TDDFT for nuclear structure and low-energy reaction

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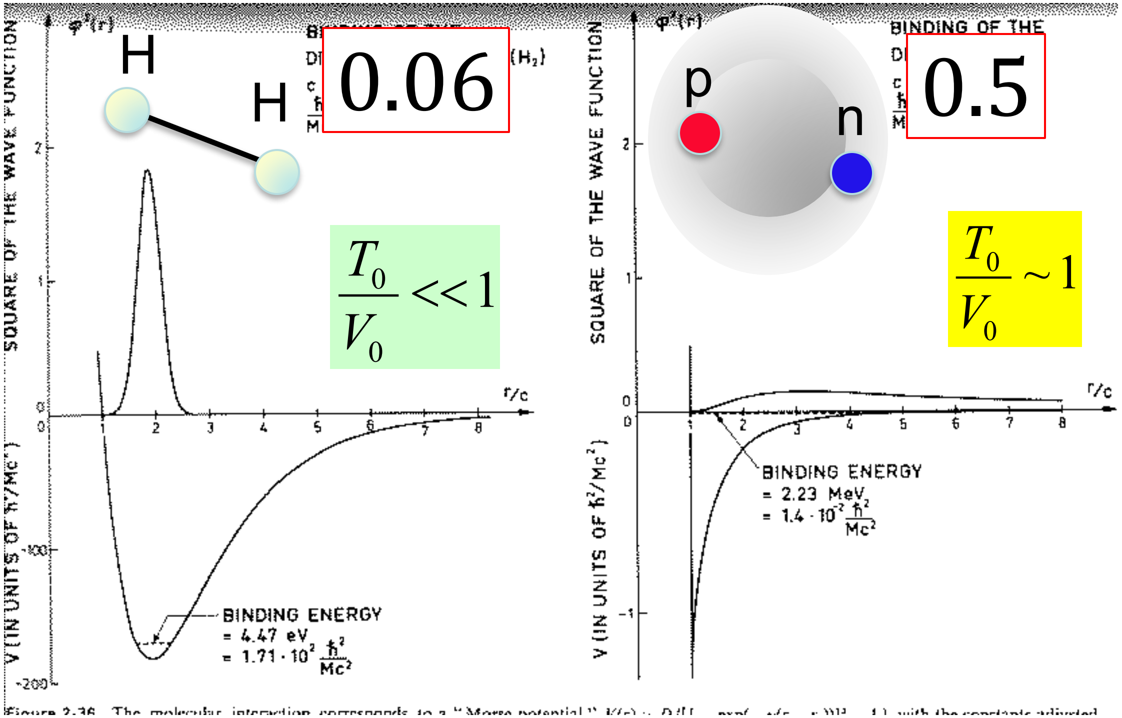
Contents

- Mean-field description of nuclei
- Linear response in TDDFT
  - Deformation & giant resonances (linear response)
  - Knockout reaction: Transition density
- LACM: Fusion reaction
  - Few-body model
  - TDDFT: LACM description of fusion reaction

(TD)DFT: (Time-dependent) density functional theory
LACM: Large amplitude collective motion

Atomic and nuclear interactions

Bohr, Mottelson, Nuclear Structure Vol.1



$$\boxed{\frac{\hbar^2}{2Mc^2}\frac{1}{V_0}}$$

“Strong interaction” but “weak” attraction

Strong quantum nature

Crystalized at low temperature

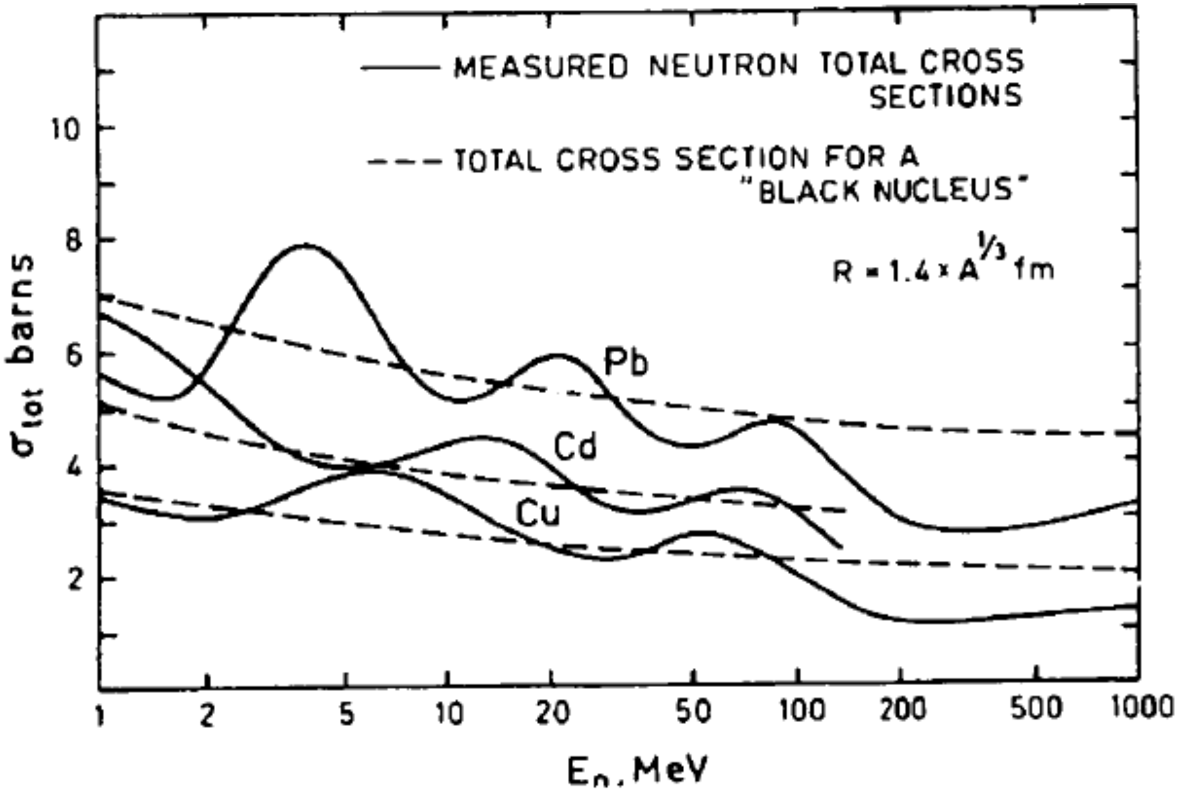
Classical nature

Liquid at zero temperature

Strong quantum nature

Total neutron cross section

From Bohr and Mottelson, Nuclear Structure Vol.1



Oscillatory behaviors

↓

Nuclear transparency

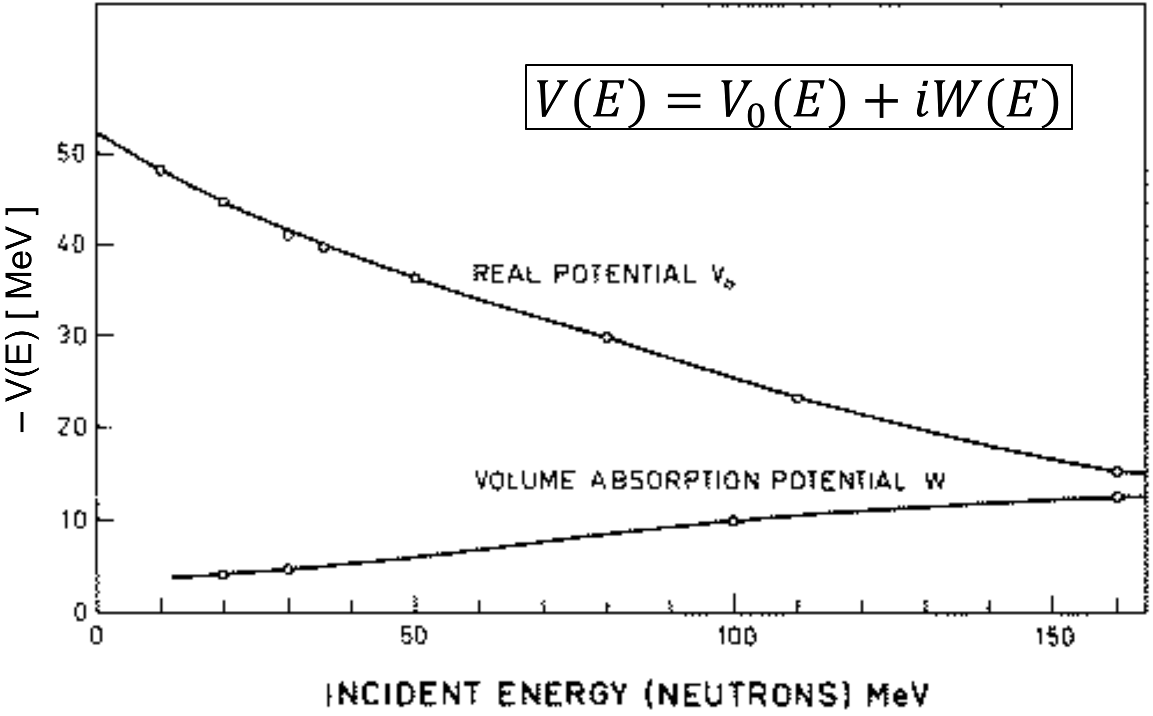
Oscillation amplitude

↓

More transparent at lower energies

Optical potential

From Bohr and Mottelson, Nuclear Structure Vol.1



Mean-free path larger than nuclear size

$$\boxed{\lambda >> R}$$

Energy dependence: $\frac{dV}{dE}$

Effective mass

$$\frac{m^*}{m} = 1 - \frac{dV_0}{dE} \approx 0.7$$

Mean-field description with effective mass

- Mean free path: $\lambda \gg R$ encourage us a mean-field description of nuclei
- However,
  - Naïve mean-field model fails.
  - TN et al., RMP 88, 045004 (2016)

Momentum-dependent potential

TN et al., Rev. Mod. Phys. 88 (2016) 045004

- State-dependent potential

$$V_F = \langle V \rangle + T_F/5 + B/A$$

Bohr-Mottelson, Vol. 1

  - Shallower for particles with a weaker binding

- Momentum dependence

Weisskopf (1957)

  - The lowest order → "Effective mass"

$$\frac{m^*}{m} = \left(\frac{3}{2} + \frac{5}{2}\frac{B}{A}\frac{1}{T_F}\right)^{-1} \approx 0.4$$

⟺

Empirically

$$\boxed{\frac{m^*}{m} = 0.7 \sim 1}$$

Known for many years

- Vautherin-Brink (1972)

$$\boxed{E = \frac{1}{2}\sum_{i=1}^{A}(t_i + e_i)}$$

  – *…, it is well-known that it is not possible to fit the radius, s.p. energies, and total binding energy of ^{16}O and ^{40}Ca …* [Kerman (1968)]

  – *However, the situation is different for Density Functional Model*

$$\boxed{E = \frac{1}{2}\sum_{i=1}^{A}(t_i + e_i) + E_R}$$

$$\boxed{E_R = E_R[\rho]}$$

Density functional
or
Density-dep. int.

Static calculation (ground state)

Pair density

Minimization of energy $\delta E[\rho, \kappa] = 0$

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -(h-\lambda)^* \end{pmatrix} \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}$$

Kohn-Sham-Bogoliubov equations

(Hartree-Fock-Bogoliubov equations)

Nuclear deformation and giant resonances

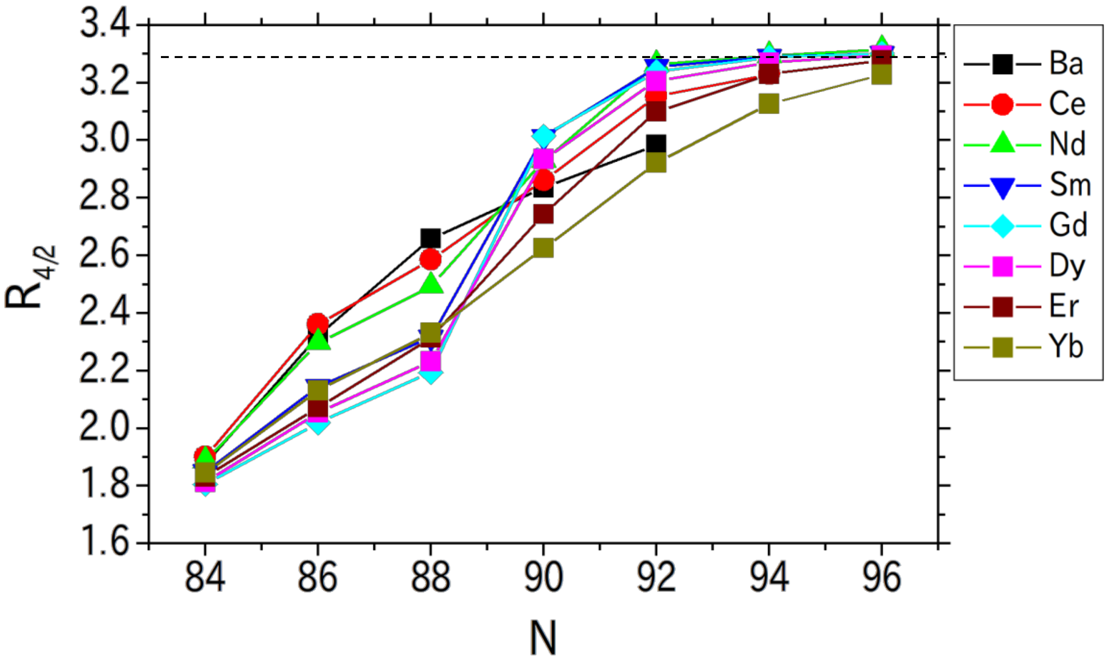
- Unified, universal, & non-empirical description
  - Universal energy density functional: $E[\rho]$
- One of the most successful applications of nuclear DFT

Shape evolution: $R_{4/2}$

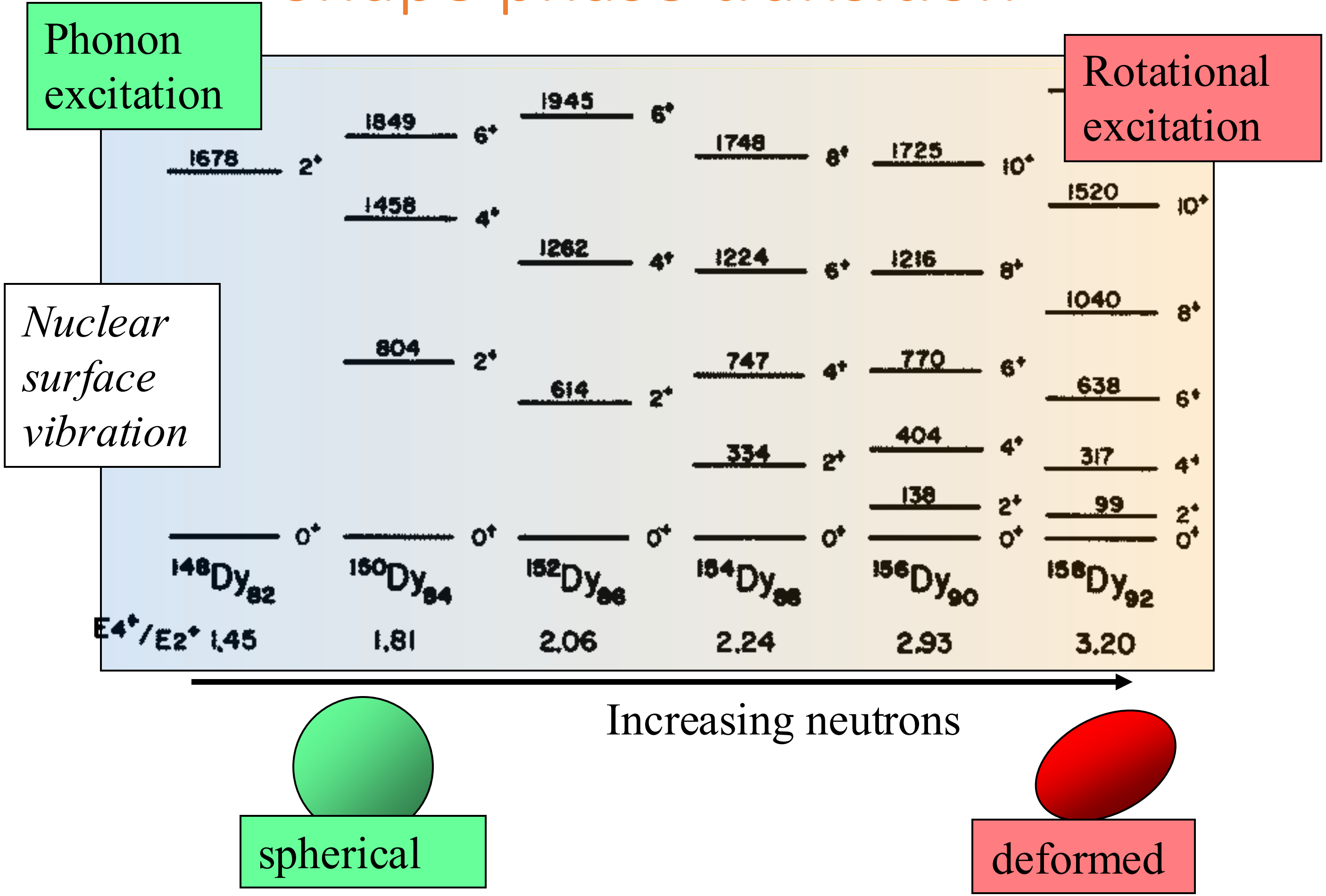
$$E_I = \frac{I(I+1)}{2\mathfrak{I}}$$

$$\Downarrow$$

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



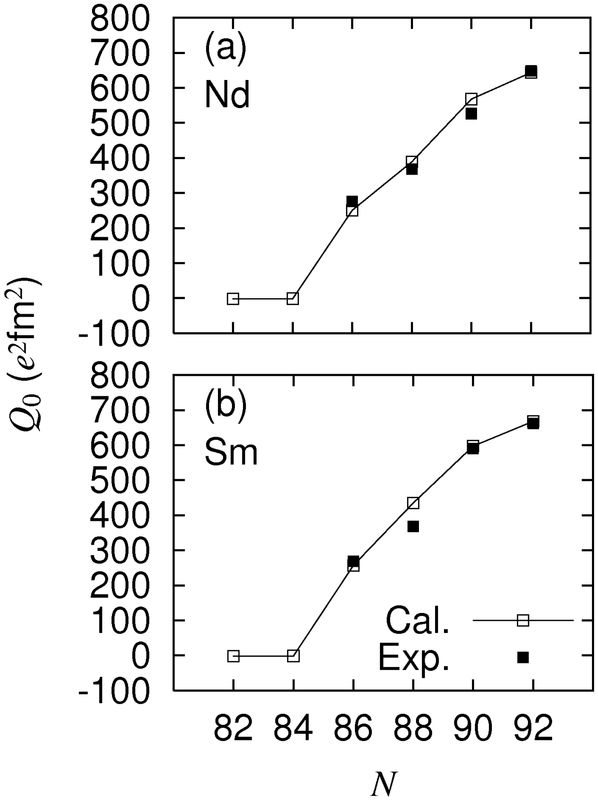
Shape phase transition

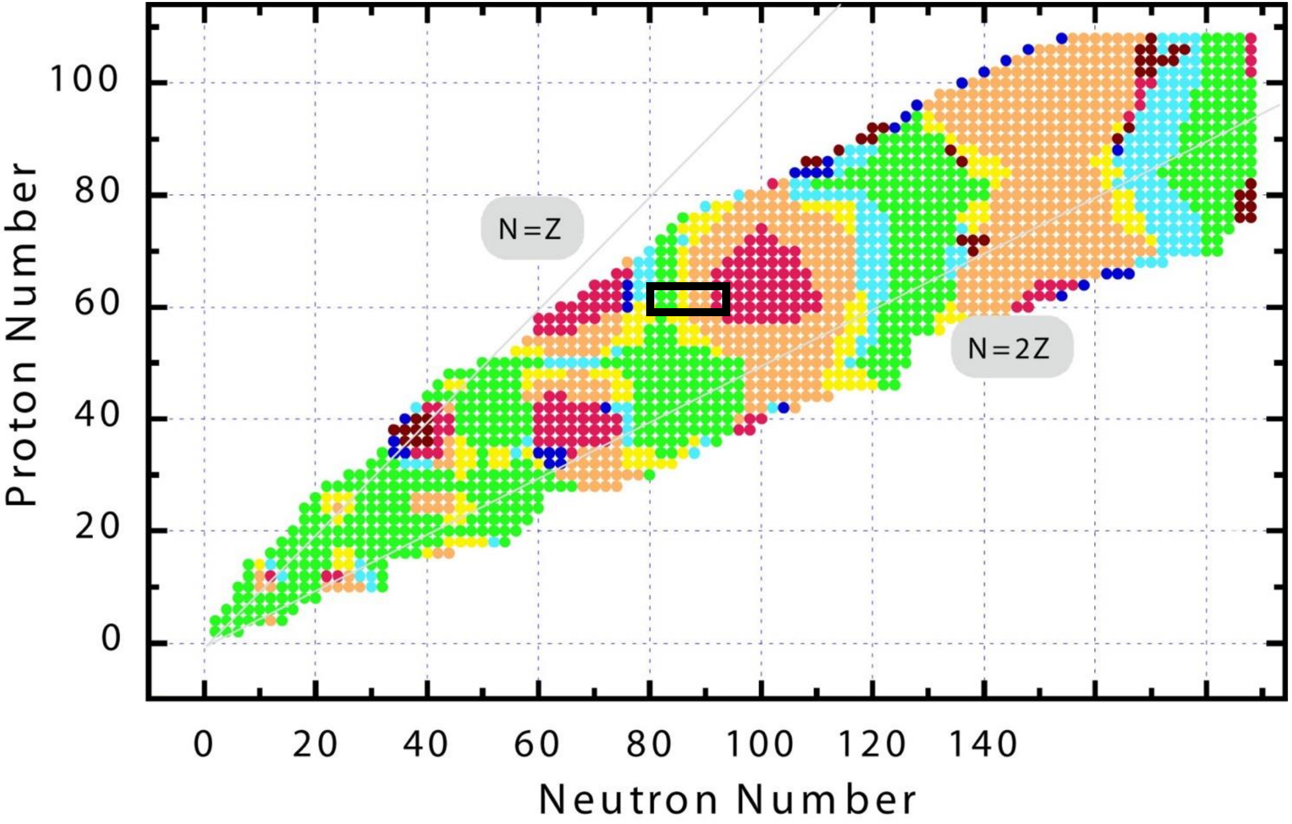


Nuclear deformation predicted by DFT

Intrinsic Q moment

$\langle \hat{Q}_{20} \rangle$





Dynamic calculation (excited states)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}U_\mu\\V_\mu\end{pmatrix}=\begin{pmatrix}h-\lambda & \Delta\\-\Delta^* & -(h-\lambda)^*\end{pmatrix}\begin{pmatrix}U_\mu\\V_\mu\end{pmatrix}$$

Linear response:

Time-dependent calculation with an initial kick

or

Quasiparticle RPA calculation

Finite amplitude method

TN, Inakura, Yabana, PRC 76, 024318 (2007)

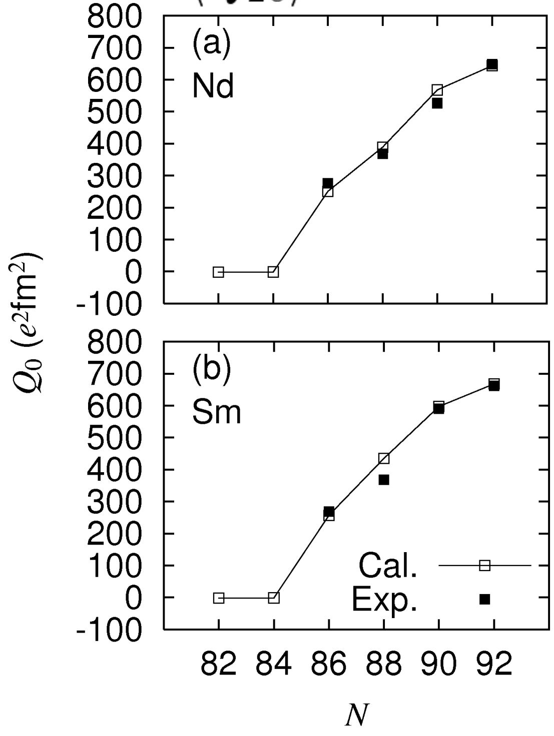
- A computationally advantageous approach to the linear response calculations
- Extensive studies of nuclear excitations, reactions, beta decays, etc.
  - Giant resonances: TN et al. (2007), Inakura&TN&Yabana (2009,2011,2013), Avogadro&TN (2011), Stoitsov et al. (2011), Niksic et al. (2013), Liang&TN (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)
  - Collective model: Wen&TN (2016,2017,2020,2022), Washiyama et al. (2021), Washiyama et al. (2024)

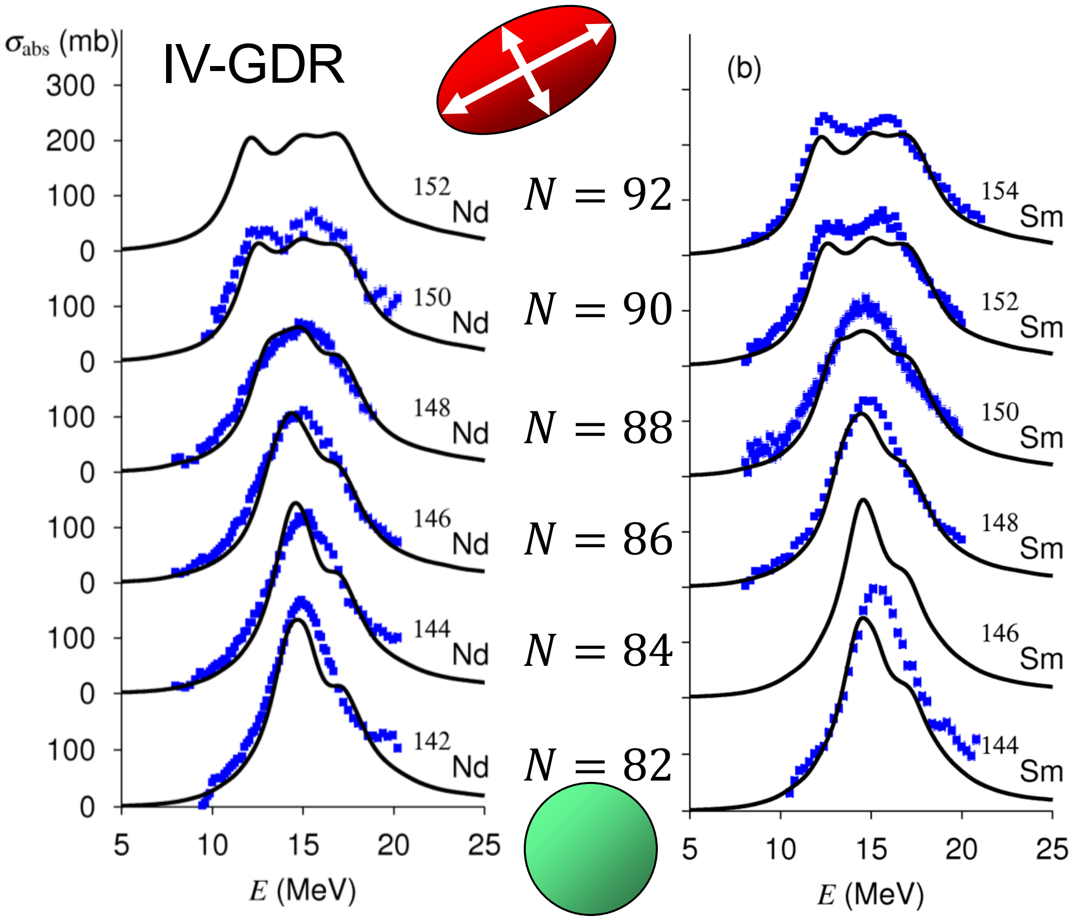
Deformation splitting of photoabsorption peaks

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

SkM* functional

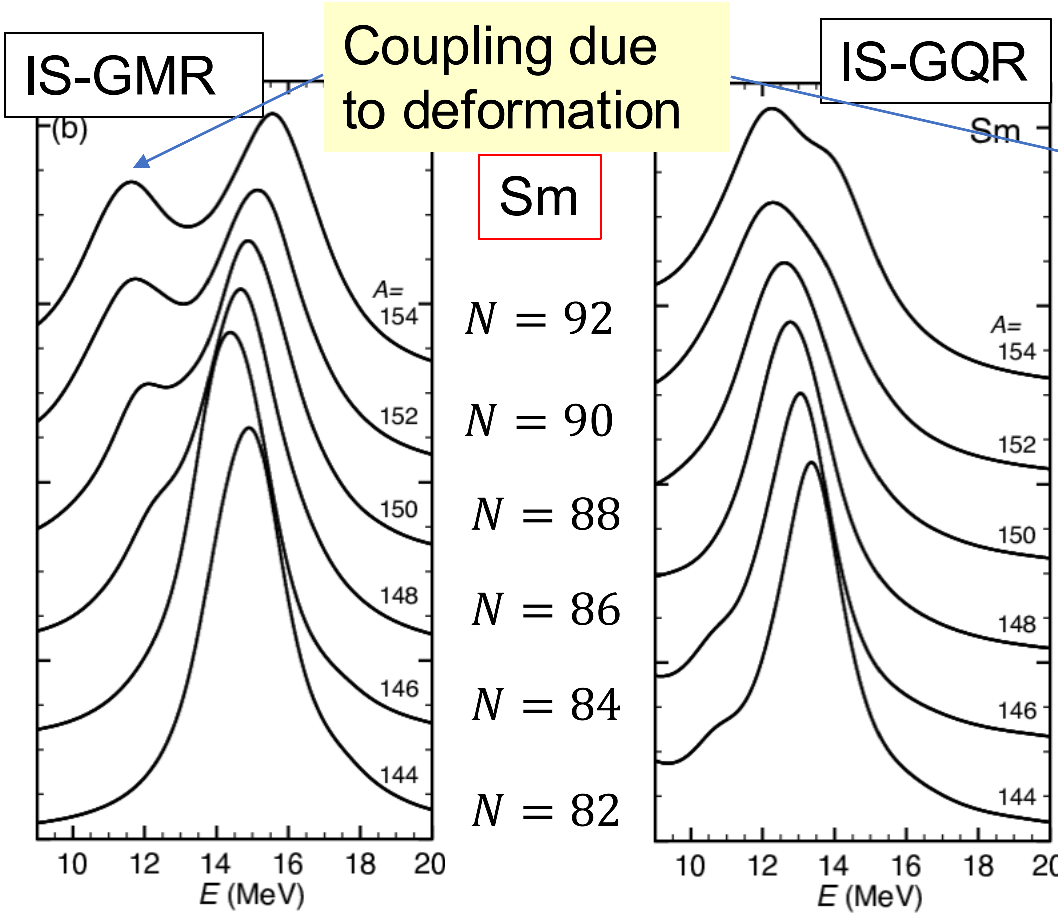
$\langle \hat{Q}_{20} \rangle$ Intrinsic Q moment

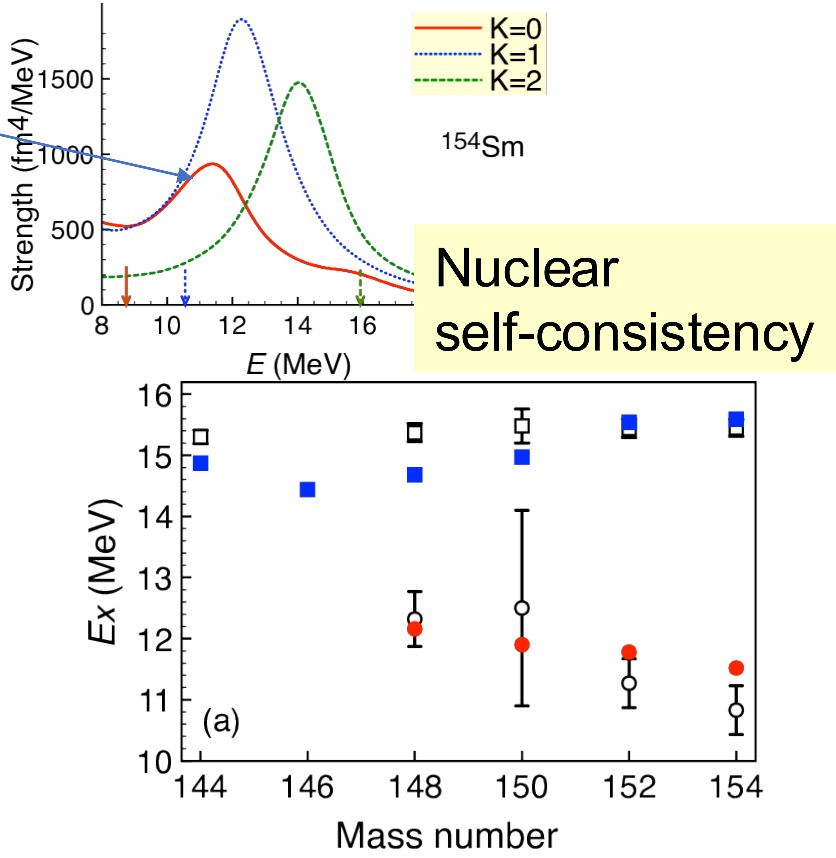




Isoscalar Giant monopole & quadrupole resonances

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





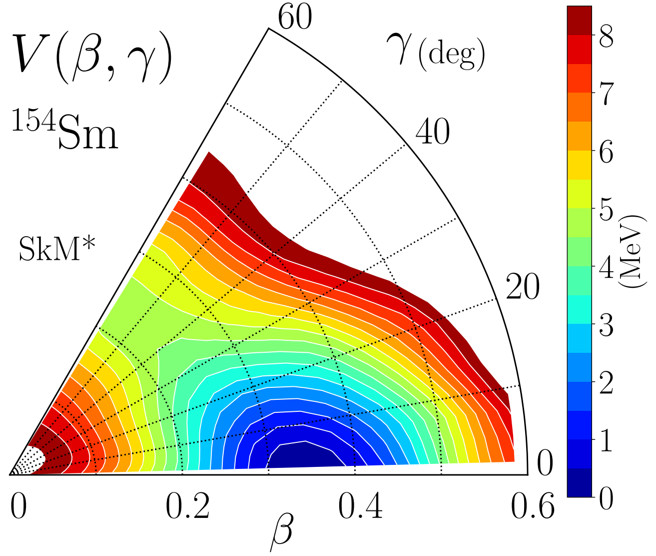
Exp: M. Itoh et al., PRC 68, 064602 (2003).

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)

Improved inertial functions

Cranking formula for collective mass

$$D_{q_1 q_2} = \sum_n \frac{\left\langle 0 \left| \frac{\partial}{\partial q_1} \right| n \right\rangle \left\langle n \left| \frac{\partial}{\partial q_2} \right| 0 \right\rangle + c.c.}{E_n - E_0}$$

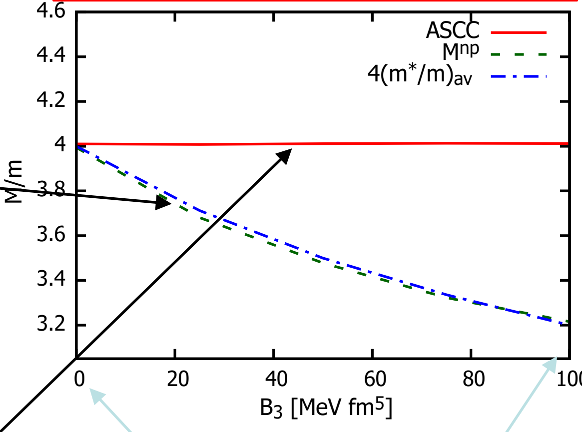
Need an artificial factor of $1.2 - 1.4$

Improved inertial functions

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} Q \\ -Q^* \end{pmatrix} = \frac{-i}{M} \begin{pmatrix} P \\ P^* \end{pmatrix}$$

Feasible with FAM
without matrix diagonalization

α particle total mass



Wrong values

Correct values

$\frac{m^*}{m} = 1$

$\frac{m^*}{m} = 0.8$

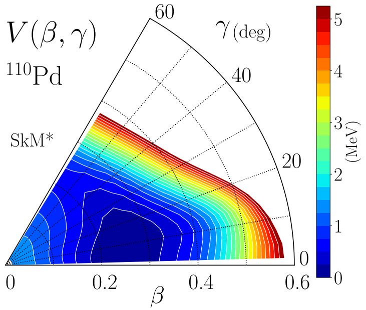
Wen, TN, PRC 105 (2022) 034603

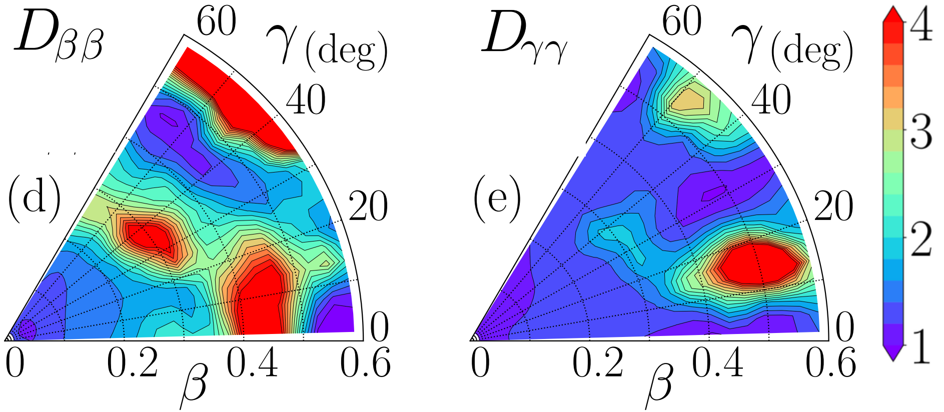
5D collective Hamiltonian with improved inertial functions

Shape fluctuation/coexistence

Washiyama, Hinohara, TN, PRC 109, L051301 (2024)

Superposition of different shapes: (β,γ)





5DCH: 5D collective Hamiltonian

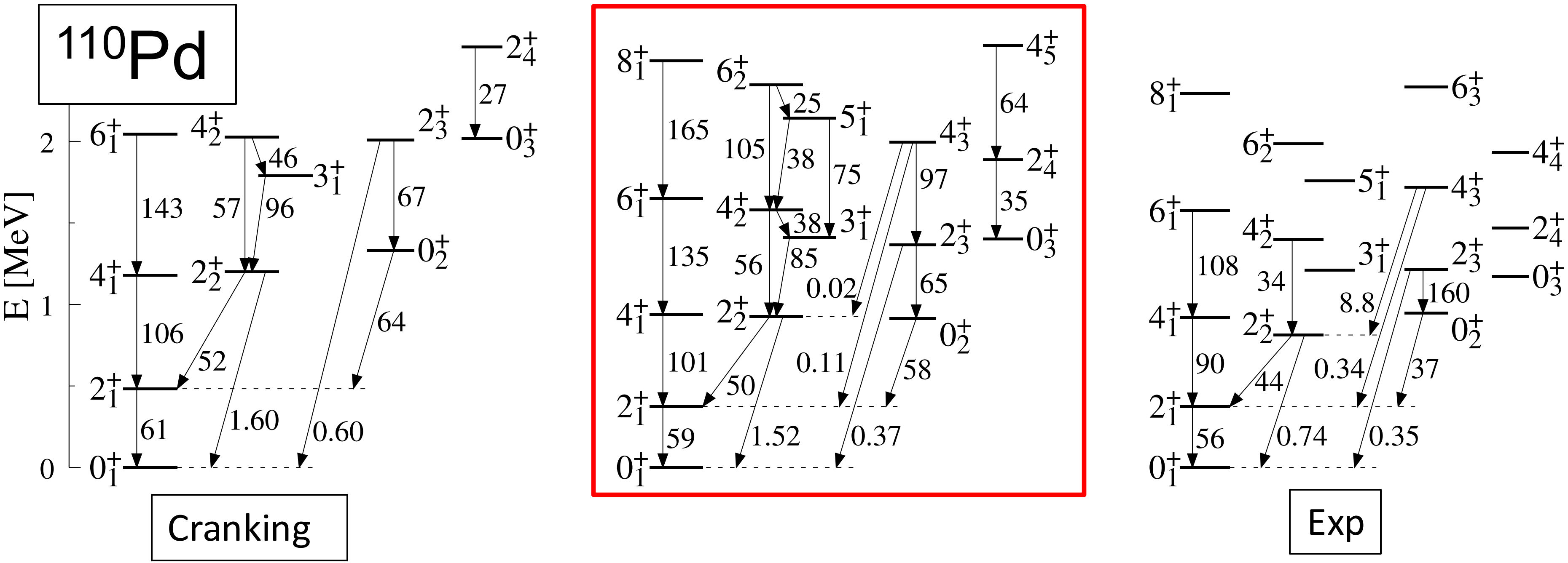
$$H = T_{\text{vib}} + T_{\text{rot}} + V(\beta,\gamma)$$

$$T_{\text{vib}} = \frac{1}{2} D_{\beta\beta}(\beta,\gamma)\dot{\beta}^2 + D_{\beta\gamma}(\beta,\gamma)\dot{\beta}\dot{\gamma} + \frac{1}{2} D_{\gamma\gamma}(\beta,\gamma)\dot{\gamma}^2$$

$$T_{\text{rot}} = \frac{1}{2} \mathcal{J}_k(\beta,\gamma)\Omega_k^2$$

$$\frac{D}{D(\text{cranking})}$$

5D collective Hamiltonian with improved inertial functions



Significant improvement over the cranking mass

Sub-barrier fusion reaction

- Few-body model
- Time-dependent wave-packet (TDWP) method
  - Neutron-halo nuclei: Fusion suppression at subbarrier energies
- TDDFT-based collective model
  - Alpha reactions
  - Fusion hindrance due to the collective mass

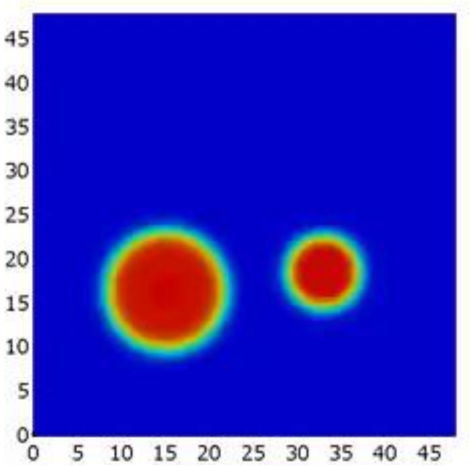
Reactions above the Coulomb barrier

"Partial"-space particle-number projection

Simenel, C., 2010, Phys. Rev. Lett. 105, 192701.

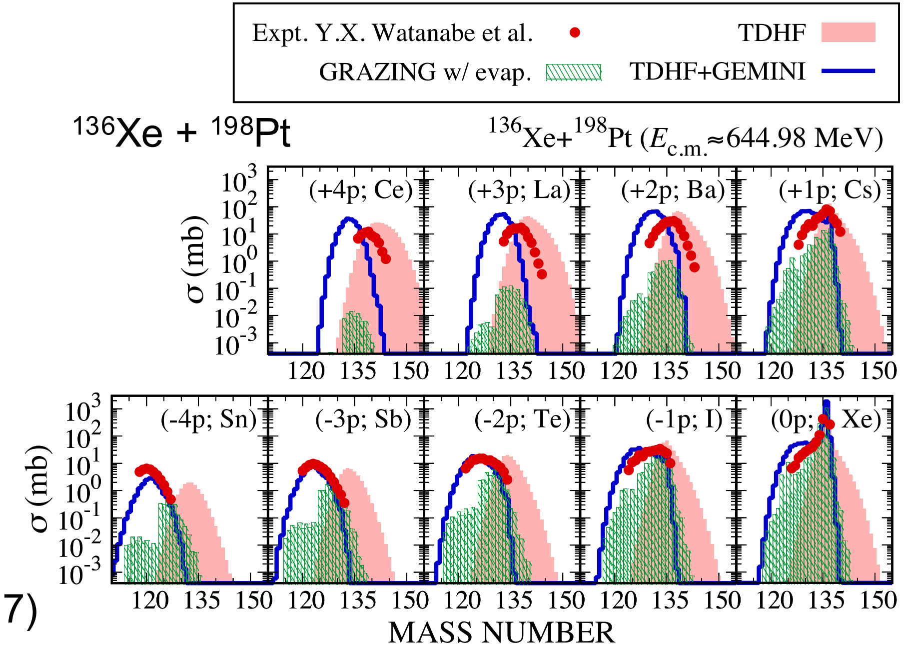
$$P_n = \langle \Phi | \hat{P}_n | \Phi \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, e^{in\theta} \det\{ \langle \phi_i | \phi_j \rangle_{\mathrm{V_T}} + e^{-i\theta} \langle \phi_i | \phi_j \rangle_{\mathrm{V_P}} \}$$

Real-time simulation



Sekizawa, PRC **96**, 014615 (2017)

^{136}Xe + ^{198}Pt



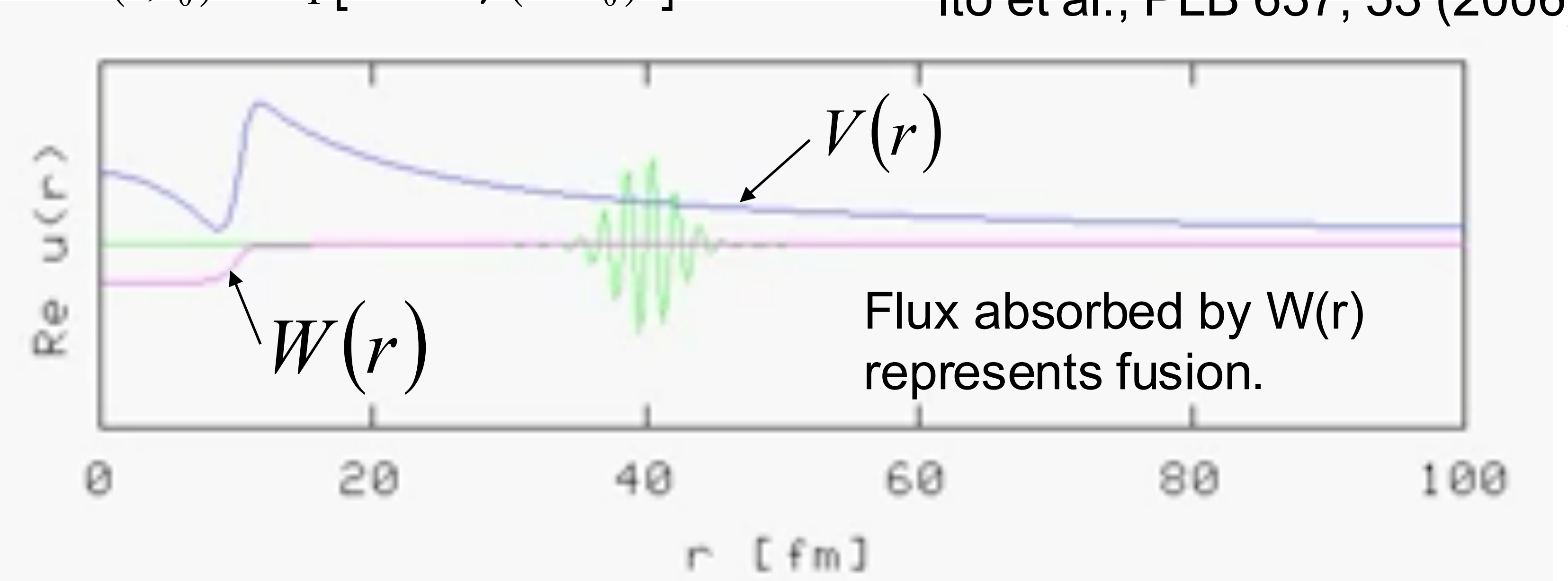
Wave packet dynamics of fusion reaction

Radial Schroedinger equation for l=0
with incident Gaussian wave packet

$$u(r,t_0) = \exp\left[-ikr - \gamma(r-r_0)^2\right]$$

$$\boxed{i\hbar\frac{\partial}{\partial t}u(r,t) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + iW(r)\right]u(r,t)}$$

Ito et al., PLB 637, 53 (2006)



Flux absorbed by W(r) represents fusion.

Construction of low-energy reaction model

Model Hamiltonian

Correspondence: $R \leftrightarrow M(R)$

$$\left\{-\frac{d}{dR}\frac{1}{2M(R)}\frac{d}{dR}+\frac{L(L+1)}{2I(R)}+V(R)\right\}\psi_L(R)=E_L\psi_L(R)$$

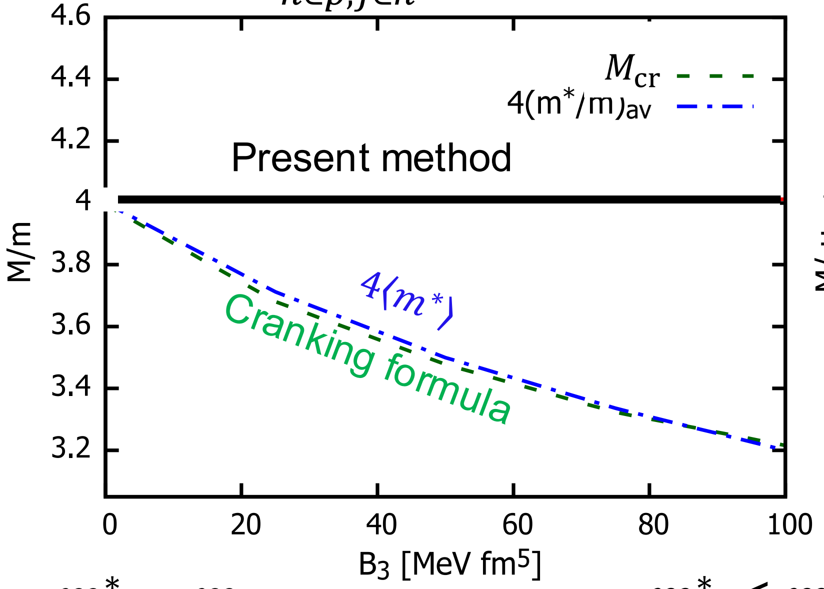
Microscopically calculating $V(R), M(R), I(R)$

Can we reproduce the following asymptotic values at $R \to \infty$?
How good is the usage of these values?

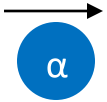
$$M(R)=\mu_R, \qquad I(R)=\mu_R R^2$$

Effect of effective mass: m^*

$$M_{\mathrm{cr}} = 2 \sum_{n \in p, j \in h} \frac{|\langle n | \hat{p}_x | j \rangle|^2}{e_n - e_j}$$

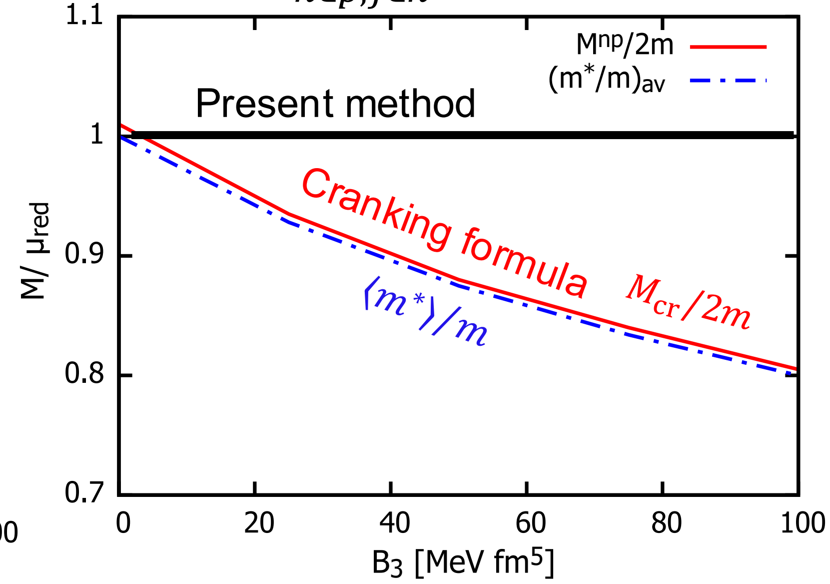


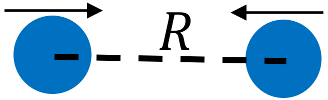
$m^* = m$



$m^* < m$

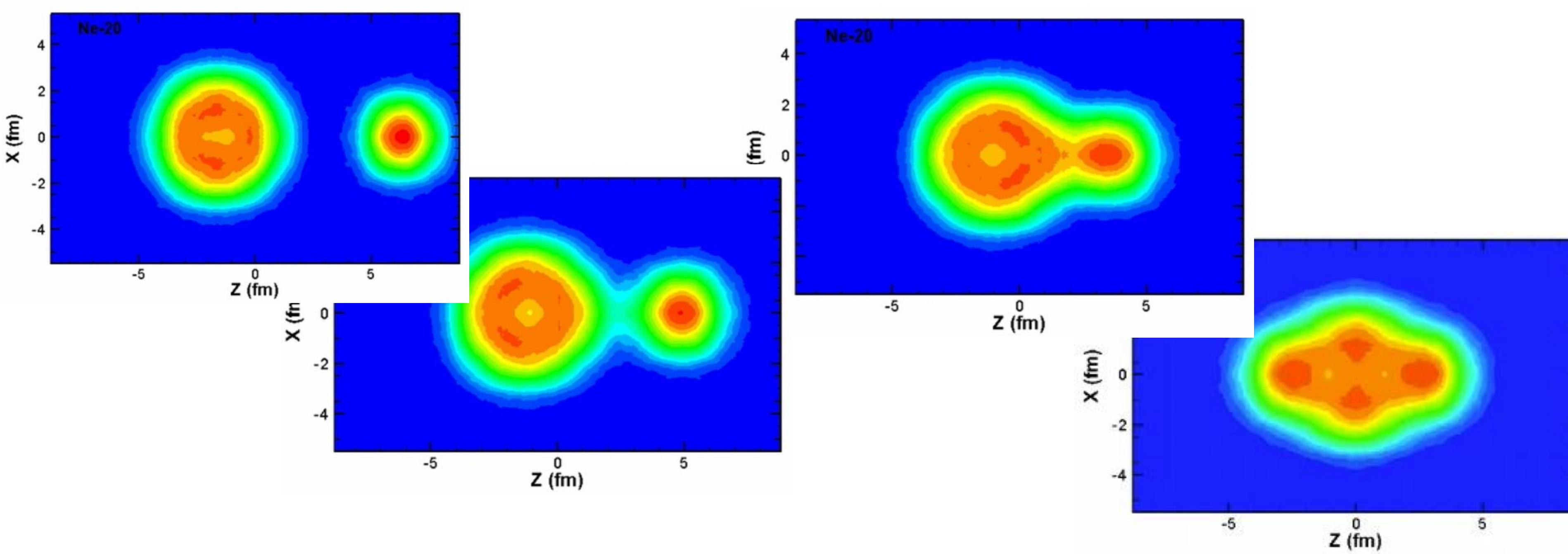
$$M_{\mathrm{cr}} = 2 \sum_{n \in p, j \in h} \frac{|\langle n | \partial / \partial R \, | j \rangle|^2}{e_n - e_j}$$





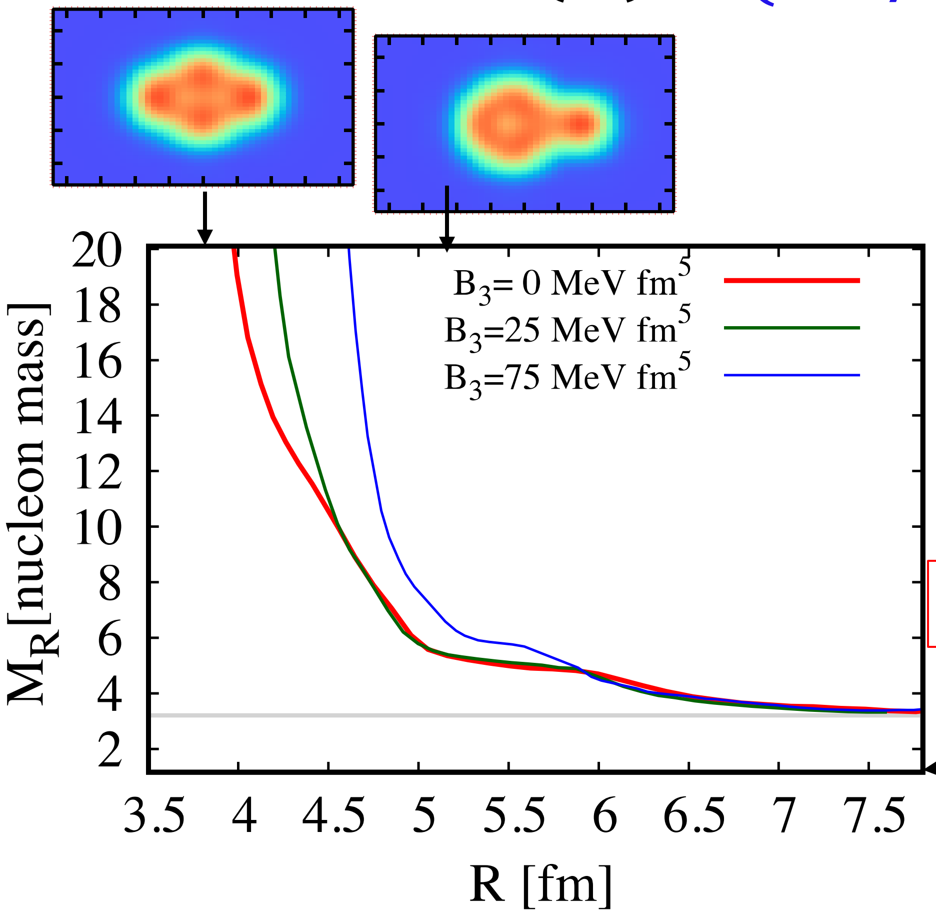
$@R = 8$ fm

α-^{16}O fusion (alpha reaction)

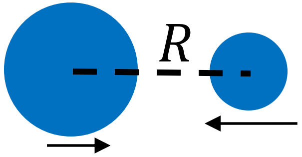


K. Wen, T. N., PRC 105 (2022) 034603; EPJWC **306**, 01006 (2024)

$M(R)$ $(m^*/m \leq 1)$

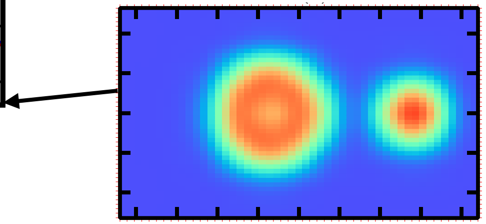


$^{16}O + \alpha$

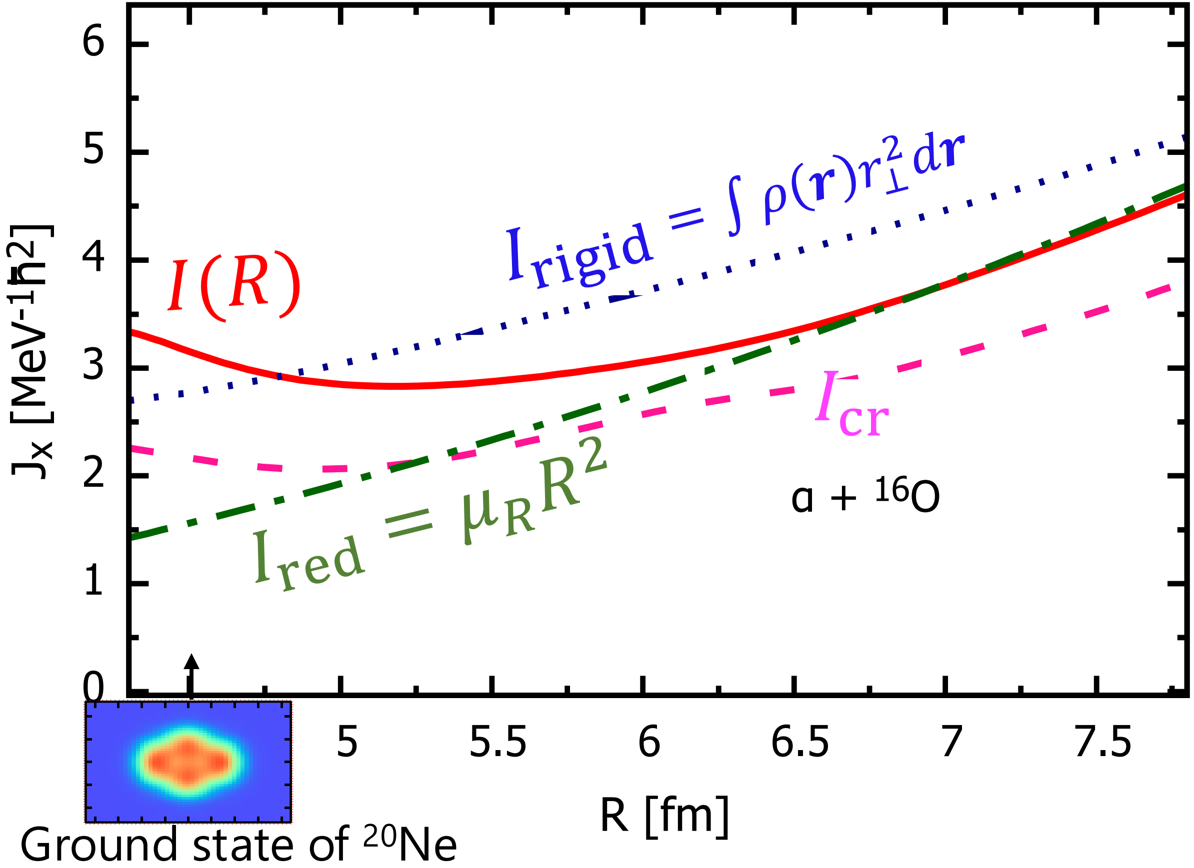


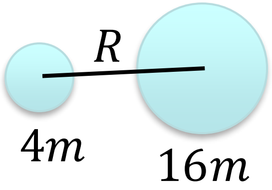
$m^* < m^* < m^* = m$

$M(R) = \mu_R \quad (R \to \infty)$



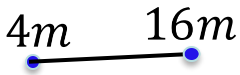
$I(R)$ $(m^*/m < 1)$





"Point-particle approx."

I_{red}



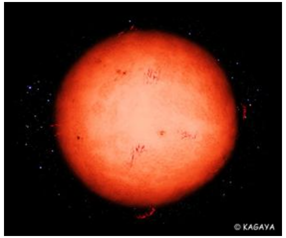
$I(R) = I_{red}$ at large R

$I_{cr} \neq I_{red}$ at large R

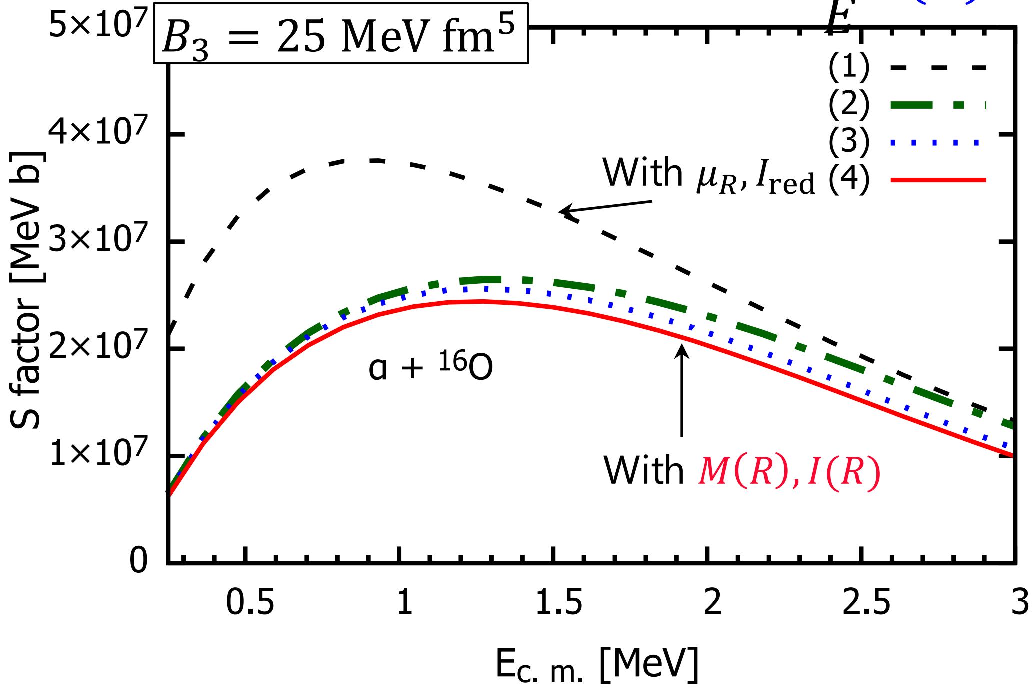
Alpha reaction: $^{16}O + \alpha$

Fusion reaction:
Astrophysical S-factor

$$\sigma(E) = \frac{1}{E} P(E) \times S(E)$$



Synthesis of ^{20}Ne



Fusion hindrance due to the inertial mass

Summary

- EDF method: Universal description of nuclear structure and reaction
- Shape phase transition & Giant resonances: Deformation splitting/coupling
- ^{16}O(p, pd)^{14}N knockout reaction (on-going)
- TDWP method for fusion: Fusion suppression for neutron-halo nuclei
- LACM: Inertial parameter effects on low-energy spectra & alpha reaction

- Collaboration
  - T. Ochi (Univ. Tsukuba; D1)
  - N. Hinohara (Univ. Tsukuba)
  - M. Ito (Kansai Univ.)
  - K. Washiyama (CiDER, Osaka Univ.)
  - K. Wen (KEK)
  - K. Yoshida (RCNP, Osaka Univ.)
  - K. Yabana (Univ. Tsukuba)