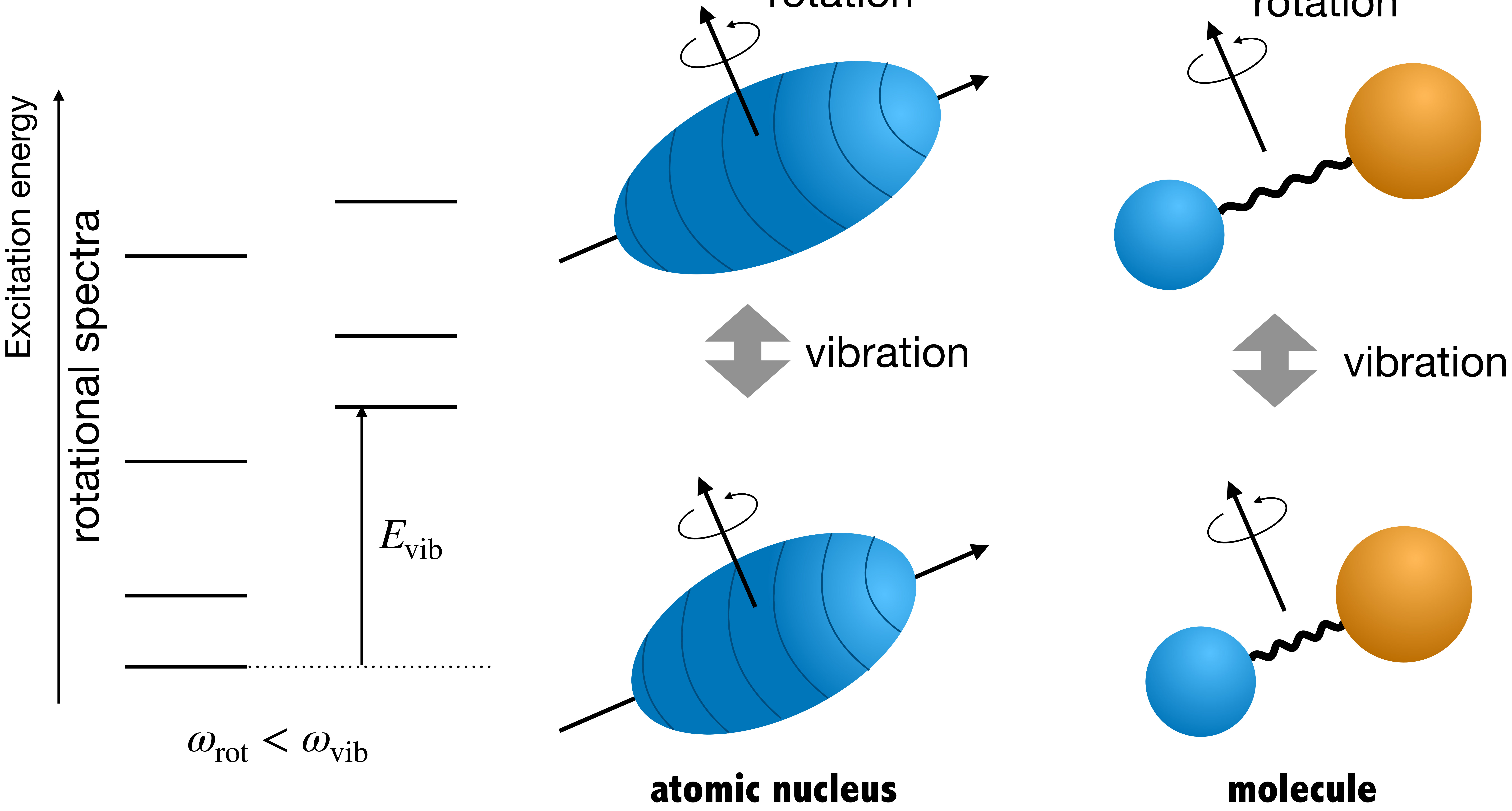
Linear-response TDDFT for rotating nuclei

—Nuclear DFT for rovibrational motions—

Kenichi Yoshida
(Kyoto U.)

Collective motions



TDDFT for vibration

vibration around the ground state: $\rho(\mathbf{r},t) = \underline{\rho_0(\mathbf{r})} + \delta\rho(\mathbf{r},t) + \mathrm{h.c.}$

Kohn–Sham (–Bogoliubov–de Gennes)

linear response to the external field: $e^{-i\omega t}\hat{F} = e^{-i\omega t}\int d\mathbf{r} f(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$

$$\delta\rho(\mathbf{r},t) \sim \delta\rho(\mathbf{r})e^{-i\omega t} \qquad \delta\rho(\mathbf{r}) = \int d\mathbf{r}'\chi_0(\mathbf{r},\mathbf{r}')\left[\frac{\delta^2 E[\rho]}{\delta^2\rho}\bigg|_{\rho=\rho_0}\delta\rho(\mathbf{r}') + f(\mathbf{r}')\right]$$

vibration in space/spin-space/isospin-space/gauge-space and coupling among them

$$\hat{F}_L = \int dr \sum_{\sigma\sigma'}\sum_{\tau\tau'} r^L Y_L(\hat{r}) O(\sigma\tau,\sigma'\tau')\hat{\psi}^\dagger(\boldsymbol{r}\sigma\tau)\hat{\psi}(\boldsymbol{r}\sigma'\tau') \quad \text{or} \quad \hat{\psi}^\dagger(\boldsymbol{r}\sigma\tau)\hat{\psi}^\dagger(\boldsymbol{r}\tilde{\sigma}'\tilde{\tau}')$$

rich variety of modes of vibration

Development and application to vibrations in deformed nuclei

Skyrme EDF

Matrix-QRPA

K. Yoshida+, PRC78(2008)064316

C. Losa+, PRC81(2010)064307

J. Terasaki+, PRC82(2010)034326

Linearized TDDFT

S. Ebata+, PRC82(2010)034306

G. Scamps+, PRC89(2014)034314

FAM-QRPA

M. Stoitsov+, PRC84(2011)041305

M. Kortelainen+, PRC92(2015)051302R

K. Washiyama+, PRC96(2017)041304R

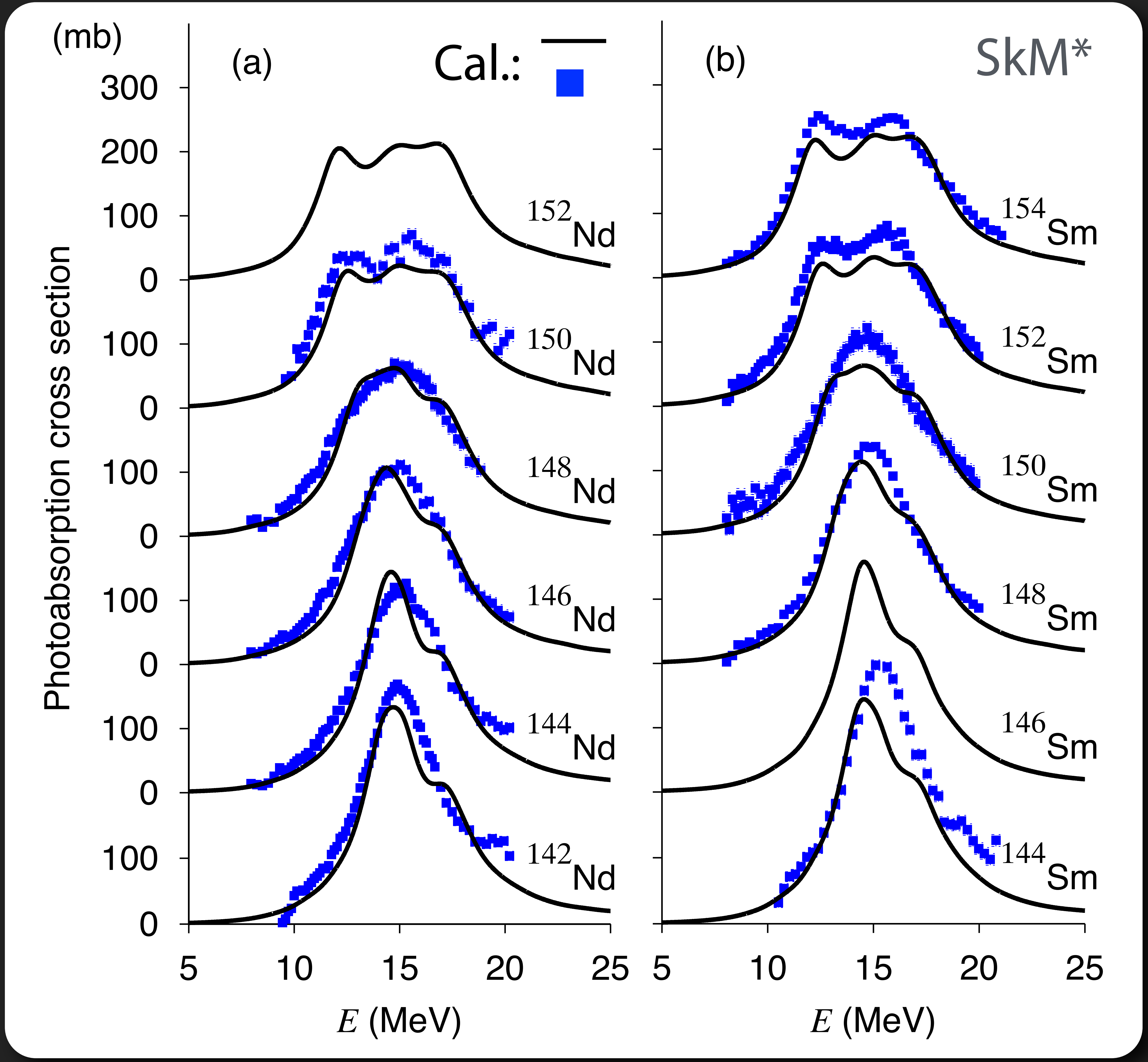
Gogny EDF

S. Péru+, PRC77(2008)044313

Relativistic EDF

D. P. Arteaga+, PRC79(2009)034311

T. Nikšić+, PRC88(2013)044327



N=92

N=82

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

TDDFT for rotation

KS Hamiltonian

TDKS eq.: $i\partial_t \phi_i(t) = h[\rho(t)]\phi_i(t)$ $\qquad h = \frac{\delta E}{\delta \rho} \qquad \rho = \Phi\Phi^*$

for collective rotations

$\Phi'(t) = U\Phi(t) = \exp[-i\omega_{\text{rot}}\hat{J}_x t]\Phi(t)$ a uniformly rotating system about the x-axis

$i\partial_t \phi_i'(t) = [h[\rho'(t)] - \omega_{\text{rot}} j_x]\phi_i'(t)$

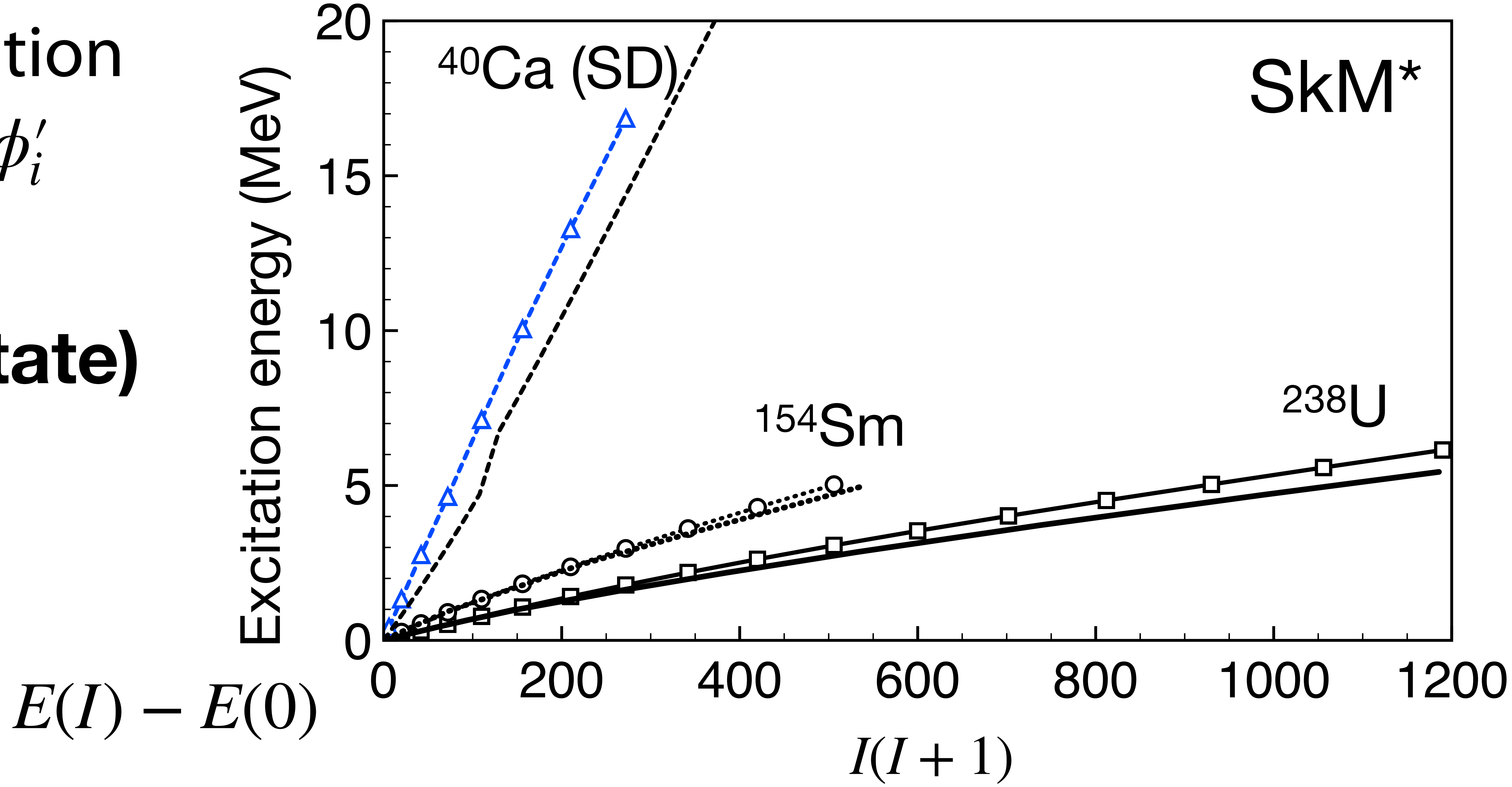
stationary ⬇ cranked KS equation

$(h - \omega_{\text{rot}} j_x)\phi_i' = e_i'\phi_i'$

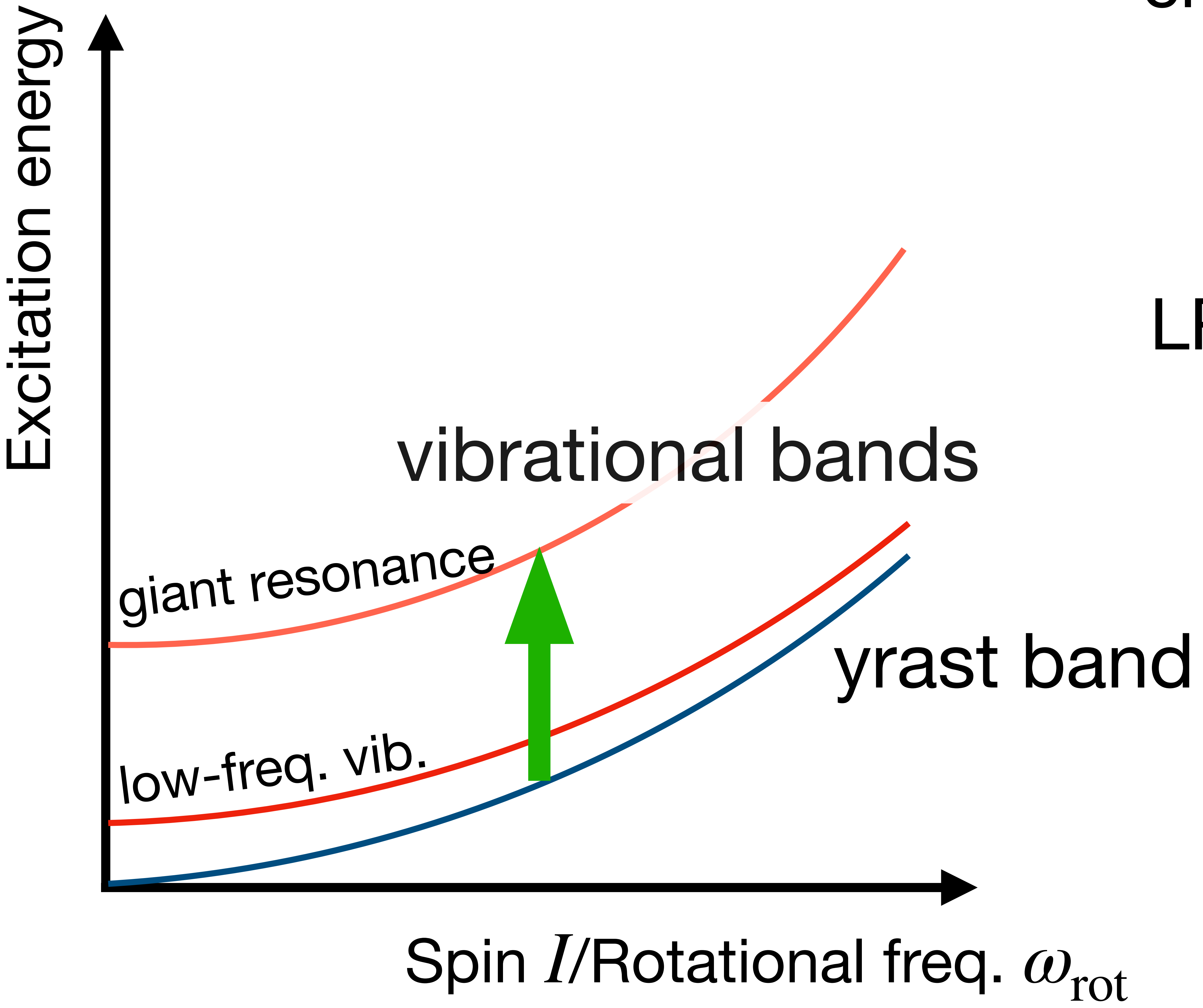
KS Routhian

yrast state (lowest energy state)

cranked KSB calculation, KY, PRC(2022)



TDDFT for vibration in a rotating nucleus



cranked KS for the yrast state $|\omega_{\rm rot}\rangle$ and $\rho_{0,\omega_{0\rm rot}}$

$$(h - \omega_{\rm rot} j_x)\phi'_i = e'_i \phi'_i$$

LR-TDDFT for vibration around the yrast state

$$\rho_{\omega_{\rm rot}}(\mathbf{r}, t) = \rho_{0,\omega_{\rm rot}}(\mathbf{r}) + \delta\rho_{\omega_{\rm rot}}(\mathbf{r}, t) + \mathrm{h.c.}$$

$$\delta\rho_{\omega_{\rm rot}}(\mathbf{r}, t) \sim \delta\rho_{\omega_{\rm rot}}(\mathbf{r}) e^{-i\omega t}$$

$$\delta\rho_{\omega_{\rm rot}}(\mathbf{r}) = \int d\mathbf{r}' \chi_{0,\omega_{\rm rot}}(\mathbf{r}, \mathbf{r}') \left[\left. \frac{\delta^2 E[\rho]}{\delta^2 \rho} \right|_{\rho=\rho_{0,\omega_{\rm rot}}} \delta\rho_{\omega_{\rm rot}}(\mathbf{r}') + f(\mathbf{r}') \right]$$

Skyrme EDF for LR-TDDFT with cranking

$$E = \int d\vec{r}\mathscr{H}(\vec{r}), \qquad \mathscr{H}(\vec{r}) = \mathscr{H}_{\text{kin}} + \mathscr{H}_{\text{Skyrme}} + \mathscr{H}_{\text{Coul}}$$

$$\mathscr{H}_{\text{Skyrme}} = \sum_{t=0,1} \sum_{t_3=-t}^{t} (\mathscr{H}_{tt_3}^{\text{even}} + \mathscr{H}_{tt_3}^{\text{odd}})$$

$$\mathcal{H}_{tt_3}^{\text{even}} = C_t^{\rho}\,\rho_{tt_3}^2 + C_t^{\Delta\rho}\,\rho_{tt_3}\Delta\rho_{tt_3} + C_t^{\tau}\,\rho_{tt_3}\tau_{tt_3} + C_t^{\nabla J}\rho_{tt_3}\,\nabla\cdot\mathbf{J}_{tt_3} + C_t^{J}\overleftrightarrow{J}_{tt_3}^2$$

$$\mathcal{H}_{tt_3}^{\text{odd}} = C_t^{s}\,\mathbf{s}_{tt_3}^2 + C_t^{\Delta s}\,\mathbf{s}_{tt_3}\cdot\Delta\mathbf{s}_{tt_3} + C_t^{T}\,\mathbf{s}_{tt_3}\cdot\mathbf{T}_{tt_3} + C_t^{\nabla s}\,(\nabla\cdot\mathbf{s}_{tt_3})^2 + C_t^{j}\,\mathbf{j}_{tt_3}^2 + C_t^{\nabla j}\,\mathbf{s}_{tt_3}\cdot\nabla\times\mathbf{j}_{tt_3}$$

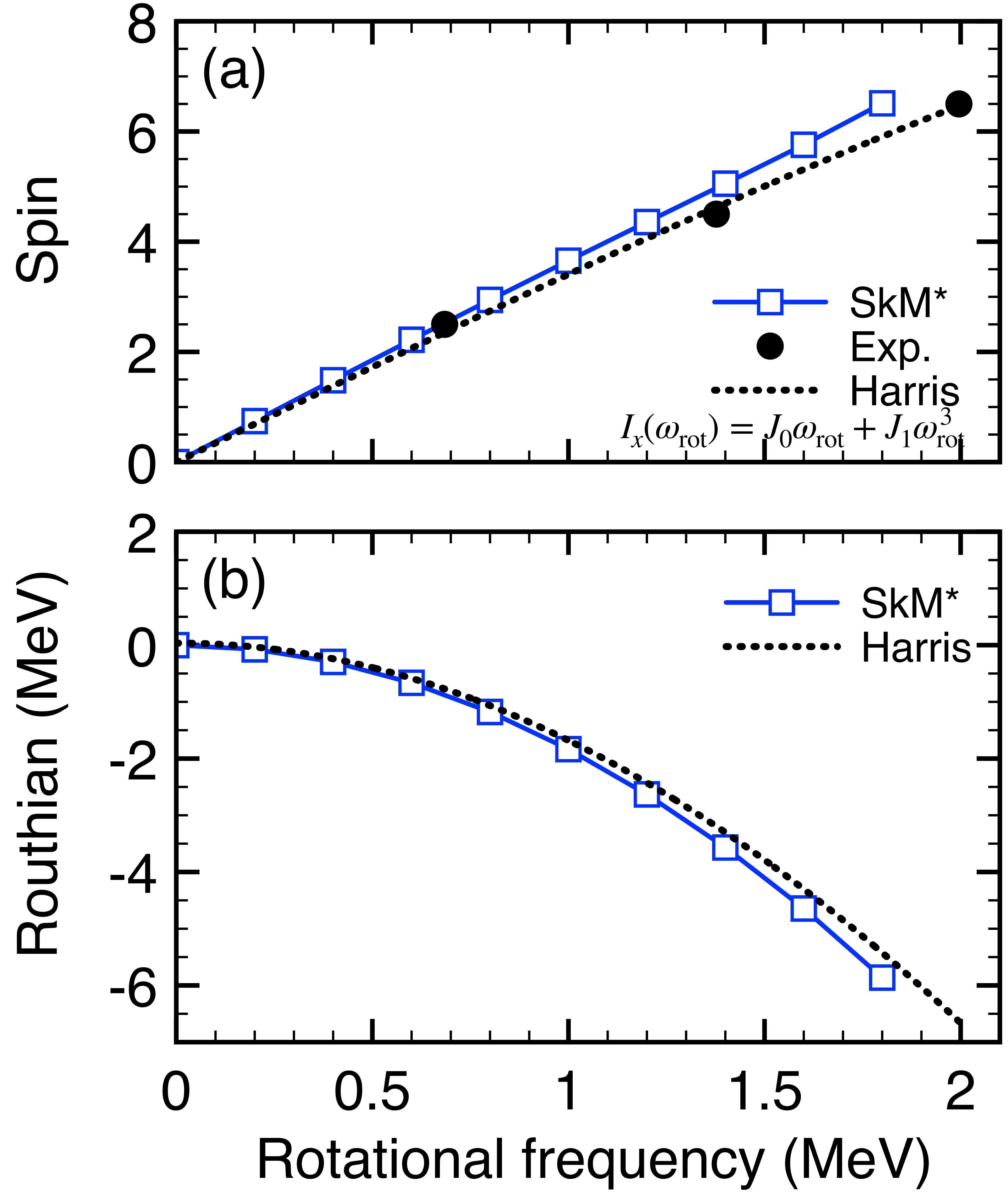
non-trivial density dependence $C_t^{\rho} = A_t^{\rho} + B_t^{\rho}\rho_{00}^{\alpha}, \quad C_t^{s} = A_t^{s} + B_t^{s}\rho_{00}^{\alpha}$

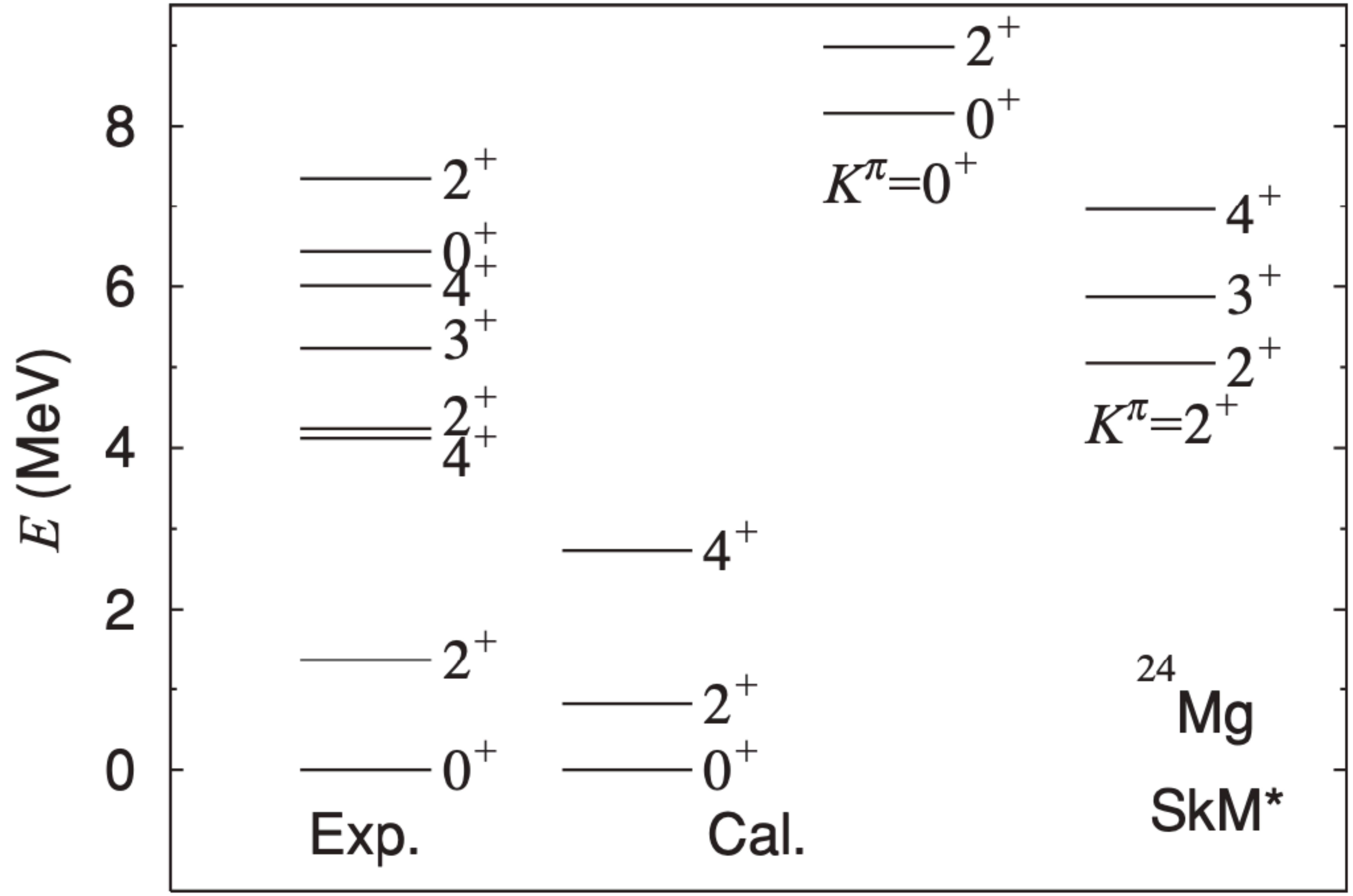
rearrangement terms

non only $\rho_{0,\omega_{\text{rot}}}$ but $\mathbf{s}_{0,\omega_{\text{rot}}}$ enter into the residual int. $\left.\frac{\delta^2 E[\rho]}{\delta^2\rho}\right|_{\rho=\rho_{0,\omega_{\text{rot}}}}$ at $\omega_{\text{rot}} \neq 0$

Numerical application

ground band



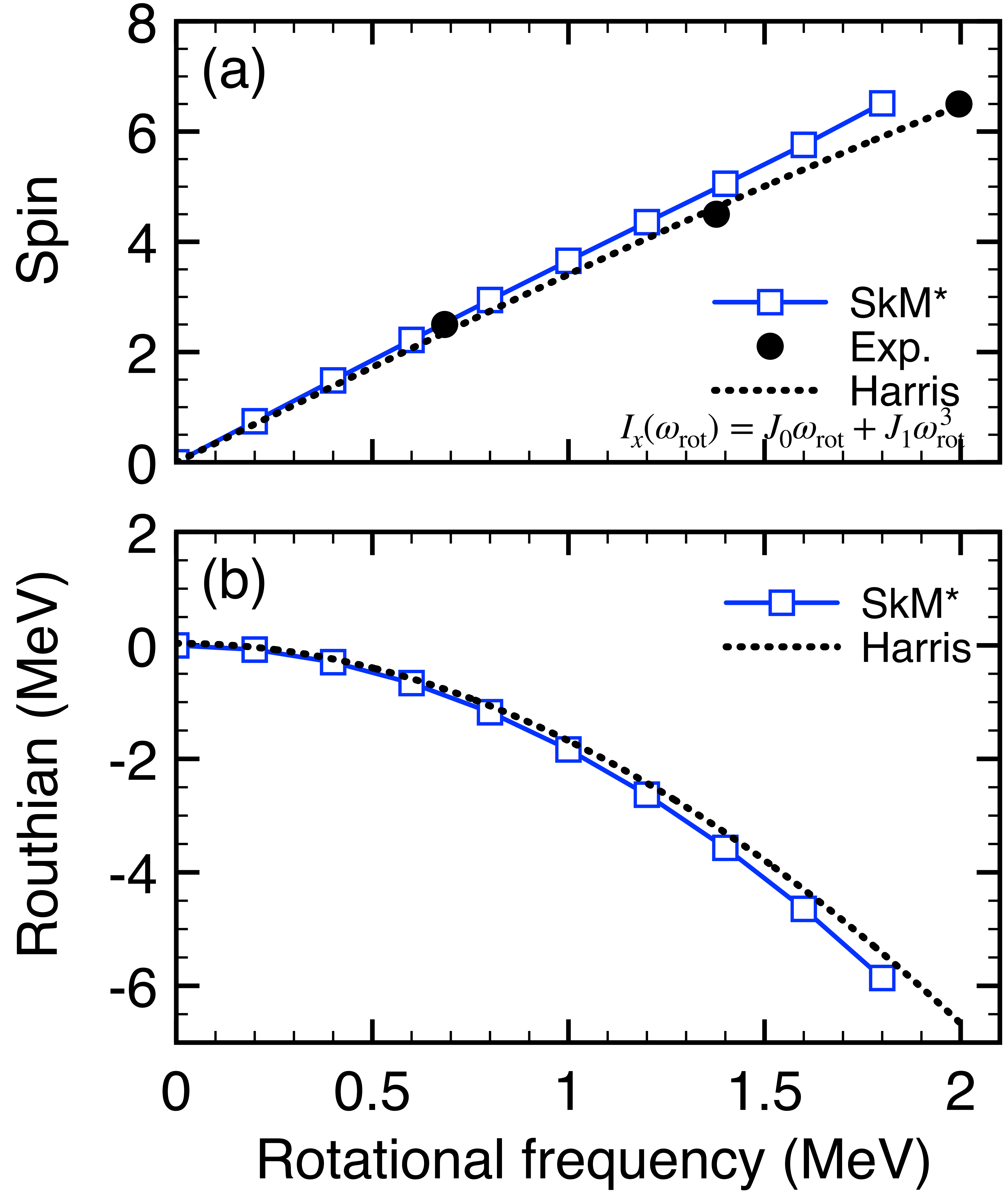


KY, N. Van Giai, PRC78(2008)064316

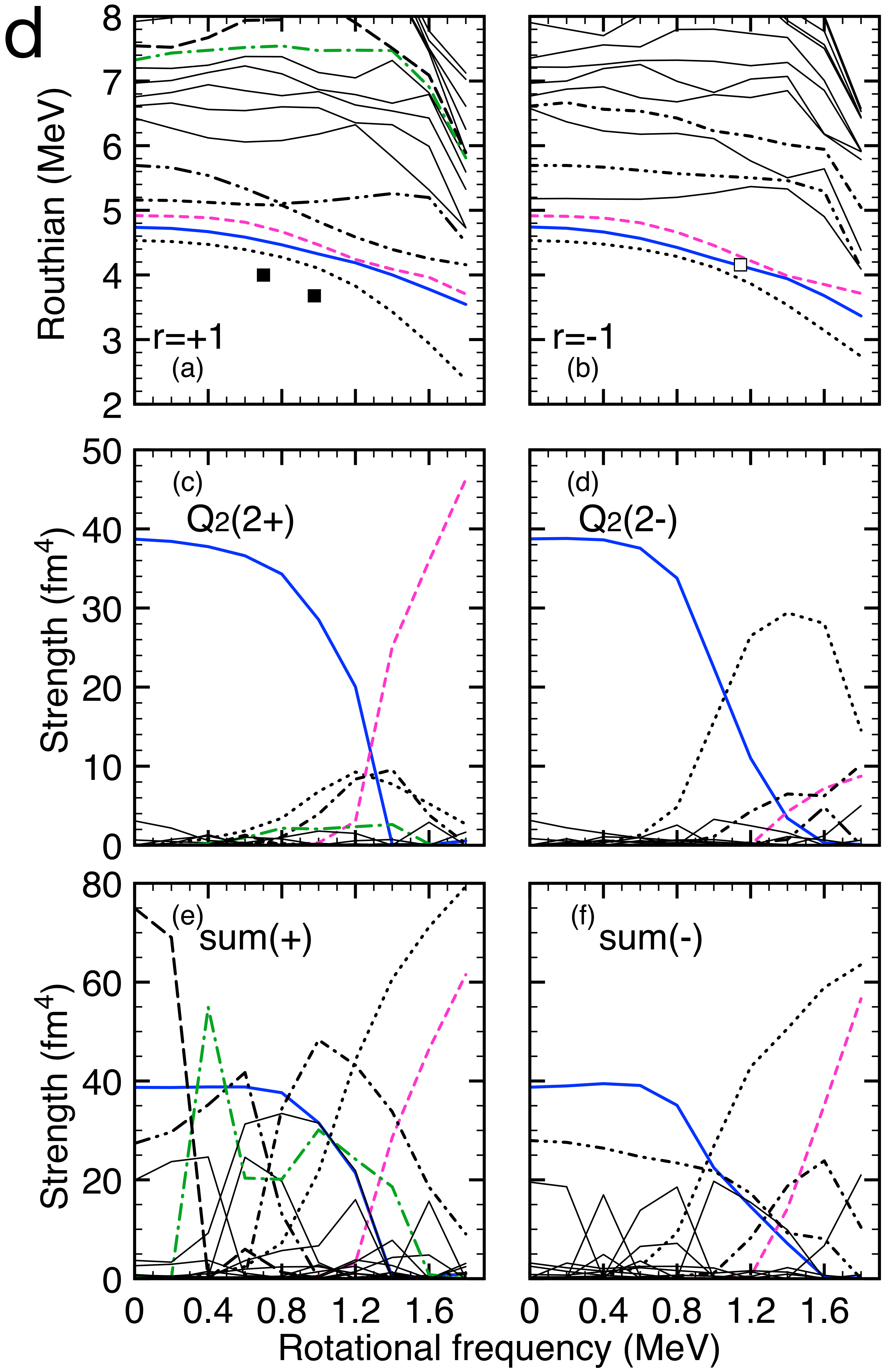
$$E(I,K) = \omega_{\rm RPA} + \frac{I(I+1)-K^2}{2\mathscr{J}_{\rm TV}}$$

Collective vibrations in rotating ^{24}Mg

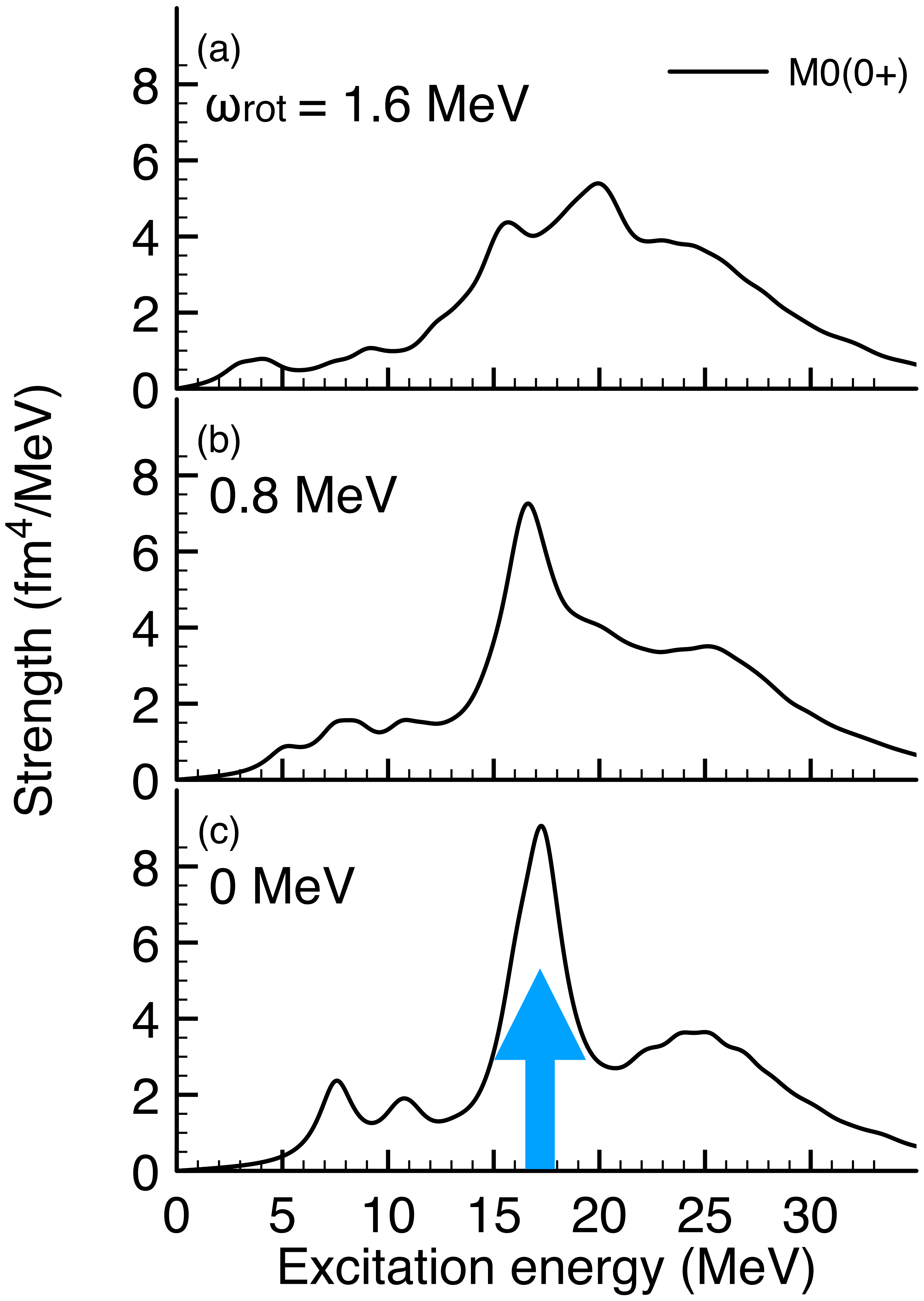
ground band

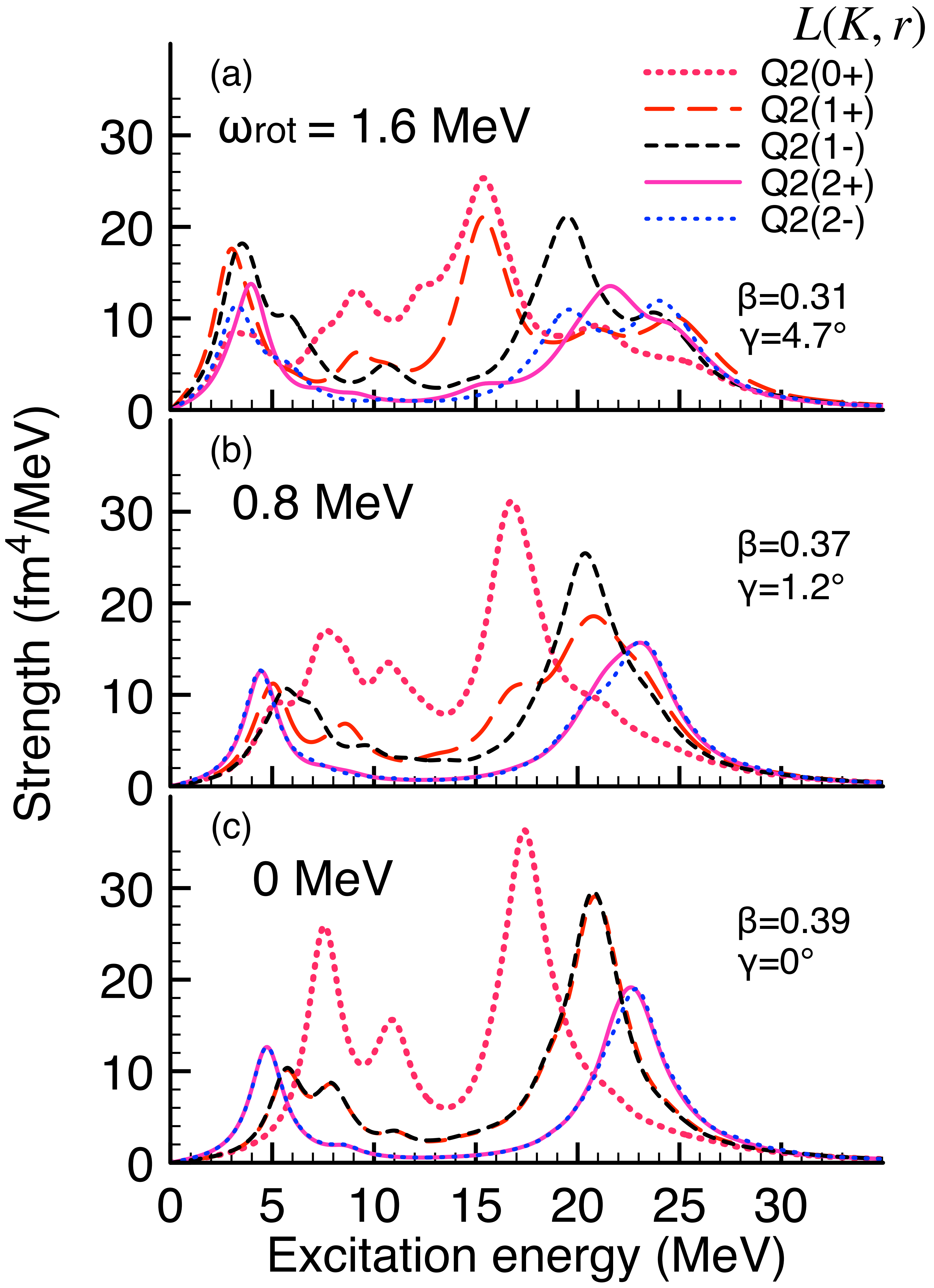


gamma band

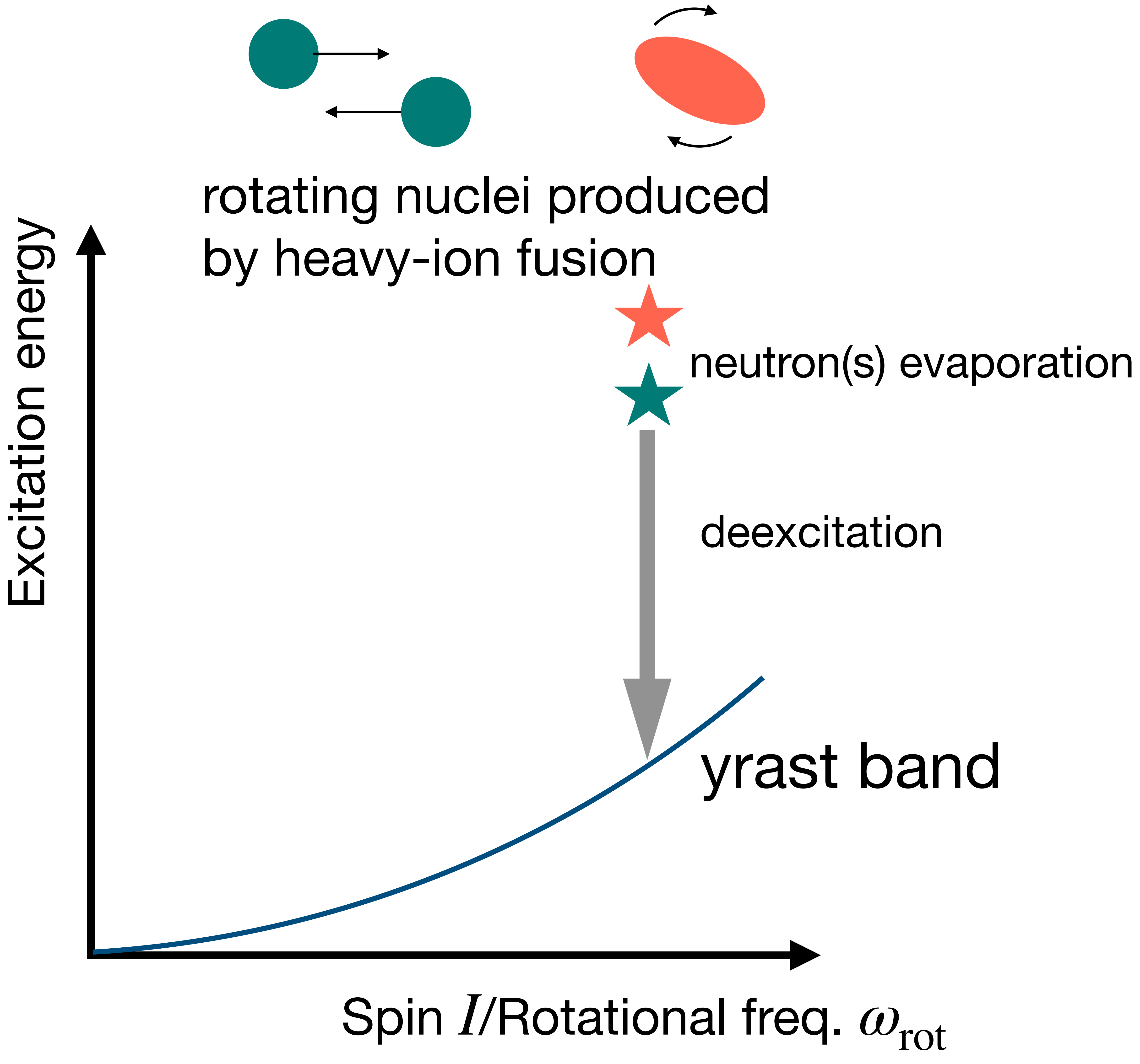


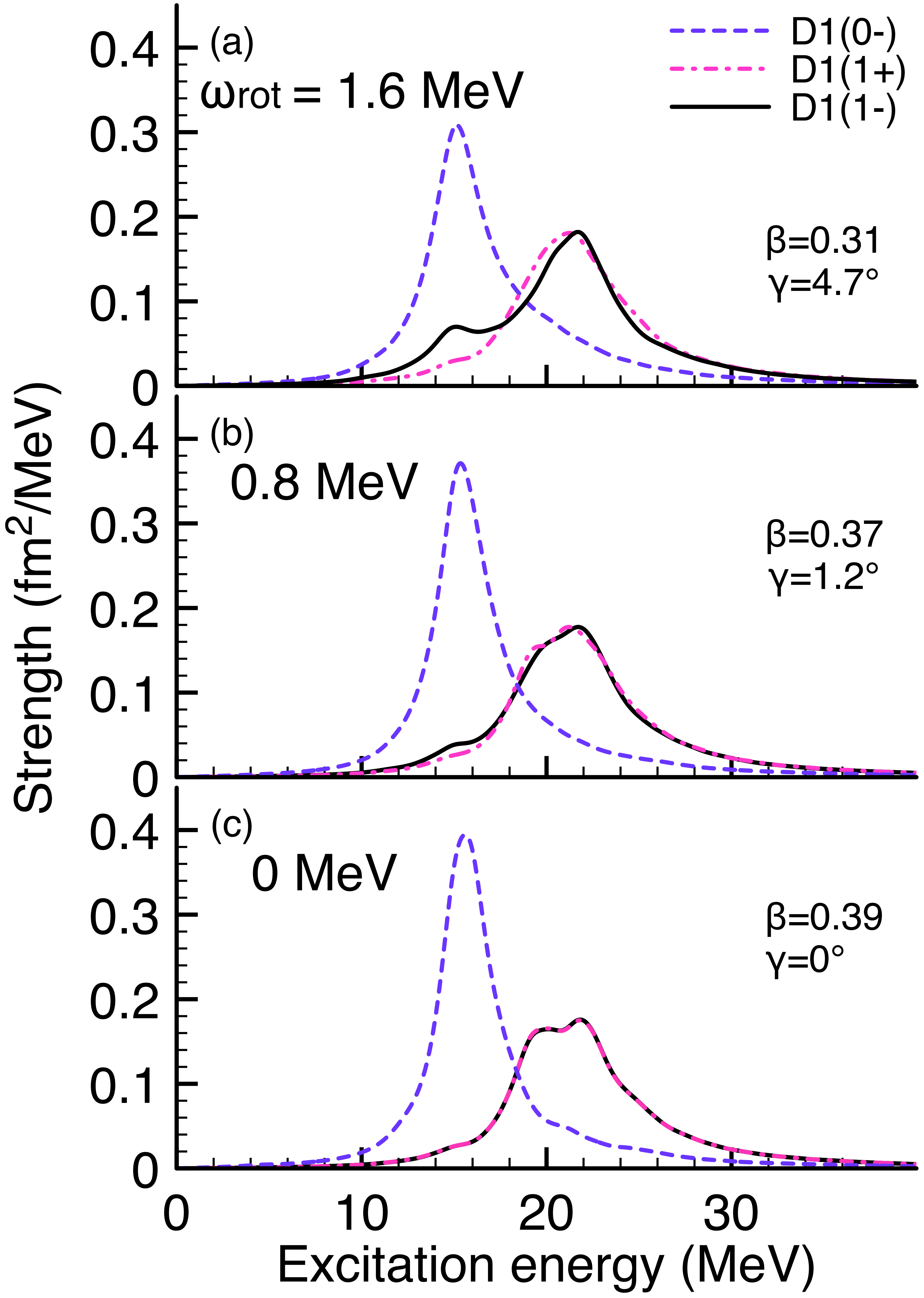
Giant monopole/quadrupole resonances





IV dipole resonance





Summary

First attempt to describe vibrations in rotating nuclei within TDDFT

Numerical application to the γ vibration and giant resonances in ^{24}Mg

- the observed γ band is well described

  c.f. GCM (multi-slater dets. calc.) overestimates the energy

- rotational effects on multipole responses
  - broadening of a width of GMR/GQR: K is no longer a good quantum number
  - GDR is less sensitive to the rotation

Triaxial GCM by M. Bender et al. (2008)