Finite amplitude method and its applications

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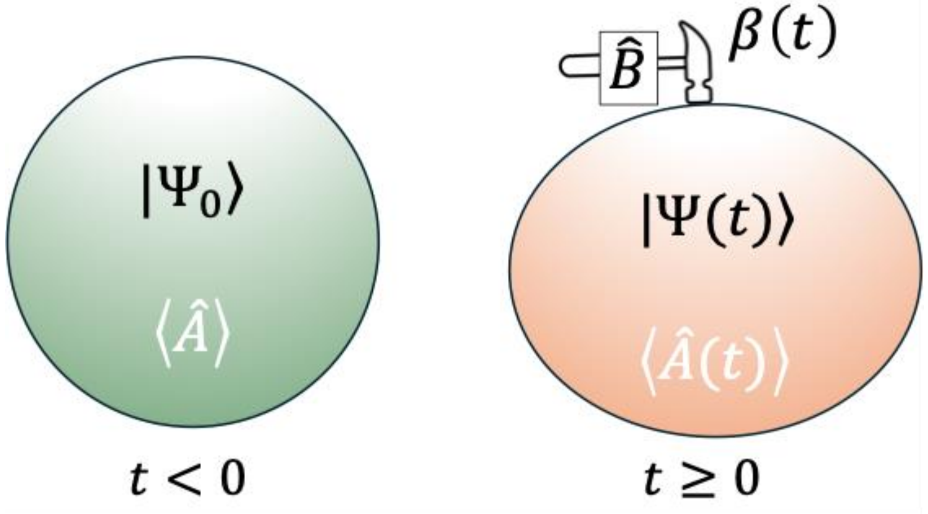
Linear response (LR) theory



Time-dependent perturbation

$$\hat{H}_P(t) = \beta(t)\hat{B}, \qquad \beta(t) = 0 \text{ for } t < 0$$

Linear response in an observable $\hat{A}$

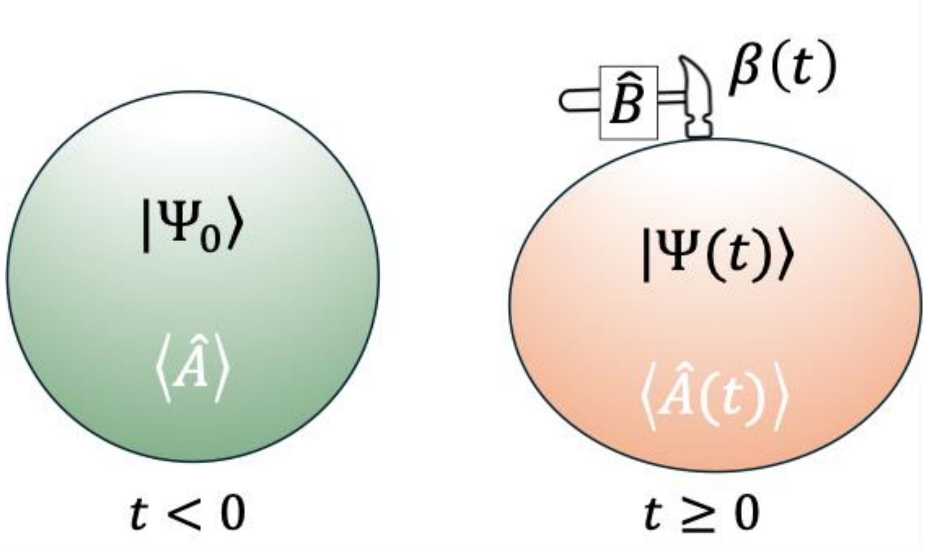
$$\delta\langle\hat{A}(t)\rangle \equiv \langle\Psi(t)|\hat{A}|\Psi(t)\rangle - \langle\Psi(t)|\hat{A}|\Psi(t)\rangle\Big|_{H_P=0}$$

$$= \int \chi_{AB}(t-t')\beta(t')dt'$$

Response function

$$i\chi_{AB}(t-t') \equiv \theta(t-t')\langle\Psi_0|[\hat{A}_I(t-t'),\hat{B}]|\Psi_0\rangle$$

Lehmann representation



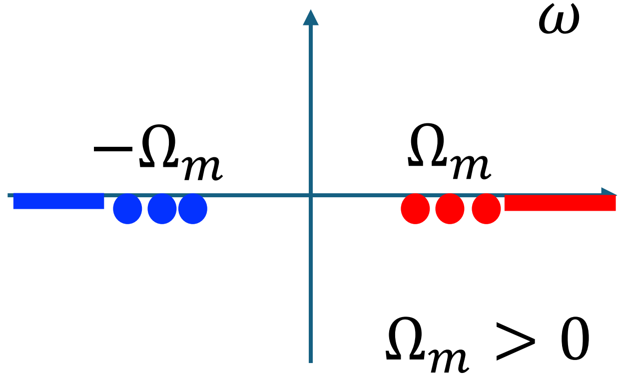
Frequency representation

$$\delta\langle \hat{A}(\omega)\rangle \equiv \chi_{AB}(\omega)\beta(\omega)$$

Response function

$$i\chi_{AB}(\omega) = \int \theta(t)\langle \Psi_0 | [\hat{A}_I(t), \hat{B}] | \Psi_0 \rangle e^{i\omega t'} dt'$$

$$\chi_{AB}(\omega) = \sum_{m>0} \left(\frac{\langle \Psi_0 | \hat{A} | \Psi_m \rangle \langle \Psi_m | \hat{B} | \Psi_0 \rangle}{\omega - \Omega_m + i\eta} - \frac{\langle \Psi_0 | \hat{B} | \Psi_m \rangle \langle \Psi_m | \hat{A} | \Psi_0 \rangle}{\omega + \Omega_m + i\eta} \right)$$

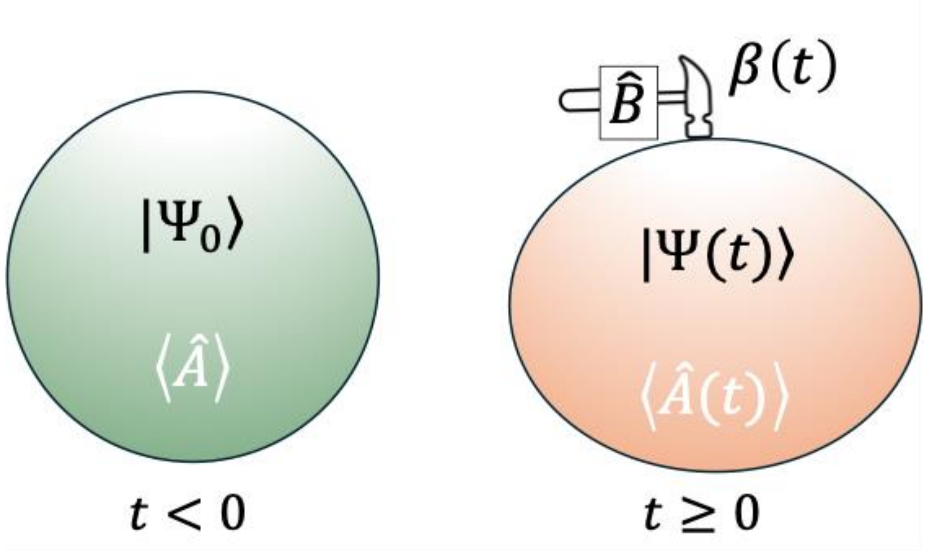


Poles at excitation energies $\Omega_m - i\eta$ and $-\Omega_m - i\eta$

$\mathrm{Im}[\chi_{AA}(\omega)] = 0 \quad \text{at } \omega \neq \pm\Omega_m$

$\omega \times \mathrm{Im}[\chi_{AA}(\omega)] \leq 0$

Energy dissipation



$$\hat{H}_P(t) = \beta(t)\hat{V} = \beta(t)\int v(\boldsymbol{r})\hat{n}(\boldsymbol{r})d\boldsymbol{r}$$

Excitation rate = work at unit time

$$\frac{dE}{dt} = \beta(t)\int\{-\nabla v(\boldsymbol{r})\}\cdot\boldsymbol{j}(\boldsymbol{r},t)d\boldsymbol{r}$$

$\boldsymbol{j}(\boldsymbol{r},t)$: Current density

Assuming a fixed frequency perturbation, $\beta(t) = \beta_0\cos\omega t$

$$\frac{d\bar{E}}{dt} = \frac{\omega}{2\pi}\int_0^{2\pi/\omega}\frac{dE}{dt}dt = -\frac{\beta_0^2}{2}\omega\times\mathrm{Im}[\chi_{VV}(\omega)]$$

$$\omega\times\mathrm{Im}[\chi_{AA}(\omega)] \leq 0$$

$$\Rightarrow \boxed{\frac{d\bar{E}}{dt} > 0}$$

Fluctuation-dissipation theorem at $T = 0$

$$\boxed{\mathrm{Im}[\chi_{VV}(\omega)] = -\pi[S_{VV}(\omega) - S_{VV}(-\omega)]}$$

Strength function ≈ "Fluctuation"

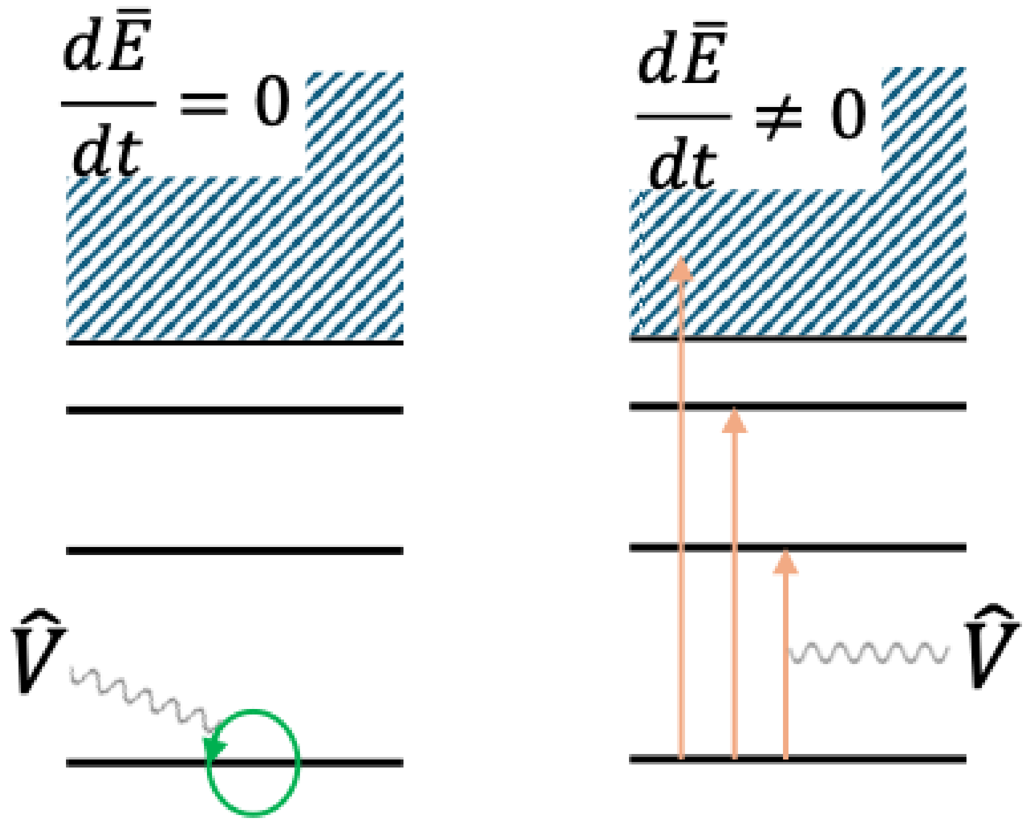
$$S_{VV}(\omega) = \sum_{m>0} \left|\langle\Psi_m|\hat{V}|\Psi_0\rangle\right|^2 \delta(\omega - \Omega_m)$$

<u>Generalized form</u>

$$\boxed{\chi^D_{AB}(\omega) = -\pi[S_{AB}(\omega) - S_{AB}(-\omega)]}$$

$$\chi_{AB}(\omega) = \chi^P_{AB}(\omega) + i\chi^D_{AB}(\omega)$$

$$S_{AB}(\omega) = \sum_{m>0} \langle\Psi_0|\hat{A}|\Psi_m\rangle\langle\Psi_m|\hat{B}|\Psi_0\rangle\delta(\omega - \Omega_m)$$



(a) $(\Delta V)^2 = 0$

(b) $(\Delta V)^2 \neq 0$

Finite temperature: $T \neq 0$

Response function

$$i\chi_{AB}(t) \equiv \theta(t)\mathrm{Tr}\left[\frac{e^{-\beta H}}{Z}\left[\hat{A}_I(t),\hat{B}\right]\right]$$

$$\chi_{AB}(\omega) = \sum_{m,n}\left(\frac{\langle\Psi_n|\hat{A}|\Psi_m\rangle\langle\Psi_m|\hat{B}|\Psi_n\rangle}{\omega-\Omega_{mn}+i\eta} - \frac{\langle\Psi_n|\hat{B}|\Psi_m\rangle\langle\Psi_m|\hat{A}|\Psi_n\rangle}{\omega+\Omega_{mn}+i\eta}\right)$$

Fluctuation-dissipation theorem

$$\boxed{\chi_{AB}^D(\omega) = -2\pi e^{-\frac{\beta\omega}{2}}\sinh\frac{\beta\omega}{2}S_{AB}(\omega)}$$

$$S_{AB}(\omega) = \sum_{m,n}\frac{e^{-\beta E_n}}{Z}\langle\Psi_n|\hat{A}|\Psi_m\rangle\langle\Psi_m|\hat{B}|\Psi_n\rangle\delta(\omega-\Omega_{mn})$$

LR in time-dep. DFT (TDDFT)

Time-dependent Kohn-Sham equations $x \equiv (\boldsymbol{r}, t)$ $[\, x \equiv (\boldsymbol{r}, t, \sigma, \tau)\,]$

$$i\frac{\partial}{\partial t}\psi_i(x) = \left\{-\frac{1}{2m}\nabla^2 + v_{\mathrm{KS}}[n](x)\right\}\psi_i(x)$$

A virtual non-interacting system with a density-dep. KS potential

External perturbation

$$\hat{H}_P(t) = \int v(x)\hat{n}(\boldsymbol{r})d\boldsymbol{r}$$

$$\delta n(x) = \int dx'\chi_{nn}(x, x')v(x')$$

$$v_{\mathrm{KS}}(x) = v[n_0](r) + v_{\mathrm{ind}}(x)$$

$$v_{\mathrm{ind}}(x) = \frac{\delta v_{\mathrm{KS}}}{\delta n}\cdot\delta n = \int f(x, x')\delta n(x')dx'$$

$$\delta n(x) = \int dx'\chi^0_{nn}(x, x')\{v(x') + v_{\mathrm{ind}}(x')\}dx'$$

<u>Density response function (DRF)</u>

$$\boxed{\chi = \chi^0 + \chi^0 \cdot f \cdot \chi}$$

χ^0: Ind.-particle DRF

Green's function method (Continuum RPA)

$$\chi^0_{nn}(\boldsymbol{r},\boldsymbol{r}';\omega) = \sum_h \phi_h^*(\boldsymbol{r})\phi_h(\boldsymbol{r}')G^{(+)}(\boldsymbol{r},\boldsymbol{r}';\epsilon_h+\omega) + \sum_h \phi_h(\boldsymbol{r})\phi_h^*(\boldsymbol{r}')G^{(+)*}(\boldsymbol{r},\boldsymbol{r}';\epsilon_h-\omega)$$

Out-going BC for $G^{(+)}$ provides a treatment of particle decays ("escape width")

For deformed systems: Double-iteration method

Nakatsukasa & Yabana,
J. Chem. Phys. 114, 2550 (2001)
Chem. Phys. Lett. 374, 613 (2003)
Phys. Rev. C 71, 024301 (2005)

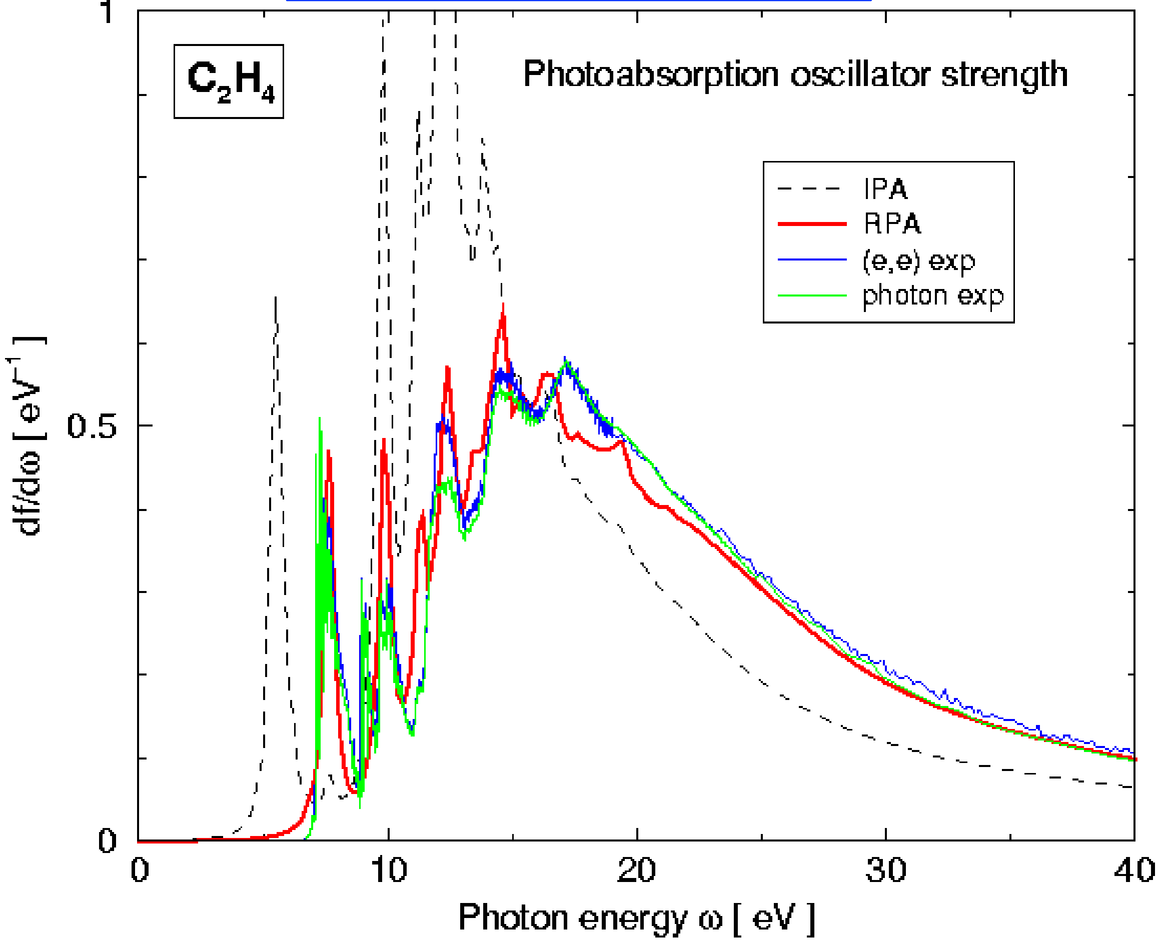
$$v = v_{\rm sph} + v_{\rm def}$$

$$\boxed{G^{(+)} = G^{(+)}_{\rm sph} + G^{(+)}_{\rm sph}\cdot v_{\rm def}\cdot G^{(+)}} \Longleftrightarrow \boxed{\chi = \chi^0 + \chi^0\cdot f\cdot\chi}$$

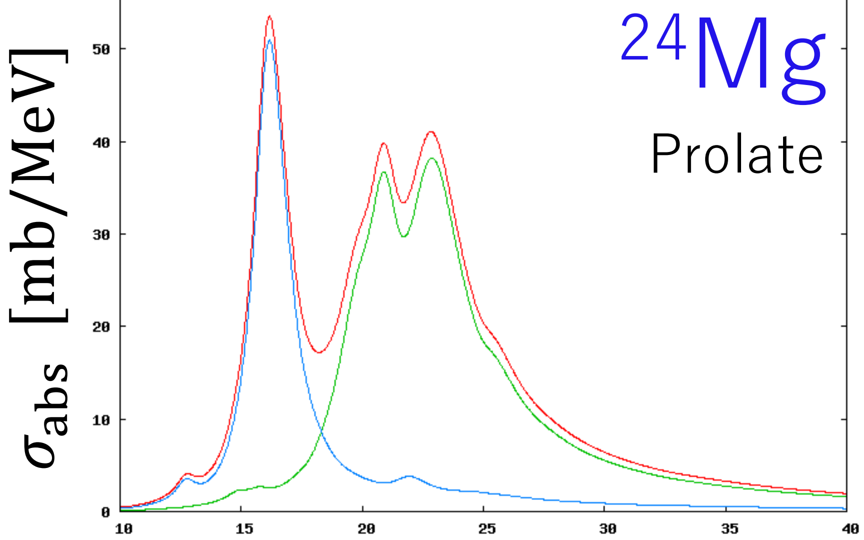
Photoabsorption

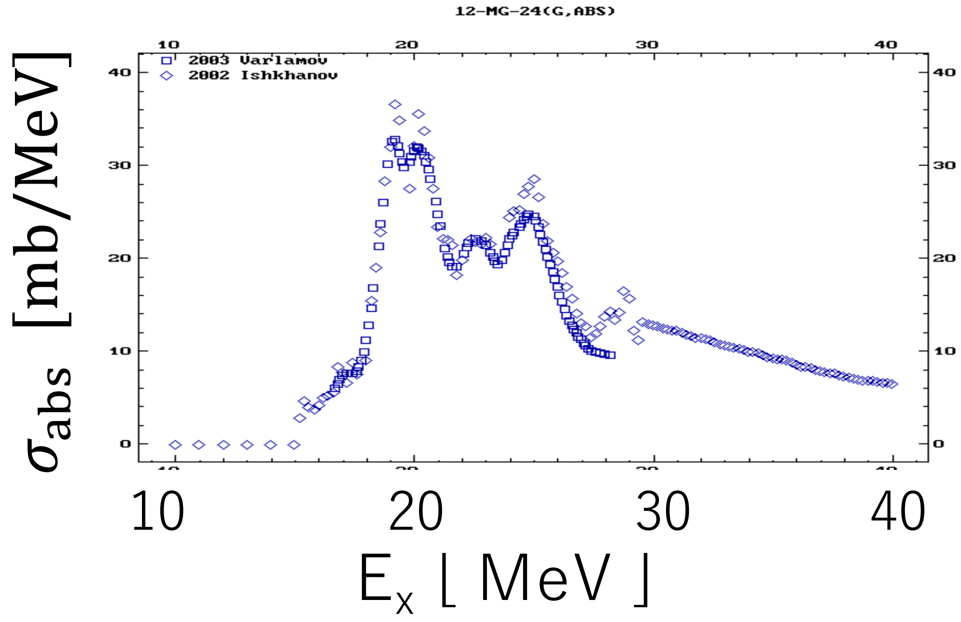
(Electric dipole)

Ethylene molecule



Magnesium nucleus





Finite amplitude method (FAM)

In nuclear physics application, we need to treat spin-orbit, spin-dep., isospin-dep., pair densities;

- Complicated residual kernel (interaction): $f \equiv \left.\frac{\delta v_{\mathrm{KS}}}{\delta n}\right|_{n=n_0}$

- Computationally demanding, especially for deformed nuclei

- FAM provides a solution for both problems.

FAM: A way to avoid calculation of "f"

Nakatsukasa, Inakura, Yabana, Phys. Rev. C 76, 024318 (2007)

Induced field: $v_{\mathrm{ind}}(\omega) = f \cdot \delta n(\omega)$

$$= \eta^{-1}\left(v_{\mathrm{KS}}[n_\eta] - v_0\right) + O(\eta^2)$$

$$n_\eta \equiv n_0 + \eta\delta n(\omega) = \sum_h |\tilde{\psi}_h\rangle\langle\bar{\psi}_h| + O(\eta^2)$$ *Non-hermitian*

with
$$|\tilde{\psi}\rangle = |\phi\rangle + \eta|X\rangle$$
$$\langle\bar{\psi}| = \langle\phi| + \eta\langle Y|$$

Next, how to obtain $|X\rangle$ and $\langle Y|$.

FAM: A way to avoid solution of LR equation

Instead of solving an RPA-like equation, $\left\{\begin{pmatrix} A(\omega) & B(\omega) \\ B^*(\omega) & A^*(\omega) \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\} \begin{pmatrix} X_\omega \\ Y_\omega \end{pmatrix} = - \begin{pmatrix} v(\omega) \\ v^*(\omega) \end{pmatrix}$

we may iteratively solve

$$\omega|X_h\rangle = (h_0 - \epsilon_h)|X_h\rangle + \{v(\omega) + v_{\mathrm{ind}}(\omega)\}|\phi_h\rangle$$

$$\omega\langle Y_h| = -\langle Y_h|(h_0 - \epsilon_h) - \langle\phi_h|\{v(\omega) + v_{\mathrm{ind}}(\omega)\}$$

$\Updownarrow$

$$v_{\mathrm{ind}}(\omega) = \eta^{-1}\big(v_{\mathrm{KS}}[n_\eta] - v_0\big) + O(\eta^2)$$

Developments in FAM

Review: TN, Hinohara, Eur. Phys. J. A 62, 133 (2026)

- A computationally advantageous approach to the linear response calculations
- Extensive studies of nuclear excitations, reactions, beta decays, etc.
  - Giant resonances: TN et al. (2007), Inakura&TN&Yabana (2009,2011,2013), Avogadro&TN (2011), Stoitsov et al. (2011), Niksic et al. (2013), Liang&TN (2014), Kortelainen et al. (2015), Oishi et al. (2016), Washiyama&TN (2017), Sun&Liu (2017), Sun et al. (2019), Sun (2021), Sun&Meng (2022), Sasaki et al. (2022), Washiyama et al. (2024)
  - Low-lying collective states: Avogadro&TN (2013), Hinohara et al. (2013)
  - NG modes: Hinohara&Nazarewicz (2016), Petrik&Kortelainen (2018)
  - (Double-)Beta decay: Mustonen et al. (2014), Mustonen&Engel (2016), Shafer et al. (2016), Ney et al. (2020), Hinohara&Engel (2022)
  - Particle-vibration coupling: Zhang et al. (2022), Liu et al. (2024)
  - Collective model: Wen&TN (2016,2017,2020,2022), Washiyama et al. (2021), Washiyama et al. (2024)

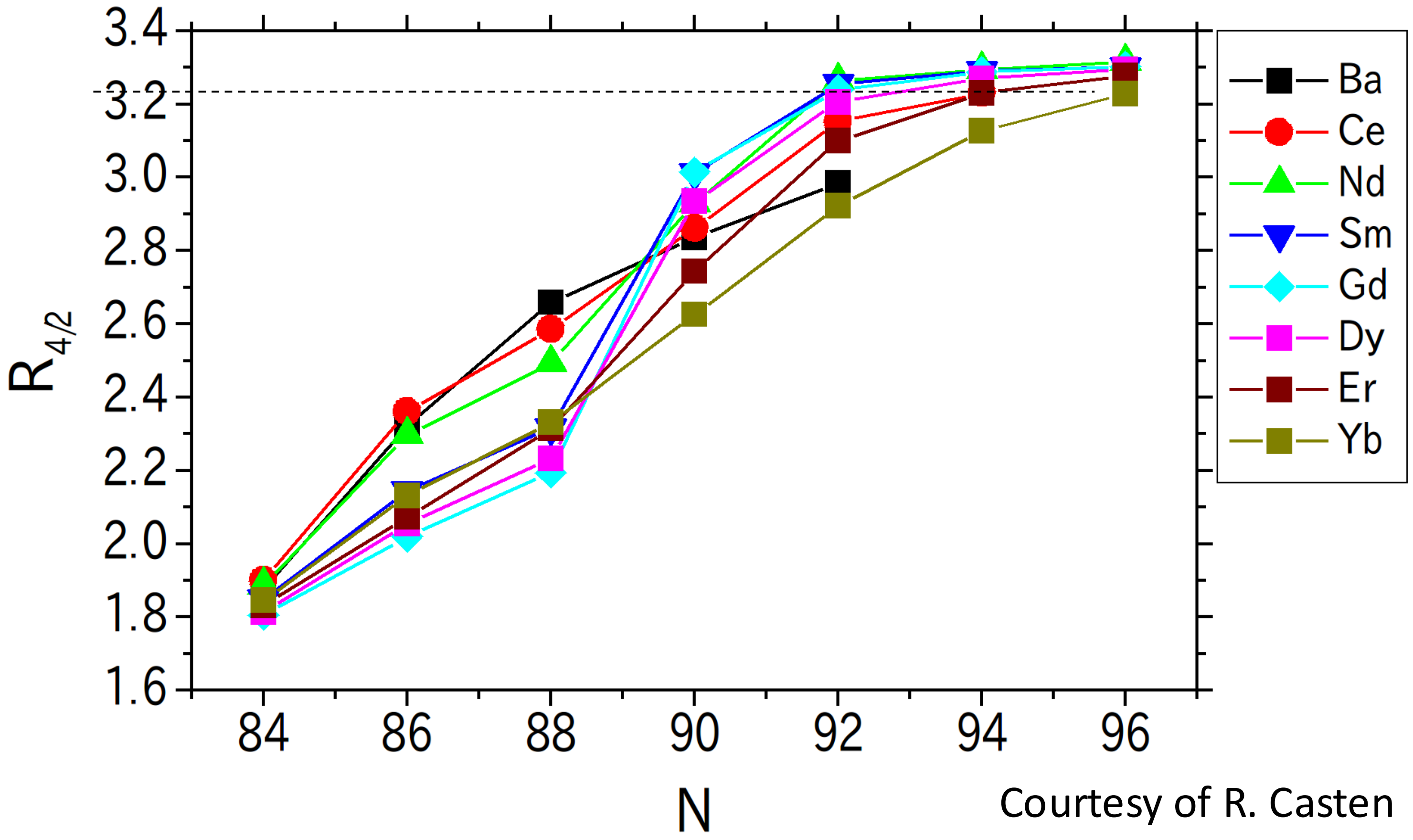
Applications of FAM to deformed nuclei

$$E_I = \frac{I(I+1)}{2\Box}$$

$\Box$

$$R_{4/2} \Box \frac{E_4}{E_2} = \frac{20}{6} = 3.33\Box$$

Pairing & deformation are essential for these isotopes

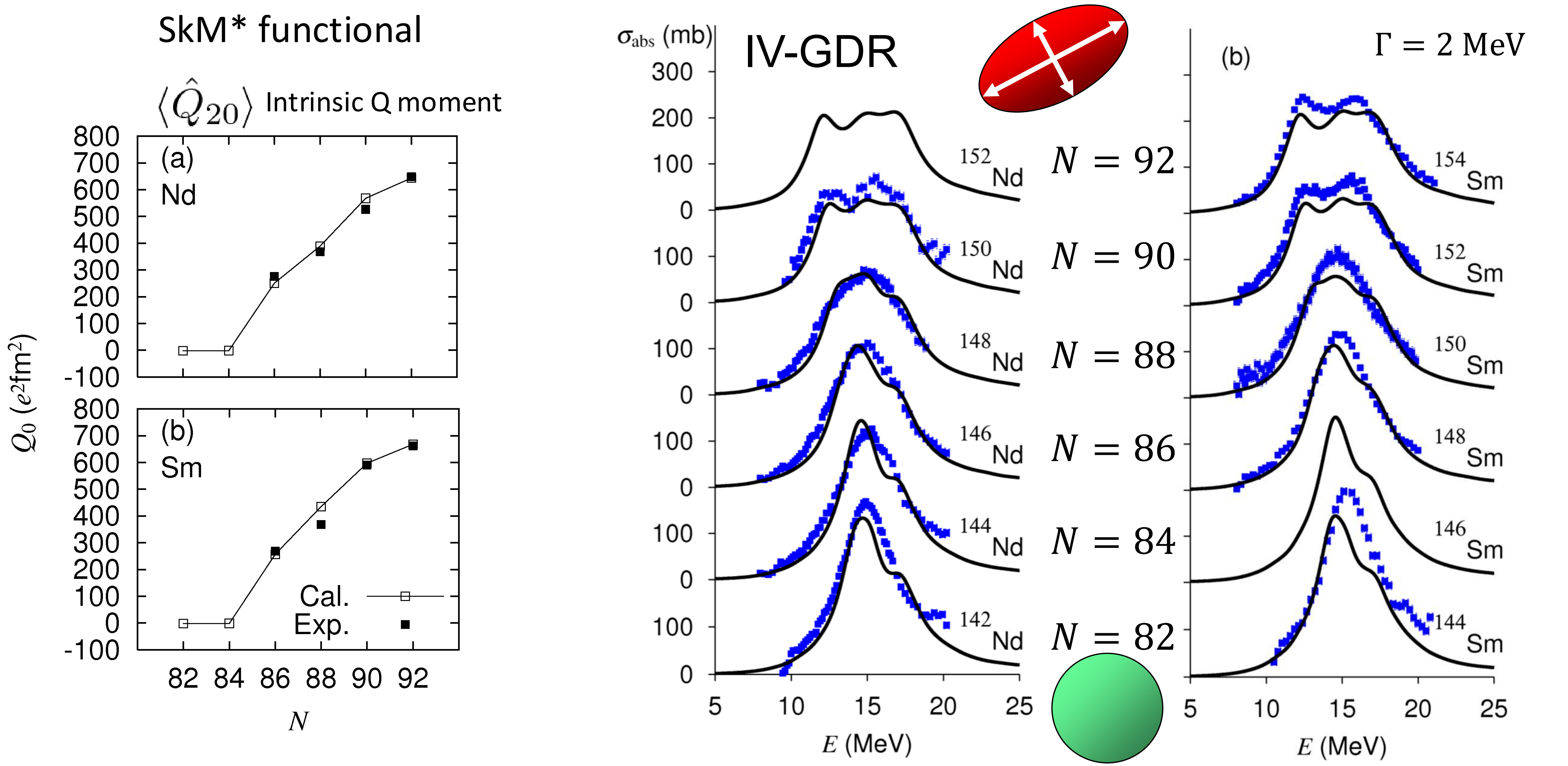


Courtesy of R. Casten

FAM to superfluid systems: Avogadro, TN, Phys. Rev. C 84, 014314 (2011)

Deformation splitting of photoabsorption peaks

Yoshida and TN, Phys. Rev. C 83, 021404 (2011)

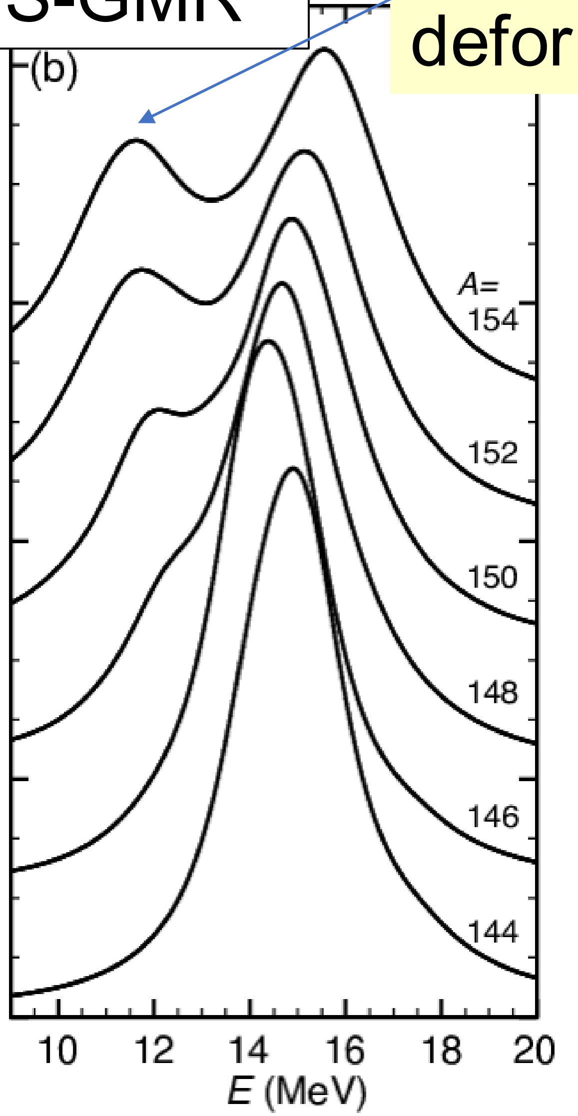


Isoscalar Giant monopole & quadrupole resonances

Yoshida and TN, Phys. Rev. C 88, 034309 (2013)

IS-GMR

Coupling due to deformation



Sm

$N = 92$

$N = 90$

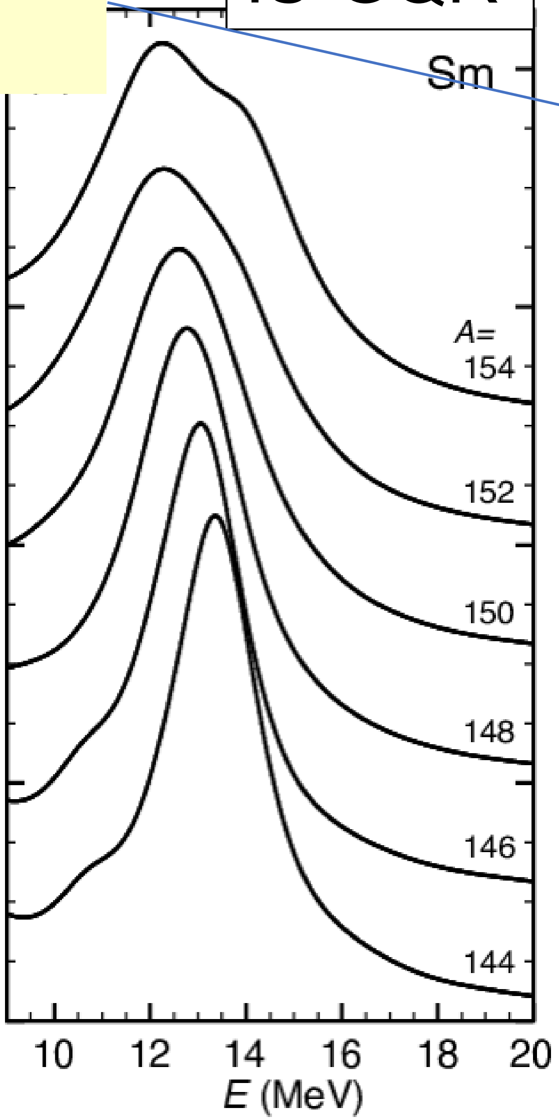
$N = 88$

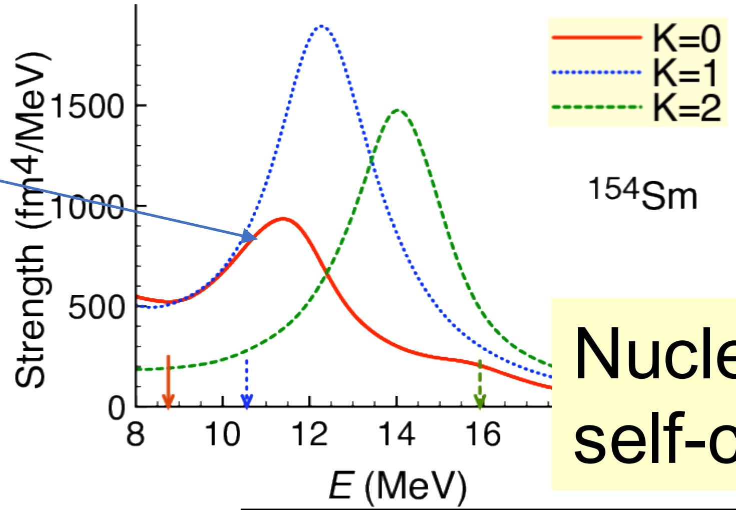
$N = 86$

$N = 84$

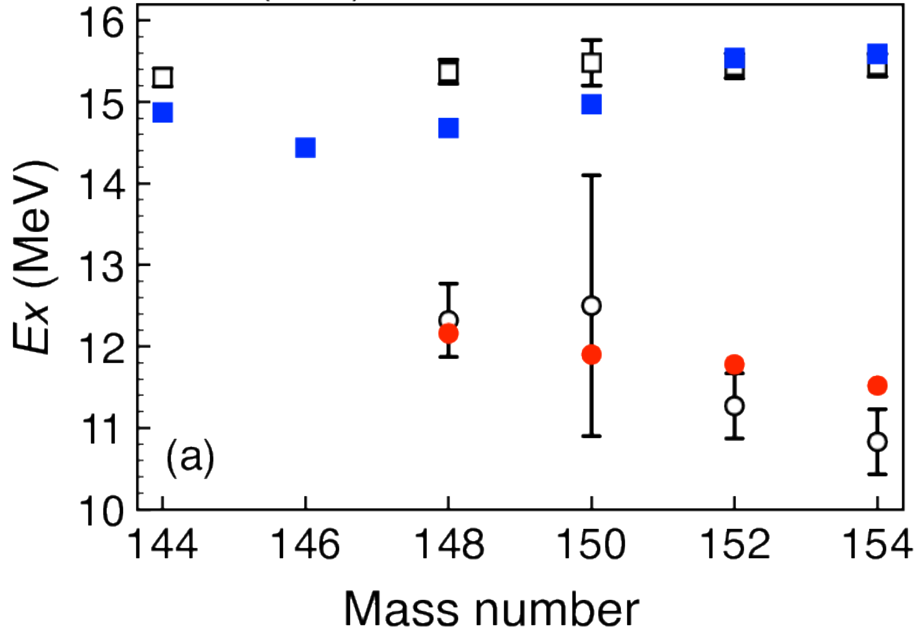
$N = 82$

IS-GQR





Nuclear self-consistency



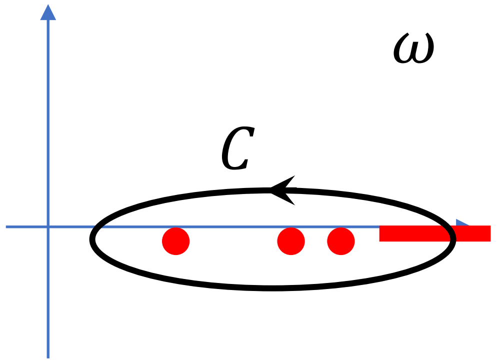
Exp: M. Itoh et al., PRC 68, 064602 (2003).

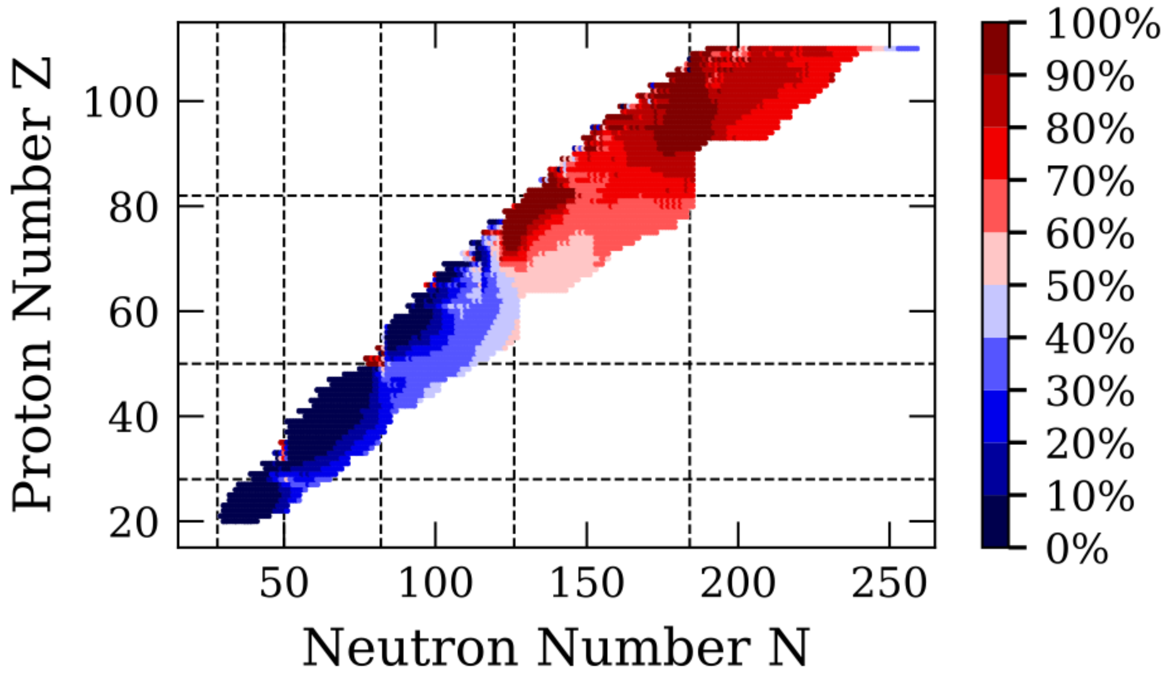
Hinohara, Kortelainen, Nazarewicz, Phys. Rev. C 87, 064309 (2013)

FAM: Eigenmodes

- Sum over eigenmodes

$$\sum_{E_i<\Omega_m<E_f} f(\Omega_m)\langle 0|\hat{A}|m\rangle\langle m|\hat{B}|0\rangle = \frac{1}{2\pi i}\oint_C f(\omega)\chi_{AB}(\omega)d\omega$$





First-forbidden contributions in β^--decay

Ney, et al., Phys. Rev. C 102, 034326 (2020)

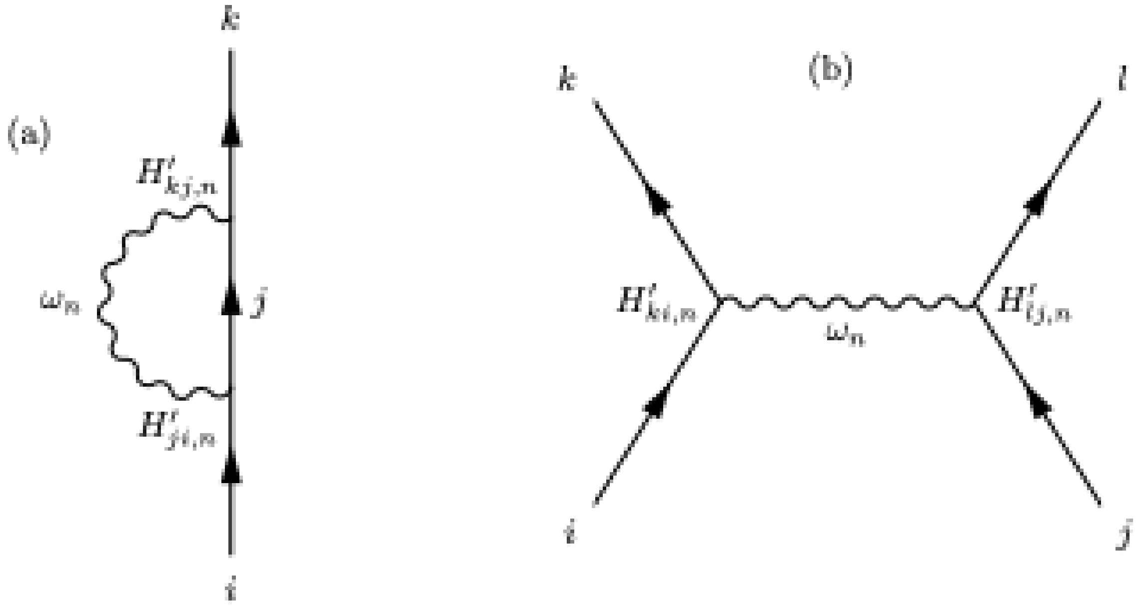
Particle-vibration coupling

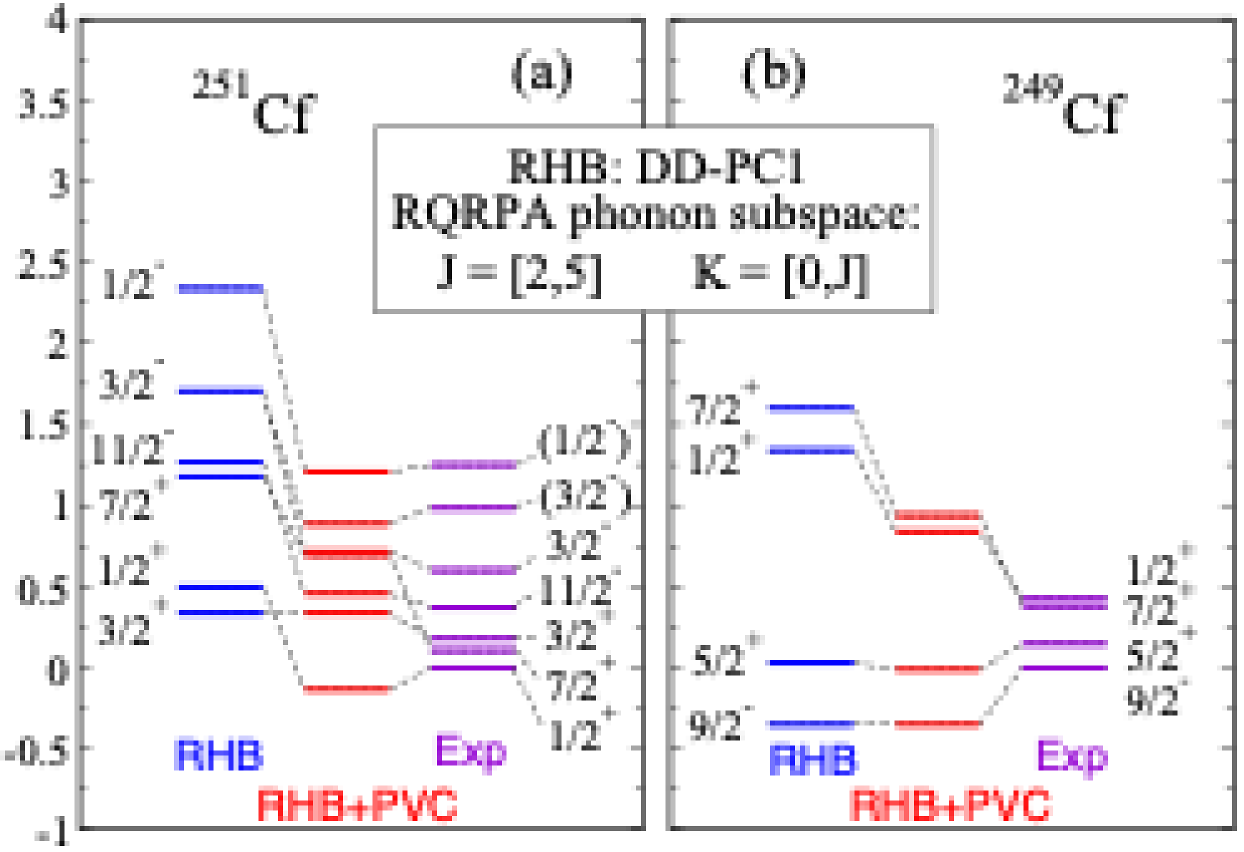
Coupling term (vertex)

$$H_{ij,m} \equiv \langle \phi_i | v_{\text{ind}}^{m} | \phi_j \rangle$$

v_{ind}^{m}: Residual field induced by δn^{m}

$$v_{\text{ind}}^{m} = \eta^{-1}\left(v_{\eta}^{m} - v_0\right)$$

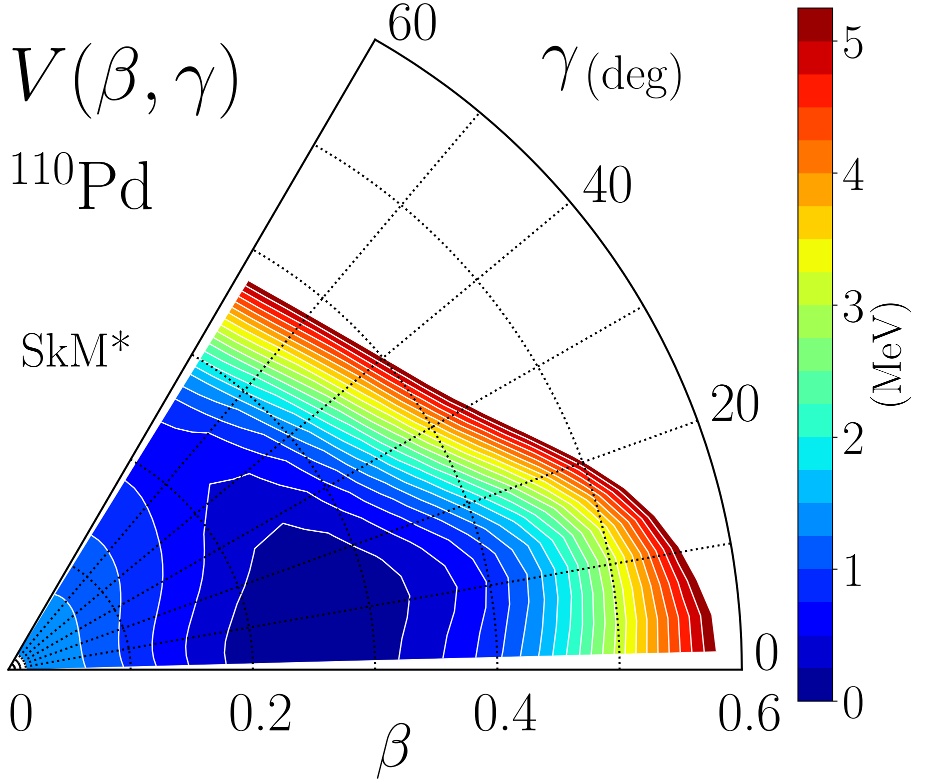




Zhang et al., Phys. Rev. C 105, 044326 (2022).

Large amplitude collective motion

- Calculation of collective mass parameters using the linear response calculation
- Shape fluctuation: ^{110}Pd
- e.g.) Quadrupole shape d.o.f.: (β, γ)



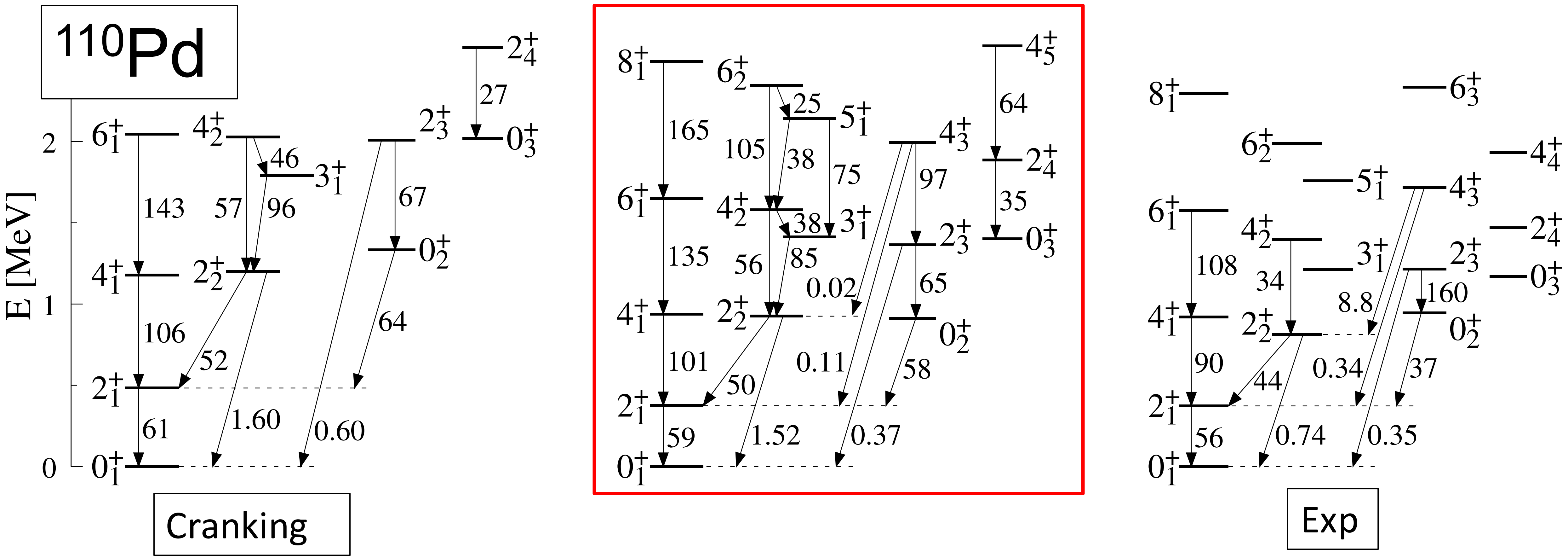
Constraint EDF

$$\delta(E[\rho,\kappa] - \lambda\hat{Q}) = 0$$

TN, Matsuyanagi, Matsuo, Yabana, RMP 88, 045004 (2016)

5D collective Hamiltonian with improved inertial functions

Washiyama, Hinohara, TN, Phys. Rev. C 109, L051301 (2024)



Significant improvement over the cranking mass

Even reducing computational cost by emulator

Hinohara, Zhang, and Engel, in preparation

Application to calculation of collective mass

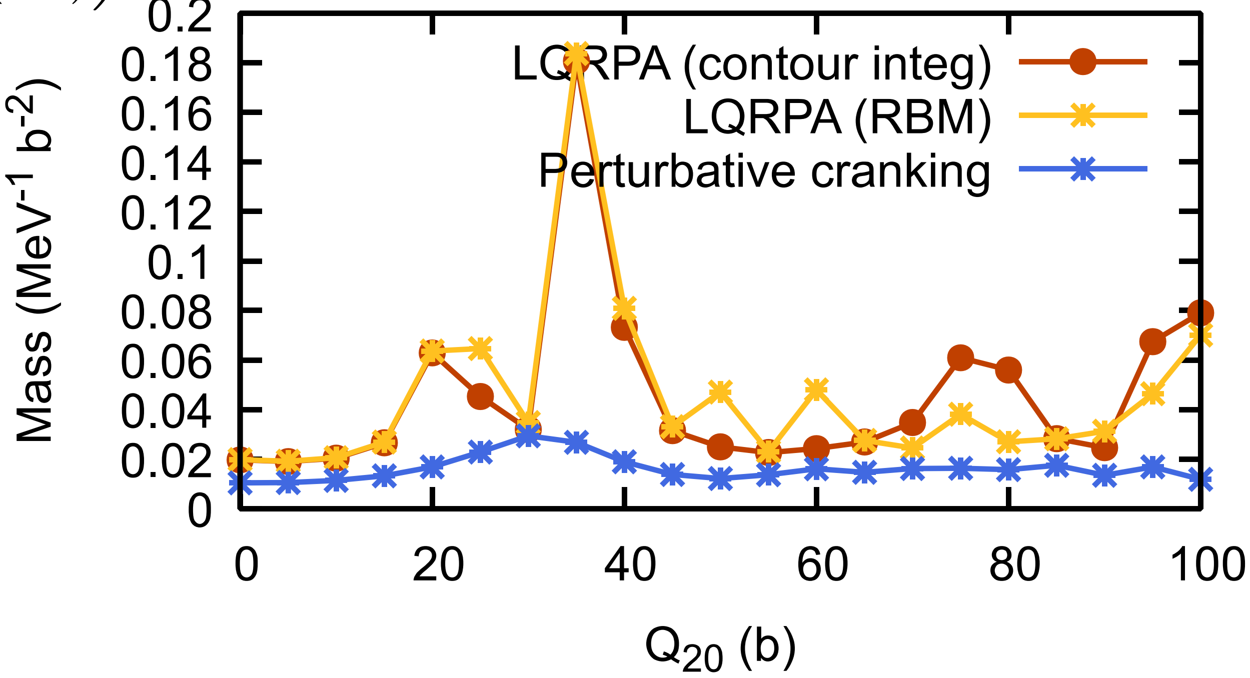
Using solutions of the finite amplitude method for n different frequencies ω_k

$$\begin{pmatrix} X_{\mu\nu}(\omega) \\ Y_{\mu\nu}(\omega) \end{pmatrix} = \sum_{k=1}^{n} a_k(\omega) \begin{pmatrix} X_{\mu\nu}(\omega_k) \\ Y_{\mu\nu}(\omega_k) \end{pmatrix} + b_k(\omega) \begin{pmatrix} Y^*_{\mu\nu}(\omega_k) \\ X^*_{\mu\nu}(\omega_k) \end{pmatrix}$$

$2n$-dimensional RPA matrix

Result with $n = 10$

Hinohara, preliminary



Summary

- Finite amplitude method provides both an easy-coding and computationally advantageous method for linear response calculations.
- Many applications
  - Strength functions, giant resonances in deformed nuclei
  - Collective masses (5DCH, fusion/fission, etc.)
  - Systematic analysis on beta decays (UNC, Chapel Hill)
  - Particle-vibration couplings, beyond RPA
- Future perspectives
  - Ab-initio approaches: Beaujeault-Taudière, et al., Phys. Rev. C 107, L021302 (2023).
  - Symmetry-restored approaches: Chen, et al., Phys. Rev. C 113, 034311 (2026)