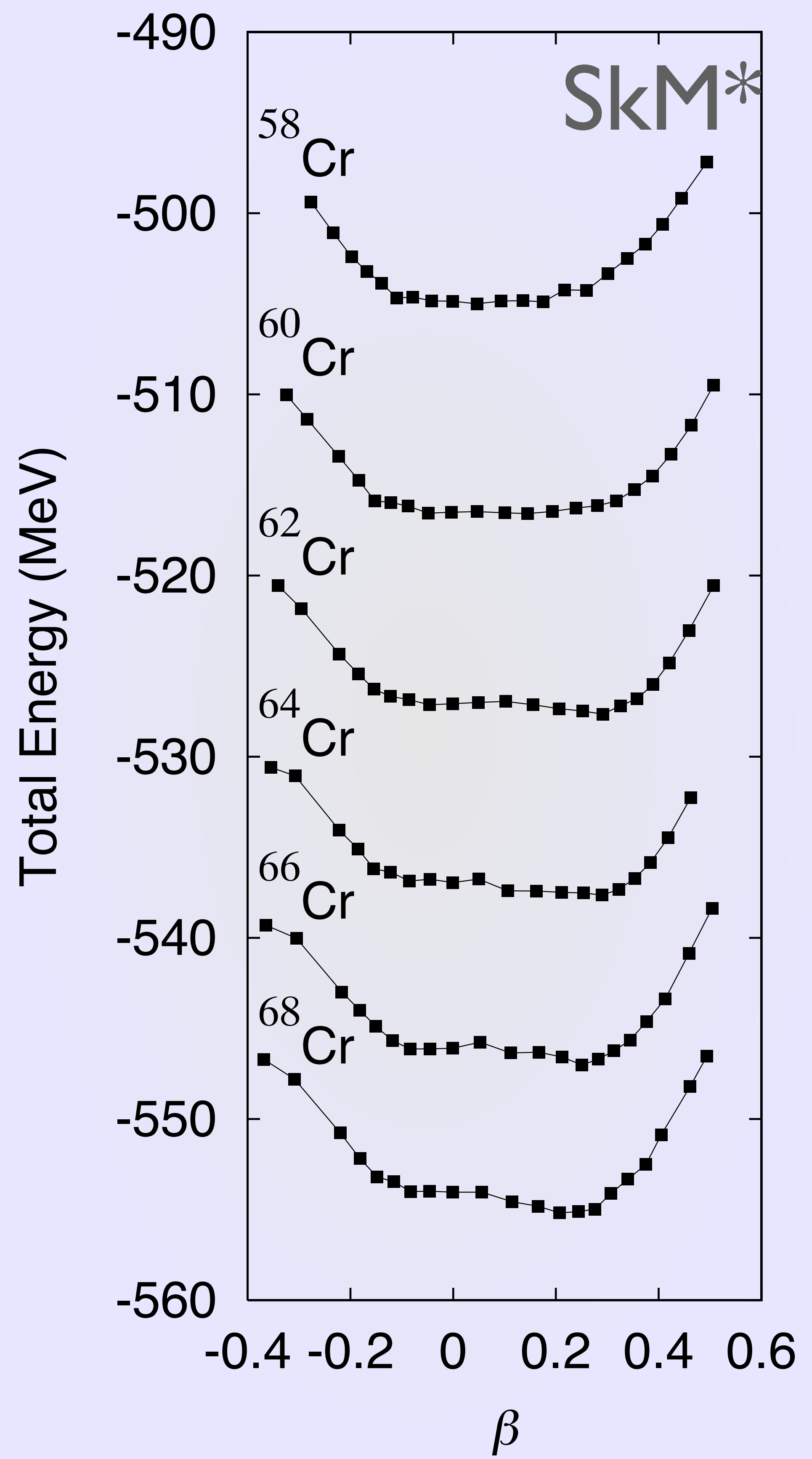
close to the critical point of the shape-phase transition from spherical to quadrupole deformed shape

Quadrupole collectivity around N=40

KY, N. HInohara, PRC83(2011)061302R

A. Gade *et al.*, PRC81(2010)051304R





Collective Hamiltonian approach

The classical collective Hamiltonian in (1+2)D:

axially symmetric rotor

$$\mathcal{H}_{\rm coll} = \frac{1}{2}\mathcal{M}_\beta(\beta)\dot{\beta}^2 + \frac{1}{2}\sum_{i=1}^{2}\mathcal{J}_i(\beta)\omega_i^2 + V(\beta)$$

Requantization with the Pauli's prescription

The collective Schrödinger equation:

$$\hat{H}_{\rm coll}\Psi_{\alpha IM}(\beta,\theta_1,\theta_2) = E_{\alpha I}\Psi_{\alpha IM}(\beta,\theta_1,\theta_2)$$

Collective wf in the lab. frame

$$\Psi_{\alpha IM}(\beta,\Omega) = \sum_{K=0}^{I}\Phi_{\alpha IK}(\beta)\langle\Omega|IMK\rangle = \Phi_{\alpha I}(\beta)\langle\Omega|IM0\rangle$$

Collective wf in the intrinsic frame

The collective Schrödinger equation in the intrinsic frame:

$$\left\{\hat{T}_{\rm vib} + \frac{I(I+1)}{2\mathcal{J}(\beta)} + V(\beta)\right\}\Phi_{\alpha I}(\beta) = E_{\alpha I}\Phi_{\alpha I}(\beta)$$

$$\hat{T}_{\rm vib} = -\frac{1}{2M_\beta(\beta)}\frac{\partial^2}{\partial\beta^2} + \frac{1}{2M_\beta(\beta)}\left[\frac{1}{2M_\beta(\beta)}\frac{\partial M_\beta(\beta)}{\partial\beta} - \frac{1}{\mathcal{J}(\beta)}\frac{\partial\mathcal{J}(\beta)}{\partial\beta}\right]\frac{\partial}{\partial\beta}$$

Normalization: $\int d\beta|G(\beta)|^{1/2}\Phi^*_{\alpha I}(\beta)\Phi_{\alpha' I'}(\beta) = \delta_{\alpha\alpha'}\delta_{II'}$ with the volume element

$$|G(\beta)| = M_\beta(\beta)\mathcal{J}^2(\beta)$$

Mass parameters of collective modes in the QRPA

Generalized momentum and coordinate operators

cf. Ring and Schuck

$$\hat{\mathcal{P}}_\nu = \frac{1}{i}\sqrt{\frac{\mathcal{M}_\nu\omega_\nu}{2}}\left(\hat{O}_\nu - \hat{O}_\nu^\dagger\right), \qquad \hat{\mathcal{Q}}_\nu = \sqrt{\frac{1}{2\mathcal{M}_\nu\omega_\nu}}\left(\hat{O}_\nu + \hat{O}_\nu^\dagger\right)$$

Hamiltonian in the RPA order

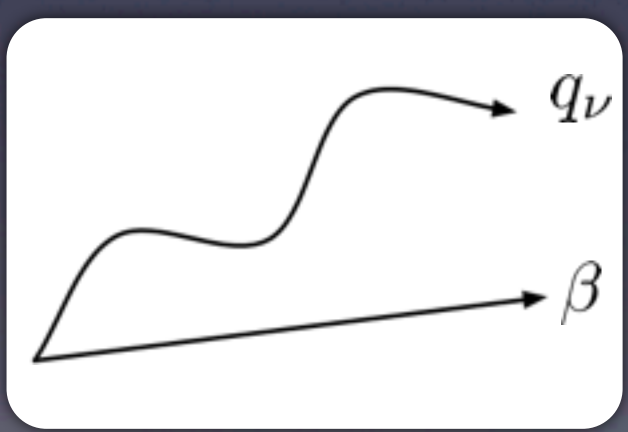
$$\hat{H}_B = \text{const.} + \sum_\nu \left(\frac{1}{2\mathcal{M}_\nu}\hat{\mathcal{P}}_\nu^2 + \frac{\mathcal{M}_\nu}{2}\omega_\nu^2\hat{\mathcal{Q}}_\nu^2\right)$$

Collective kinetic energy for the beta vibration

ν :The most collective $K^\pi = 0^+$ mode

$$T = \frac{1}{2}\dot{q}_\nu^2, \quad \mathcal{M}_\nu = 1 \quad \rightarrow \quad T = \frac{1}{2}\mathcal{M}_\beta\dot{\beta}^2$$

projection onto a coordinate β



$$\mathcal{M}_\beta = \left(\frac{dq_\nu}{d\beta}\right)^2 = \frac{1}{\eta^2}\left(\frac{dq_\nu}{dQ_{20}}\right)^2 \qquad \beta = \eta\langle\hat{Q}_{20}\rangle$$

$$\frac{dQ_{20}}{dq_\nu} = \frac{d}{dq_\nu}\langle\hat{Q}_{20}\rangle = \langle[\hat{Q}_{20}, \frac{1}{i}\hat{\mathcal{P}}_\nu]\rangle$$

Local QRPA mass: extension to the non-equilibrium point

N. Hinohara *et al.*, PRC82(2010)064313

Kohn-Sham-Bogoliubov eq with a constraint:

$$h = \frac{\delta \mathcal{E}}{\delta \varrho} - \mu \hat{q}_{20} \rightarrow |\phi(\beta)\rangle$$

QRPA on the constrained-HFB state

$$\delta \langle \phi(\beta) | [\hat{H}_{\mathrm{CHFB}}, \hat{\mathcal{Q}}_\nu] - \frac{\hat{\mathcal{P}}_\nu}{i} | \phi(\beta) \rangle = 0,$$

$$\delta \langle \phi(\beta) | [\hat{H}_{\mathrm{CHFB}}, \frac{\hat{\mathcal{P}}_\nu}{i}] - \omega_\nu^2 \hat{\mathcal{Q}}_\nu | \phi(\beta) \rangle = 0,$$

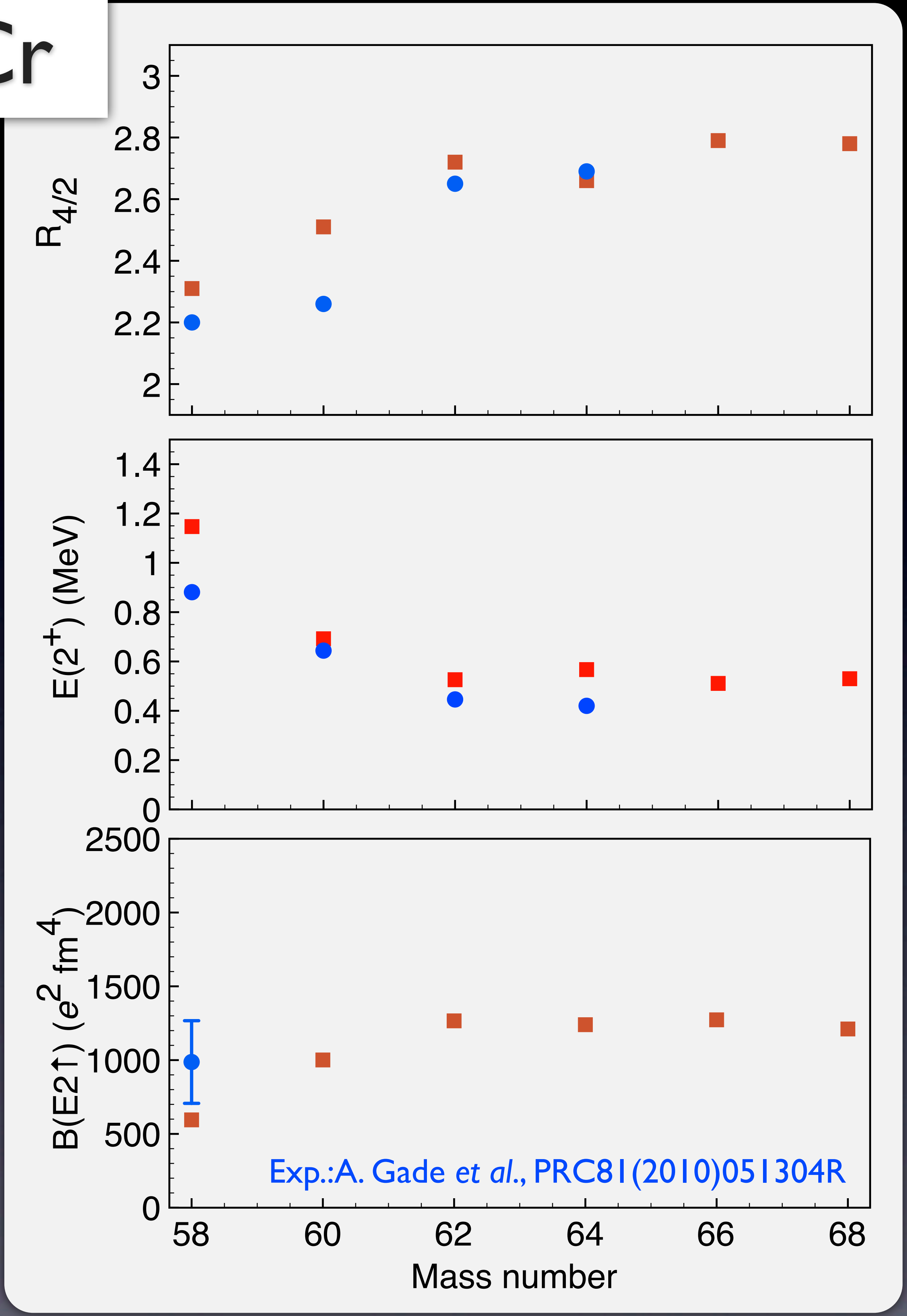
$$\langle \phi(\beta) | [\hat{\mathcal{Q}}_\mu, \frac{\hat{\mathcal{P}}_\nu}{i}] | \phi(\beta) \rangle = \delta_{\mu\nu}$$

Vibratonal mass along the collective coordinate

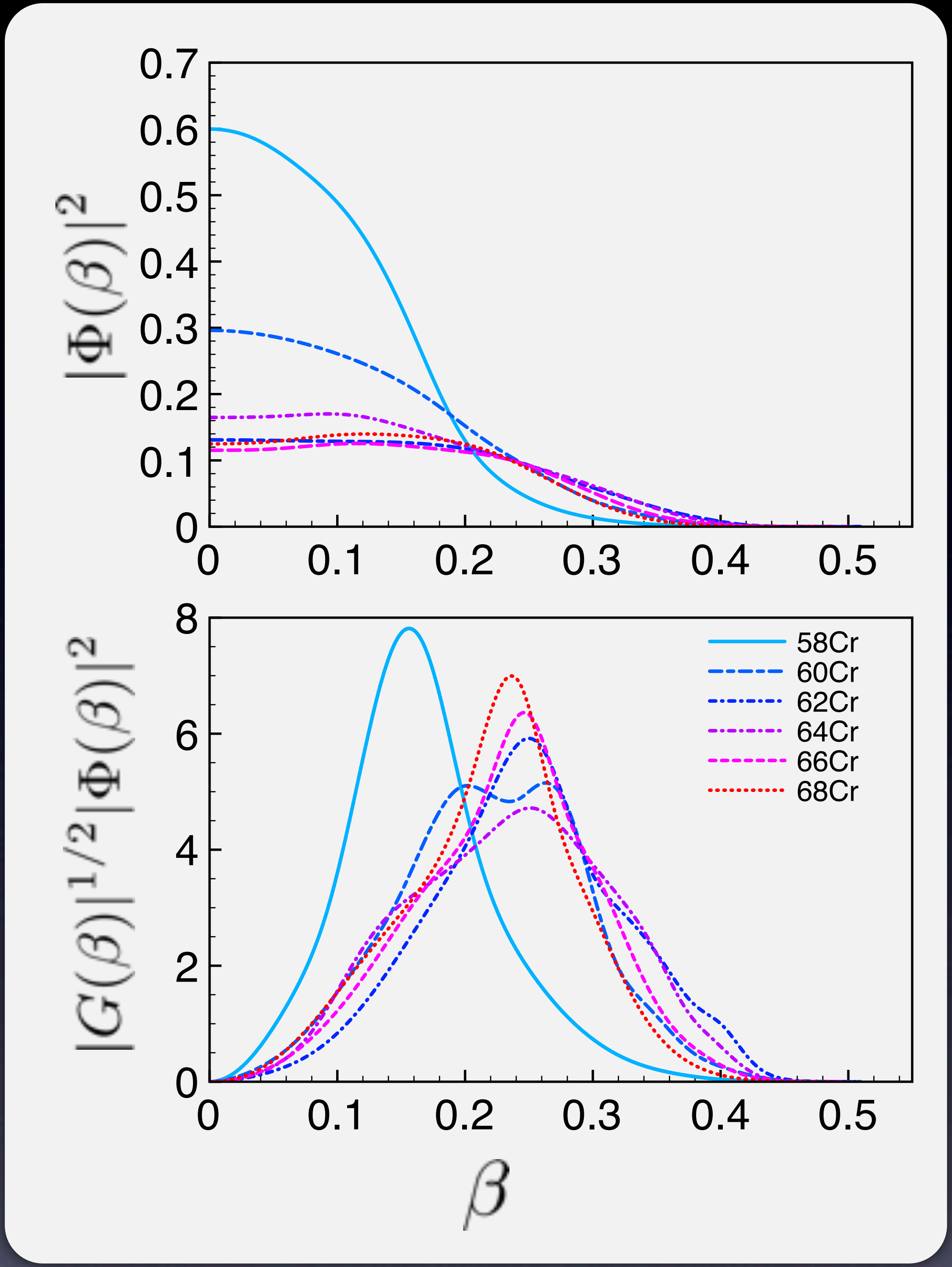
$$\mathcal{M}_\beta = \left(\frac{dq_\nu}{d\beta} \right)^2 = \frac{1}{\eta^2} \left(\frac{dq_\nu}{dQ_{20}} \right)^2$$

$$\frac{dQ_{20}}{dq_\nu} = \frac{d}{dq_\nu} \langle \hat{Q}_{20} \rangle = \langle [\hat{Q}_{20}, \frac{1}{i} \hat{\mathcal{P}}_\nu] \rangle$$

Cr

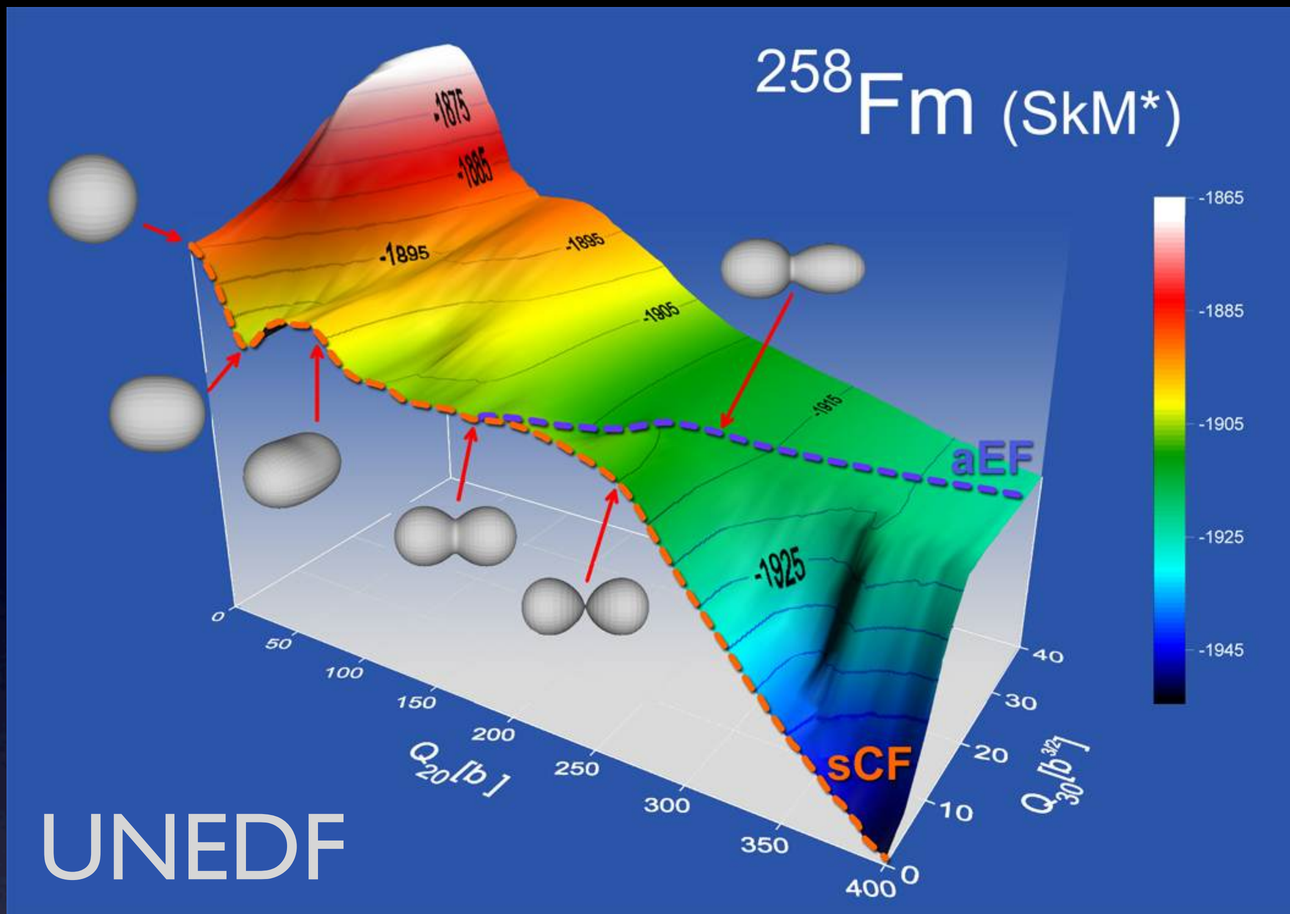


critical point at ^{60}Cr



KY, N. HInohara, PRC83(2011)061302R

Toward a microscopic description of fission dynamics

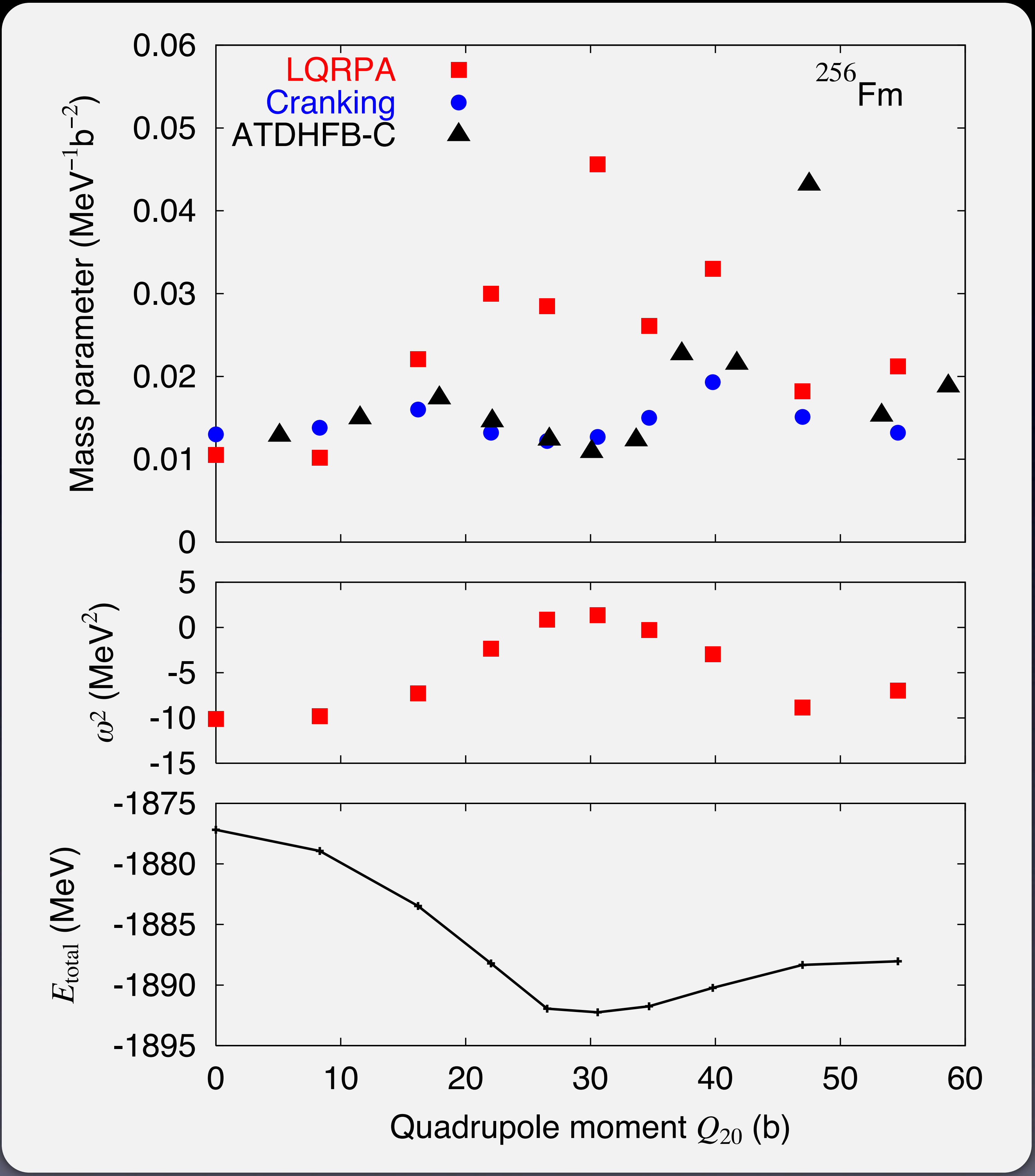


Collective Hamiltonian for fission

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

Parameters we need to evaluate microscopically

Vibrational mass parameter of the fissioning ^{256}Fm



comparison with

ATDHFB-cranking

SkM* + mixed-type pairing

A. Baran *et al*., PRC84(2011)054321

Cranking

$$M_\beta^{\mathrm{cr}} = \frac{1}{2}(S_1^{-1} S_3 S_1^{-1})$$

$$S_n = \sum_{\mu\nu} \frac{|\langle \mu\nu | \hat{Q}_{20} | \phi \rangle|^2}{(E_\mu + E_\nu)^n}$$

Summary

Skyrme-EDF based QRPA for deformed nuclei

- enhanced dipole strength in low-energy region
- deformation: coupling between the IS dipole and LEOR

Skyrme-EDF based Collective Hamiltonian

- shape-phase transition in neutron-rich Cr isotopes
- critical point from spherical to quadrupole deformed shape at around ^{60}Cr

Toward a microscopic description of fission dynamics based on Skyrme EDF