Requantizing the time-dependent density functional dynamics

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- Nuclear saturation and mean-field approach
- TDDFT for nuclear collective motion
  Success & failure
- Requantization of TDDF dynamics
  Low-energy nuclear reaction

2022.12.8 @DFT2022, YITP

Nuclear Saturation
"Liquid"-like property

B/A ~ 8 MeV

(B/A ~ 16 MeV for nuclear matter)

Density $\rho \approx 0.16\ \text{fm}^{-3}$

→ Liquid drop model

Bethe-Weizsäcker mass formula

$$B(N,Z) = a_V A - a_S A^{2/3} - a_{sym}\frac{(N-Z)^2}{A} - a_C \frac{Z^2}{A^{1/3}} + \delta(A)$$

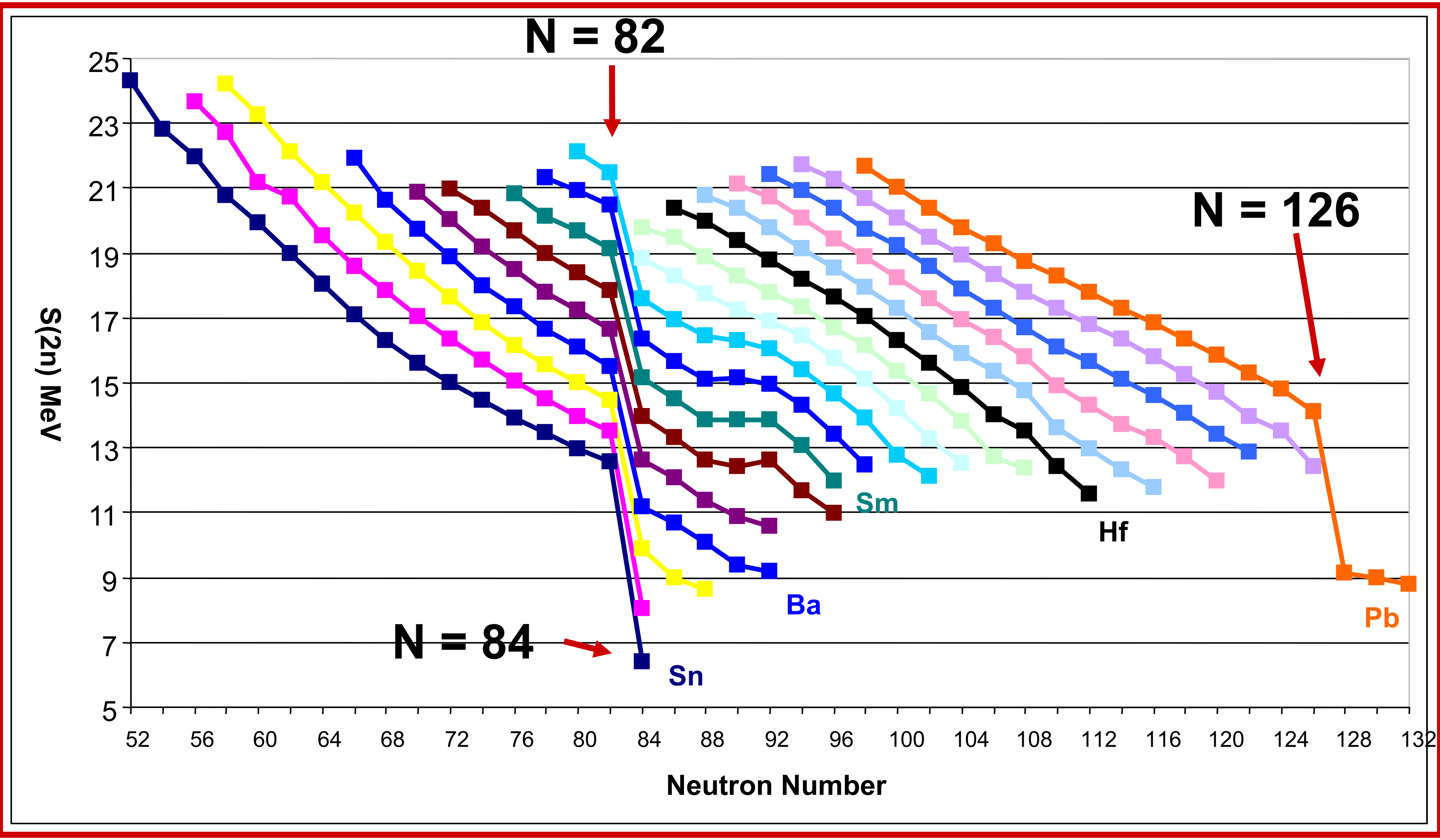
Single-particle motion
“Gas”-like picture

- Nuclear shell model
  - Strong spin-orbit coupling (Mayer-Jensen)

- Mean free path in nuclei
  - Neutron scattering

Energy required to remove two neutrons from nuclei

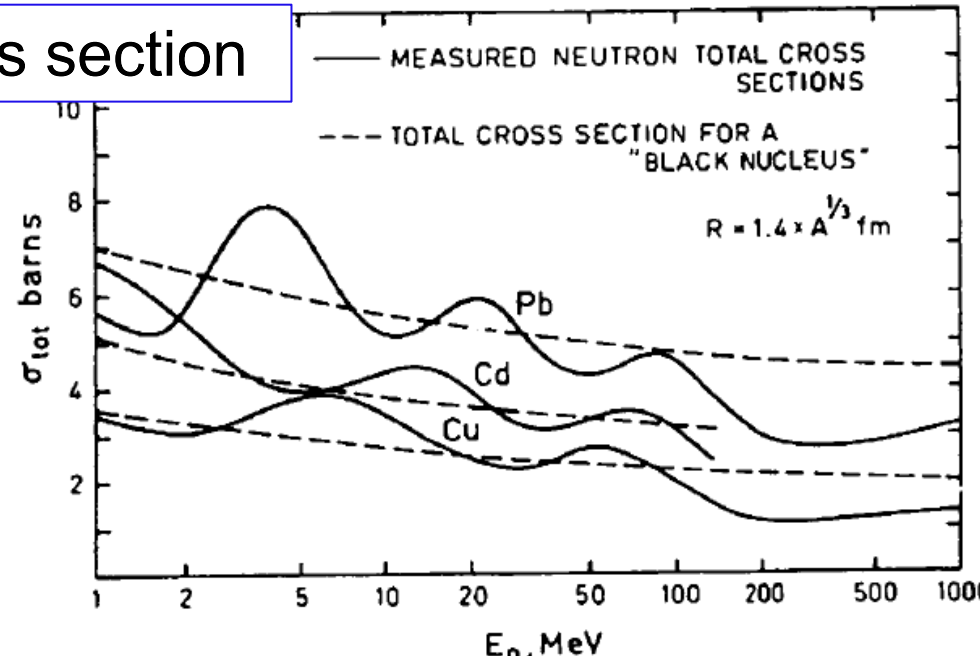
(2-neutron binding energies = 2-neutron “separation” energies)



R. Casten

Nuclear "transparency"

Neutron scattering cross section



Bohr and Mottelson, *Nuclear Structure I* (1969)

Optical-model analysis

$$V + iW \Rightarrow k_{in} + \frac{i}{2\lambda}$$

Real and imaginary potentials

$$-V \approx 50 - 0.3E, \quad -W \approx (0 \sim 2) + 0.1E$$

in units of MeV

For *low-energy* neutrons

$$\lambda \gg R$$

λ: mean free path of neutrons
R: Size of nucleus

$$m^* \approx 0.7m$$ ($m^* \approx m$ around $k \approx k_F$)

Mean-field approach

- In order to be consistent with the saturation,
  - Need momentum dependent potential
  - The lowest order → "Effective mass"

$$V = U_0 + U_1 k^2 \quad \Rightarrow m^*/m = \left(1 + U_1 k_F^2 / T_F\right)^{-1}$$

$$B/A \approx S_{n(p)} \approx 16\,\mathrm{MeV}$$

$$T_F = \frac{\hbar^2 k_F^2}{2m} \approx 40\,\mathrm{MeV}$$

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

  - Inconsistent with experiments!

A possible solution for the inconsistency

- Energy density functional

$$E[\rho] \Rightarrow \quad h[\rho]|\phi_i\rangle = \varepsilon_i|\phi_i\rangle$$

$$h[\rho] \equiv \frac{\delta E}{\delta \rho}$$

- State-dependent effective interaction
  - Rearrangement terms

Nuclear energy density functional

- Energy functional for the intrinsic states
- Spin & isospin degrees of freedom
  - Spin-current density is indispensable.
- Nuclear superfluidity → Kohn-Sham-Bogoliubov eq.
  - Pair density (tensor) is necessary for heavy nuclei.

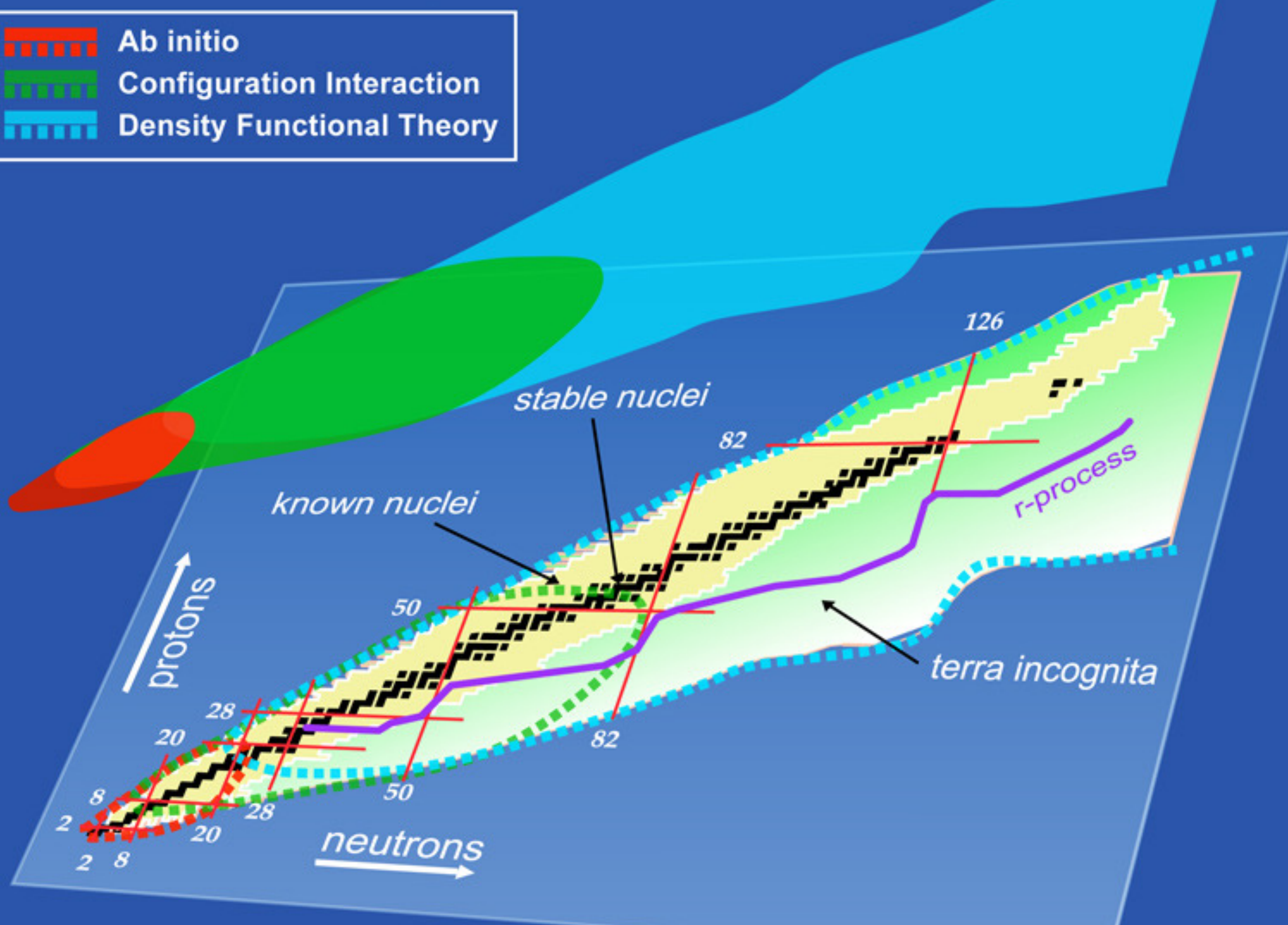
$$E\left[\rho_q, \tau_q, \overleftrightarrow{J}_q; \kappa_q\right]$$

kinetic

spin-current

pair density

Nuclear Landscape



From SciDAC-UNEDF project

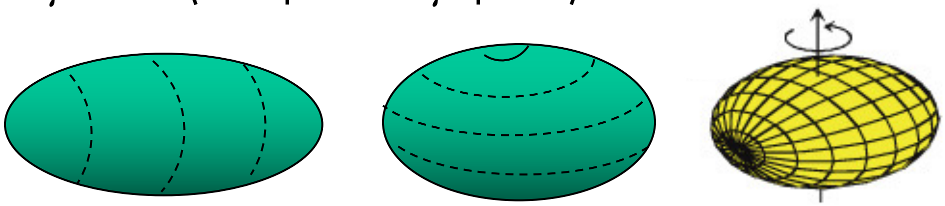
Nuclear deformation as symmetry breaking

$$e^{i\phi J}|\Psi\rangle \neq |\Psi\rangle$$

$$e^{i\phi N}|\Psi\rangle \neq |\Psi\rangle$$

Quadrupole deformation

$$\beta_{2\mu} = \langle\Psi|r^2 Y_{2\mu}|\Psi\rangle$$



prolate oblate triaxial

Pairing deformation (superfluidity)

$$\Delta = \langle\Psi|\hat{\psi}\hat{\psi}|\Psi\rangle$$

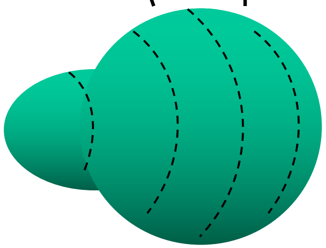
Deformation in the gauge space

Nuclear Superconductivity
Nuclear Superfluidity

Octupole deformation

$$\beta_{30} = \langle\Psi|r^3 Y_{30}|\Psi\rangle$$

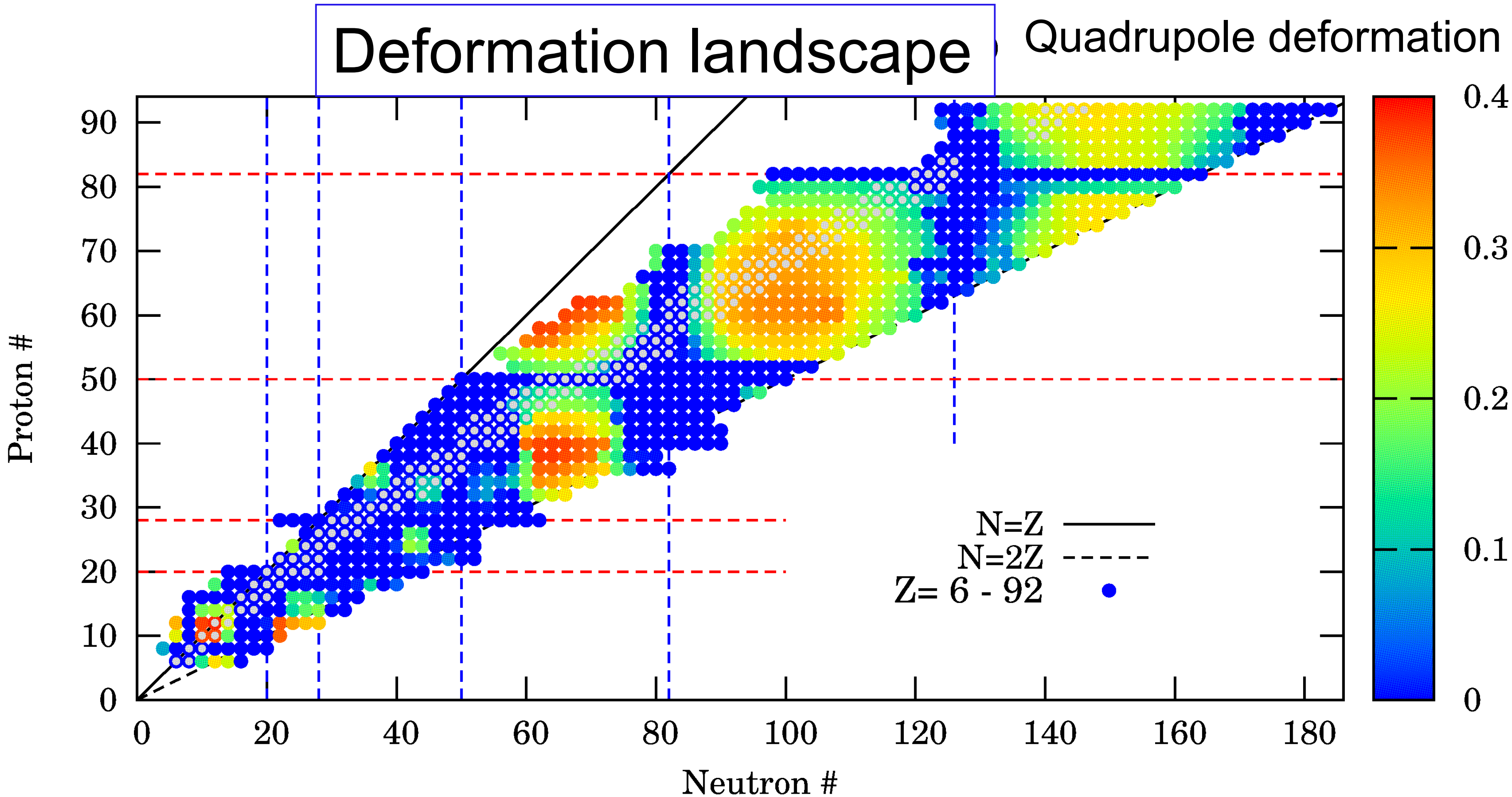
$$\hat{P}|\Psi\rangle \neq \pm|\Psi\rangle$$



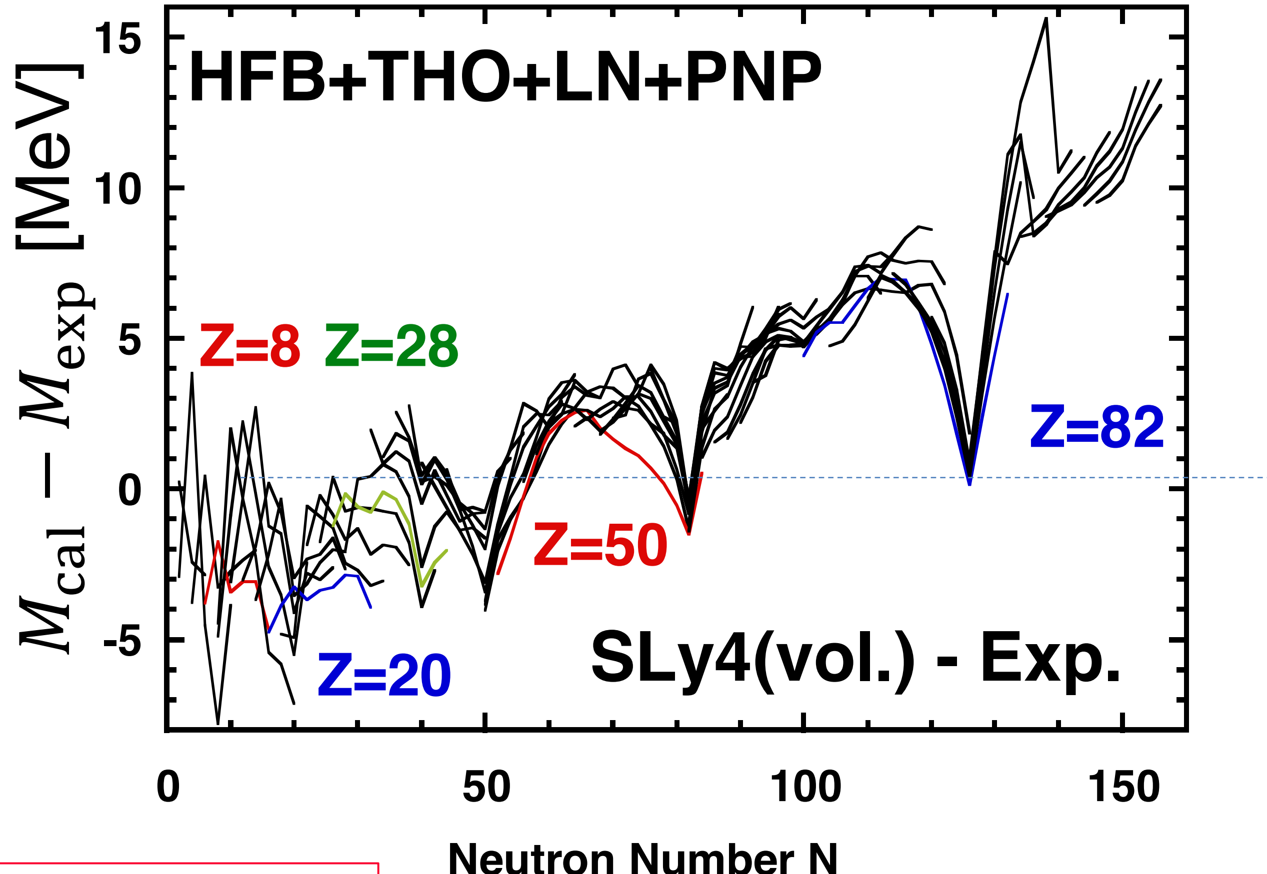
Pear shape (μ=0)

Nuclear deformation

Ebata and T.N., Phys. Scr. 92 (2017) 064005



Predicted nuclear mass



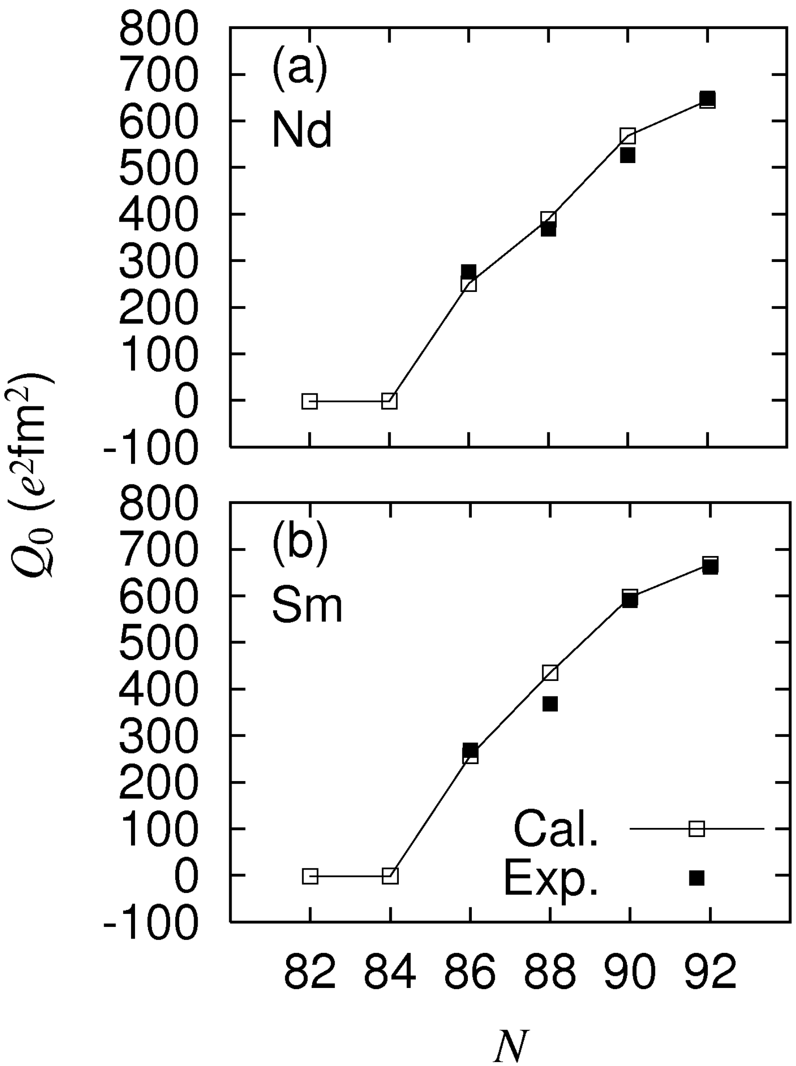
Dobaczewski et al., 2004

Missing correlations for open-shell nuclei

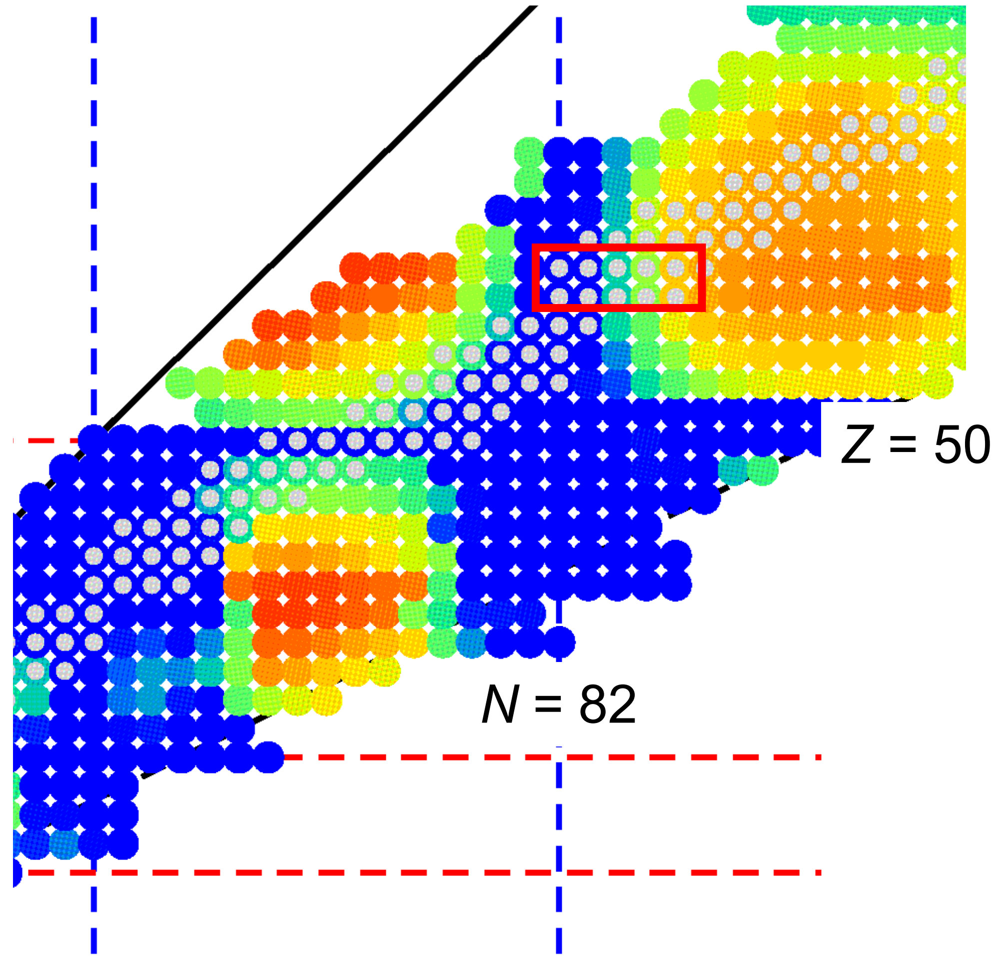
Nuclear deformation predicted by DFT

Intrinsic Q moment

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



Deformation landscape



Time-dependent density functional theory (TDDFT) for nuclei

- Time-odd densities (current density, spin density, etc.)

$$E\left[\rho_q(t),\tau_q(t),\overleftrightarrow{J}_q(t),\vec{j}_q(t),\vec{s}_q(t),\vec{T}_q(t);\kappa_q(t)\right]$$

kinetic, spin-current, current, spin, spin-kinetic, pair density

- TD Kohn-Sham-Bogoliubov-de-Gennes eq.

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

Linear response calculation

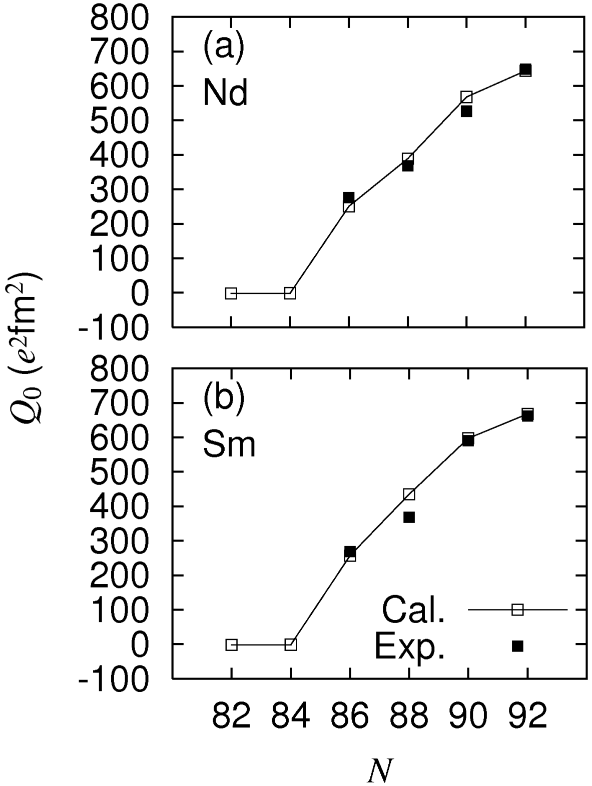
Deformation effects for photoabsorption cross section

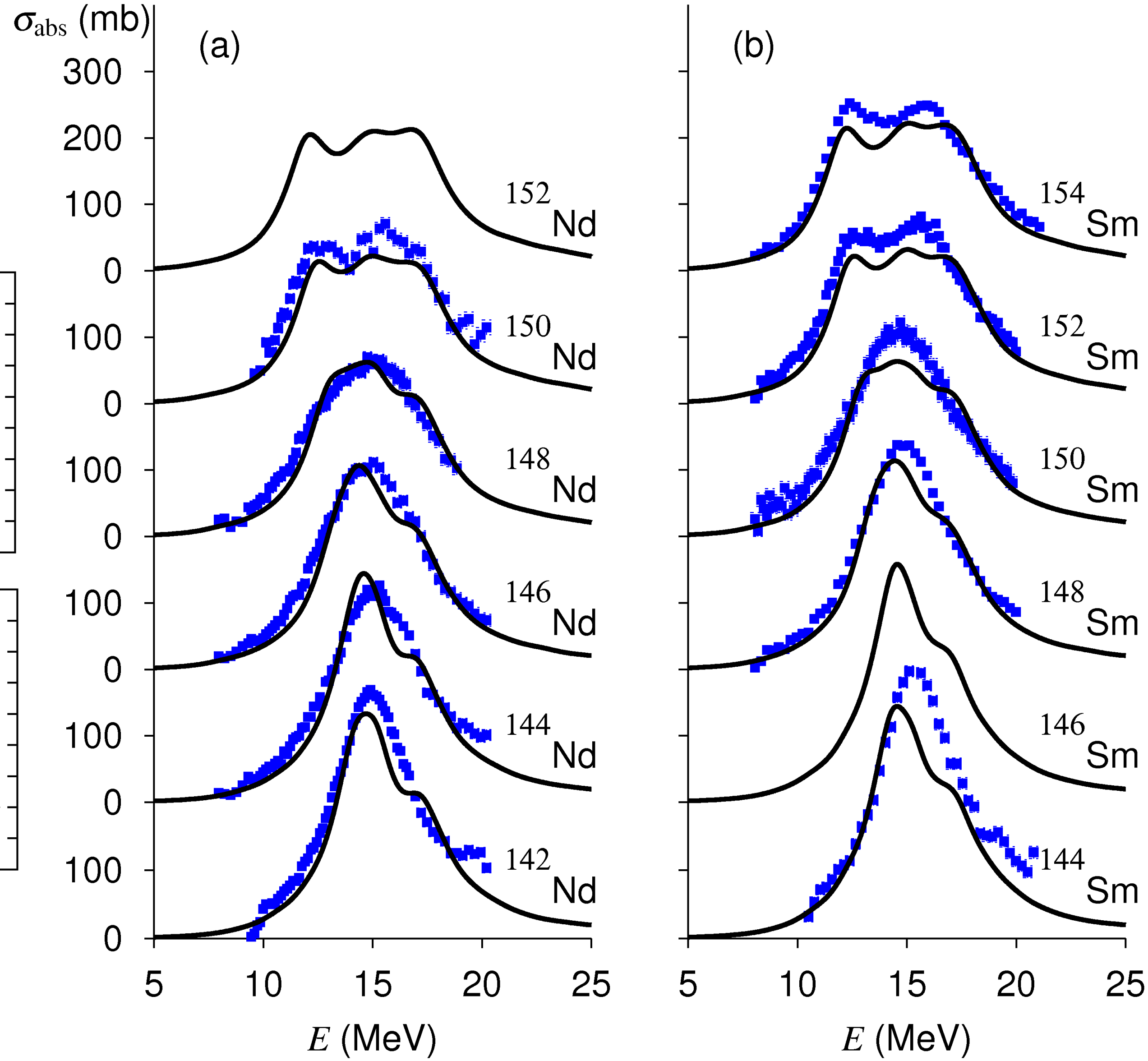
SkM* functional

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

Intrinsic Q moment

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





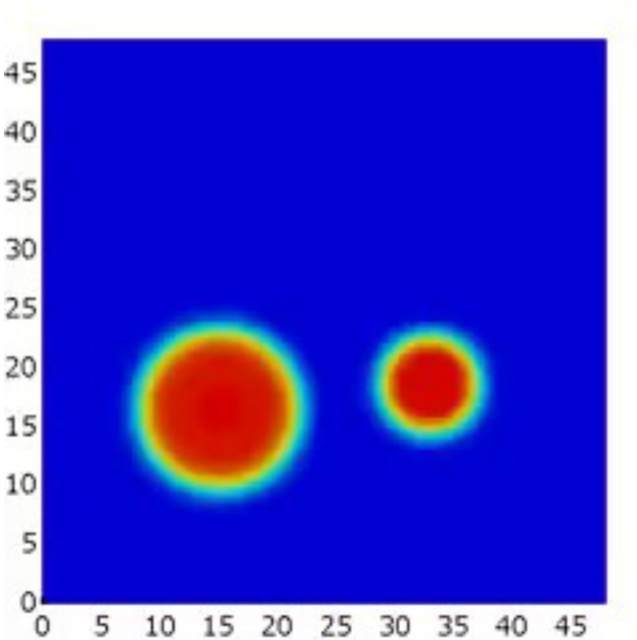
Reaction above the Coulomb barrier

"Partial"-space particle-number projection

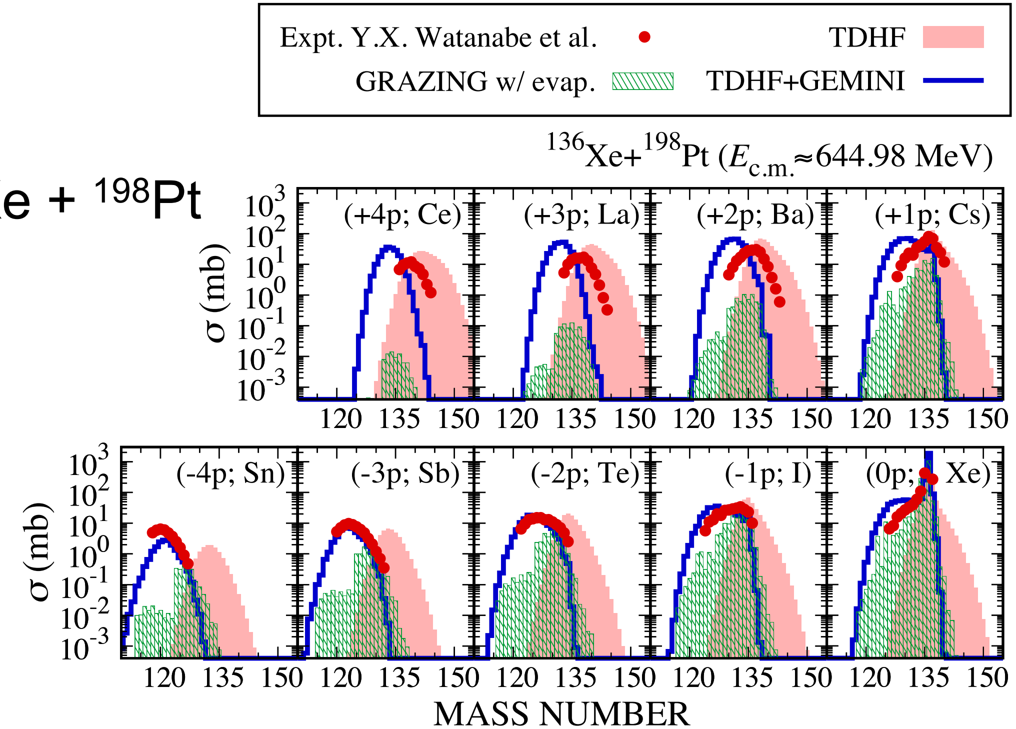
Simenel, C., 2010, Phys. Rev. Lett. 105, 192701.

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

Real-time simulation



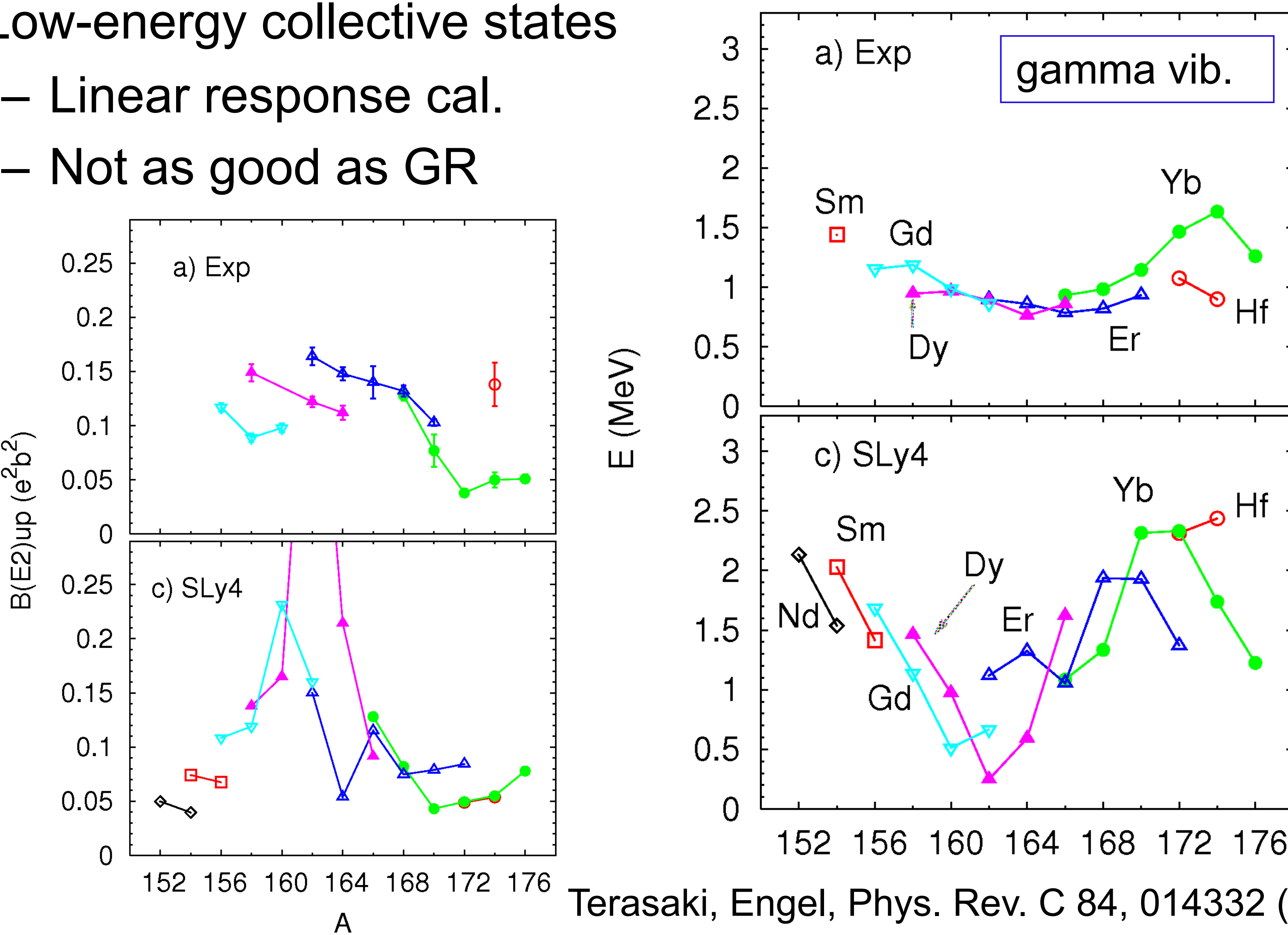
^{136}Xe + ^{198}Pt



Sekizawa, Phys. Rev. C **96**, 014615 (2017)

Low-energy states

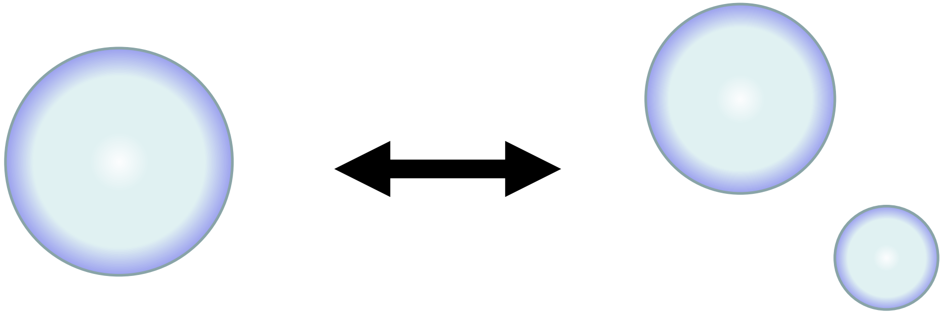
- Low-energy collective states
  - Linear response cal.
  - Not as good as GR



Terasaki, Engel, Phys. Rev. C 84, 014332 (2011)

Large amplitude collective motion

- Decay modes
  - Spontaneous fission
  - Alpha decay
- Low-energy reaction
  - Sub-barrier fusion reaction
  - Alpha capture reaction (element synthesis in the stars)



Success & failure

- Success of nuclear (TD)DFT
  - Unified picture of liquid-like and gas-like properties (*saturation* and *indep. part. motion*)
  - Giant resonances (*linearized TDDFT*)
- Problems
  - Low-energy collective motion
  - Many-body tunneling (spontaneous fission, sub-barrier fusion, astrophysical reaction)
- Possible solutions
  - Improving DF (ω-dep., beyond LDA, etc.)
  - *Re*-quantization of TDDFT

Strategy

- Purpose
  - Recover quantum fluctuation effect associated with "slow" collective motion
- Difficulty
  - *Non-trivial* collective variables
- Procedure
  1. Identify the collective subspace of such slow motion, with canonical variables (q, p)
  2. Quantize on the subspace $[q, p] = i\hbar$

Classical Hamilton's form

Blaizot, Ripka, "Quantum Theory of Finite Systems" (1986)
Yamamura, Kuriyama, Prog. Theor. Phys. Suppl. 93 (1987)

The TDDFT can be described by the classical form.

$$\dot{\xi}^{ph} = \frac{\partial H}{\partial \pi_{ph}}$$

$$\dot{\pi}_{ph} = -\frac{\partial H}{\partial \xi^{ph}}$$

$$H(\xi, \pi) = E[\rho(\xi, \pi)]$$

The canonical variables (ξ^{ph}, π_{ph})

$$\rho_{pp\prime} = \left[(\xi + i\pi)(\xi + i\pi)^{\dagger}\right]_{pp\prime} \qquad \rho_{hh\prime} = \left[1 - (\xi + i\pi)^{\dagger}(\xi + i\pi)\right]_{hh\prime}$$

$$\rho_{ph} = \left[(\xi + i\pi)\{1 - (\xi + i\pi)^{\dagger}(\xi + i\pi)\}\right]_{ph}$$

Number of variables = Number of *ph* degrees of freedom

Expansion for "slow" motion

- Hamiltonian

$$H = H(\xi, \pi) \approx \frac{1}{2} B^{\alpha\beta}(\xi)\pi_\alpha \pi_\beta + V(\xi)$$

expanded up to 2nd order in π $\quad [\alpha, \beta = (ph)]$

- Transformation $(\xi^\alpha, \pi_\alpha) \rightarrow (q^\mu, p_\mu)$

$$p_\mu = \frac{\partial \xi^\alpha}{\partial q^\mu}\pi_\alpha, \qquad \pi_\alpha = \frac{\partial q^\mu}{\partial \xi^\alpha} p_\mu$$

- Hamiltonian

$$\bar{H} = \bar{H}(q, p) \approx \frac{1}{2} \bar{B}^{\mu\nu}(q) p_\mu p_\nu + V(q)$$

Decoupled submanifold

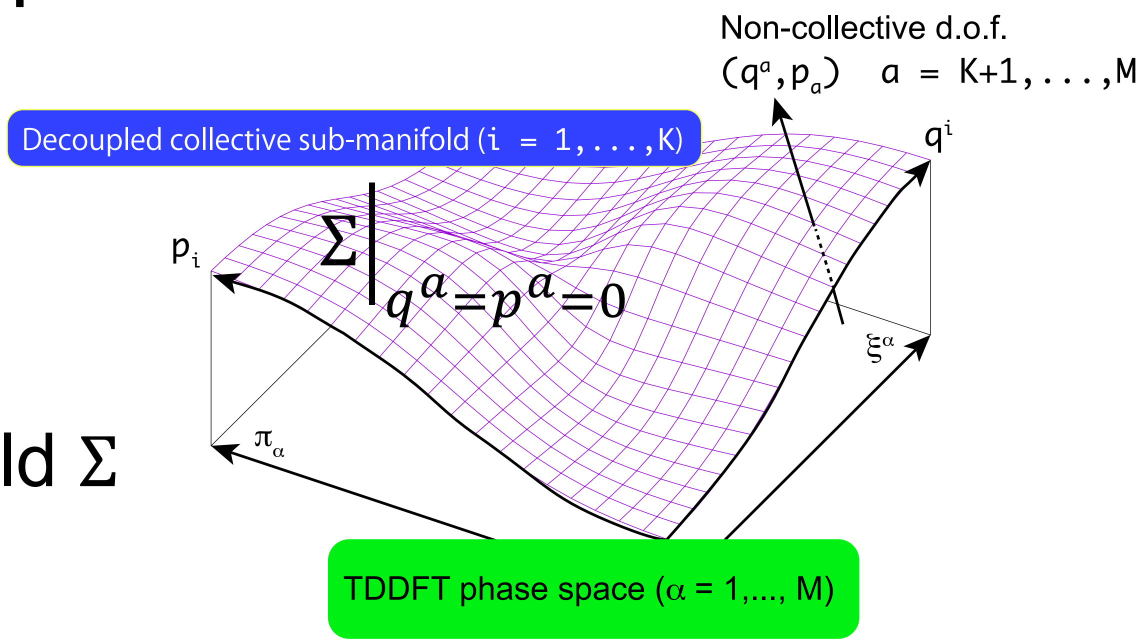
Klein, Do Dang, Walet, Phys. Rep. 335, 93 (2000)
Nakatsukasa, Prog. Theor. Exp. Phys. 2012, 01A207 (2012)

- Collective canonical variables (q,p)
  - $\{\xi^\alpha, \pi_\alpha\} \rightarrow \{q, p;\ q^a, p_a;\quad a = 2, \cdots, N_{ph}\}$
- Finding a decoupled submanifold Σ

$$\dot{q}^a = \left.\frac{\partial H}{\partial p}\right|_\Sigma \approx 0$$

$$\dot{p}^a = -\left.\frac{\partial H}{\partial q}\right|_\Sigma \approx 0$$

on the submanifold Σ



ASCC (adiabatic self-consistent collective coordinate) method

Matsuo, et al., PTP 103, 959 (2000)
Nakatsukasa, et al., RMP 88, 045004 (2016)
Nakatsukasa, Prog. Theor. Exp. Phys. 2012, 01A207 (2012)

- Collective canonical variables (q, p)
  - $\{\xi^\alpha, \pi_\alpha\} \to \{q, p; \, q^a, p_a; \quad a = 2, \cdots, N_{ph}\}$
- Finding a decoupled submanifold

$$\frac{\partial V}{\partial \xi^\alpha} - \frac{\partial V}{\partial q}\frac{\partial q}{\partial \xi^\alpha} = 0$$

Moving mean-field eq.

$$B^{\beta\gamma}\left(\nabla_\gamma \frac{\partial V}{\partial \xi^\alpha}\right)\frac{\partial q}{\partial \xi^\beta} = \omega^2 \frac{\partial q}{\partial \xi^\alpha}$$

Moving RPA eq.

$$\nabla_\gamma \frac{\partial V}{\partial \xi^\alpha} \equiv \frac{\partial^2 V}{\partial \xi^\gamma \partial \xi^\alpha} - \Gamma^\beta_{\alpha\gamma}\frac{\partial V}{\partial \xi^\beta}$$

$$\Gamma^\beta_{\alpha\gamma} = \frac{1}{2}B^{\beta\delta}\left(B_{\delta\gamma,\alpha} + B_{\delta\alpha,\gamma} - B_{\alpha\gamma,\delta}\right)$$: Affine connection

Numerical procedure

$$\frac{\partial V}{\partial \xi^{\alpha}} - \frac{\partial V}{\partial q}\frac{\partial q}{\partial \xi^{\alpha}} = 0$$

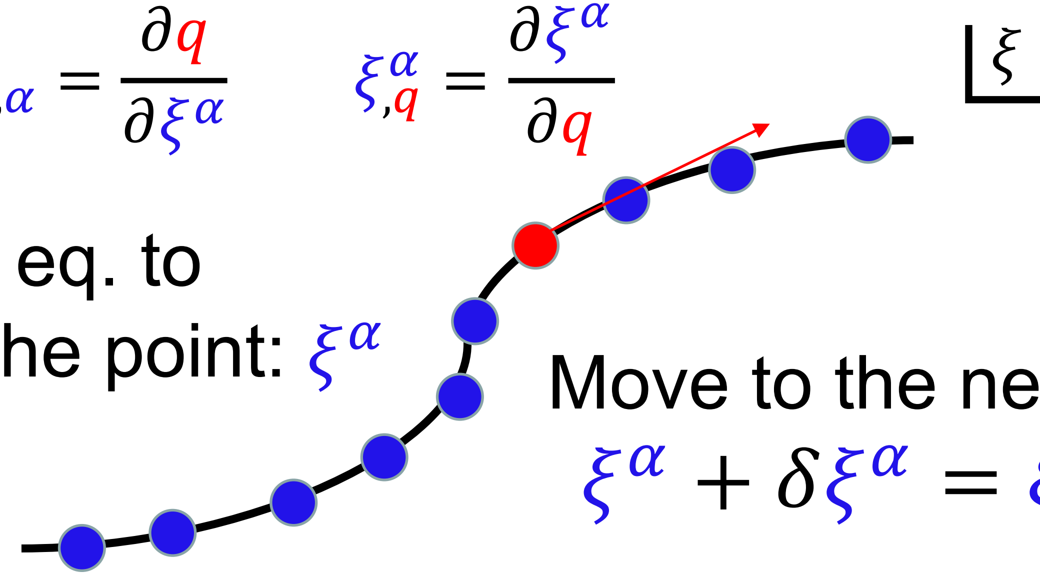
Moving mean-field eq.

$$B^{\beta\gamma}\left(\nabla_{\gamma}\frac{\partial V}{\partial \xi^{\alpha}}\right)\frac{\partial q}{\partial \xi^{\beta}} = \omega^{2}\frac{\partial q}{\partial \xi^{\alpha}}$$

Moving RPA eq.

Tangent vectors (Generators)

$$q_{,\alpha} = \frac{\partial q}{\partial \xi^{\alpha}} \qquad \xi^{\alpha}_{,q} = \frac{\partial \xi^{\alpha}}{\partial q}$$



Moving MF eq. to determine the point: ξ^{α}

Move to the next point

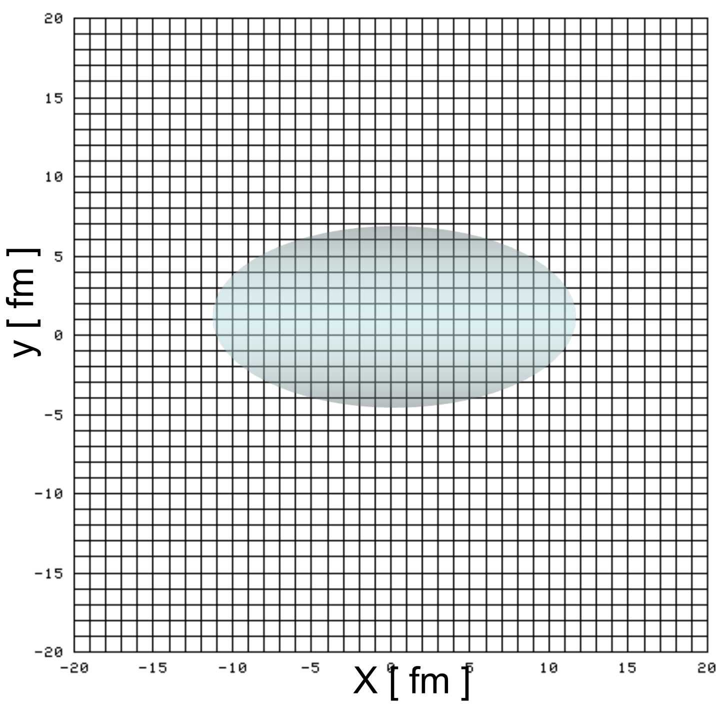
$$\xi^{\alpha} + \delta\xi^{\alpha} = \xi^{\alpha} + \varepsilon\xi^{\alpha}_{,q}$$

Canonical variables and quantization

- Solution
  - 1-dimensional state: $\xi(q)$
  - Tangent vectors: $\frac{\partial q}{\partial \xi^\alpha}$ and $\frac{\partial \xi^\alpha}{\partial q}$
  - Fix the scale of q by making the inertial mass $\bar{B} = \frac{\partial q}{\partial \xi^\alpha} B^{\alpha\beta} \frac{\partial q}{\partial \xi^\alpha} = 1$
- Collective Hamiltonian
  - $\bar{H}_{\mathrm{coll}}(q,p) = \frac{1}{2}p^2 + \bar{V}(q), \qquad \bar{V}(q) = V(\xi(q))$
  - Quantization $[q, p] = i\hbar$

3D real space representation

- 3D space discretized in lattice
- BKN functional
- Moving mean-field eq.: Imaginary-time method
- Moving RPA eq.: Finite amplitude method (PRC 76, 024318 (2007))

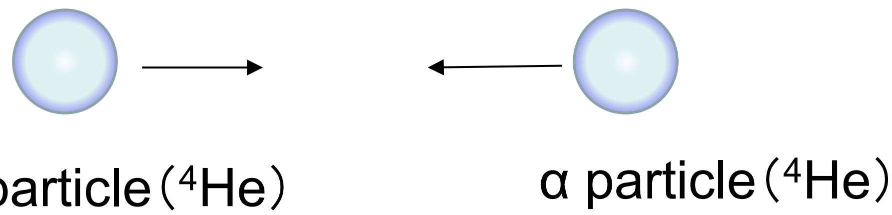


Wen, T.N., Phys. Rev. C 105 (2021) 034603; Phys. Rev. C 96 , 014610 (2017); PRC 94, 054618 (2016).

At a moment, no pairing

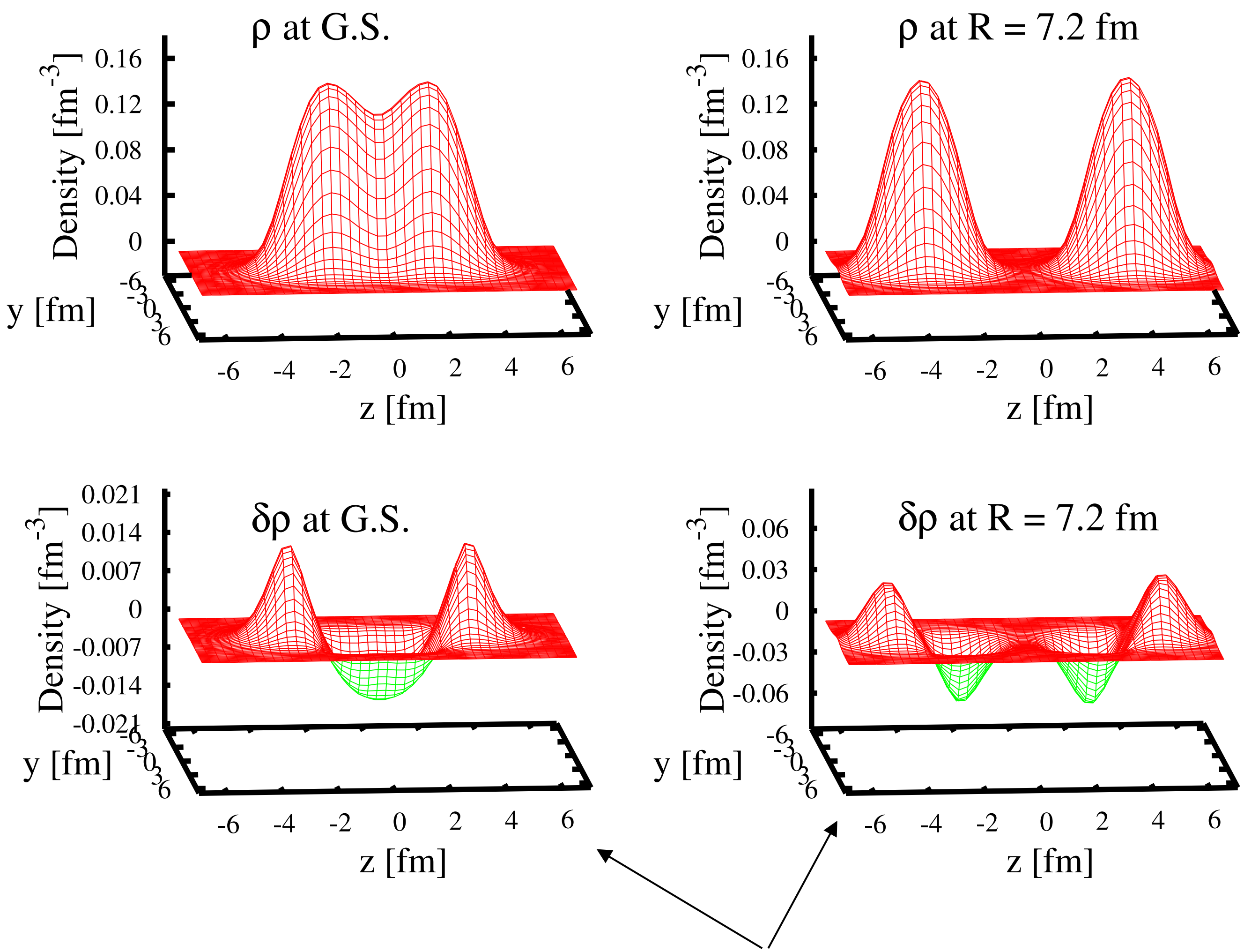
1-dimensional reaction path extracted from the Hilbert space of dimension of $10^4 \sim 10^5$.

Simple case: α + α scattering



- Reaction path
- After touching
  – No bound state, but
  – a resonance state in ^{8}Be

^{8}Be: Tangent vectors (generators)



$\rho(\vec{r})$

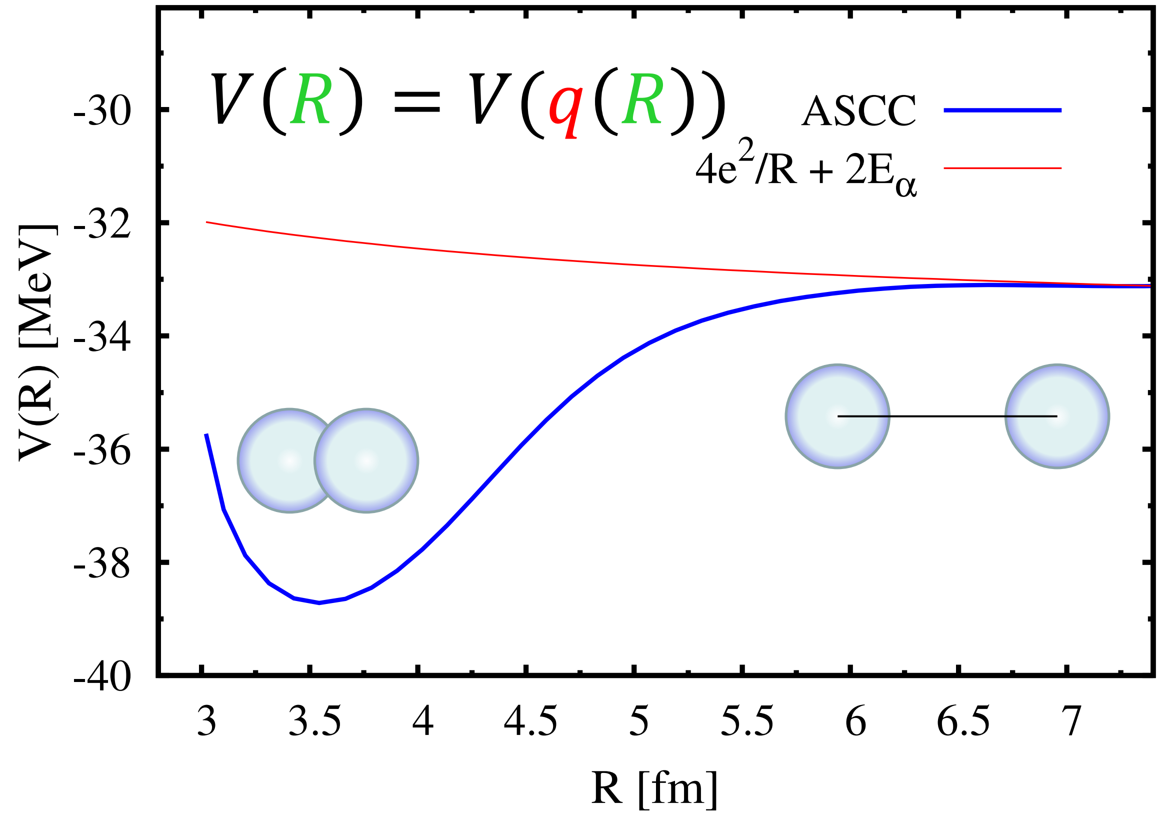
$\delta\rho(\vec{r})$

Tangent vectors (Generators)

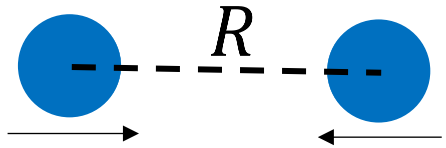
$V(R)$: collective potential

Represented by the relative distance R

Transformation: $q \rightarrow R$

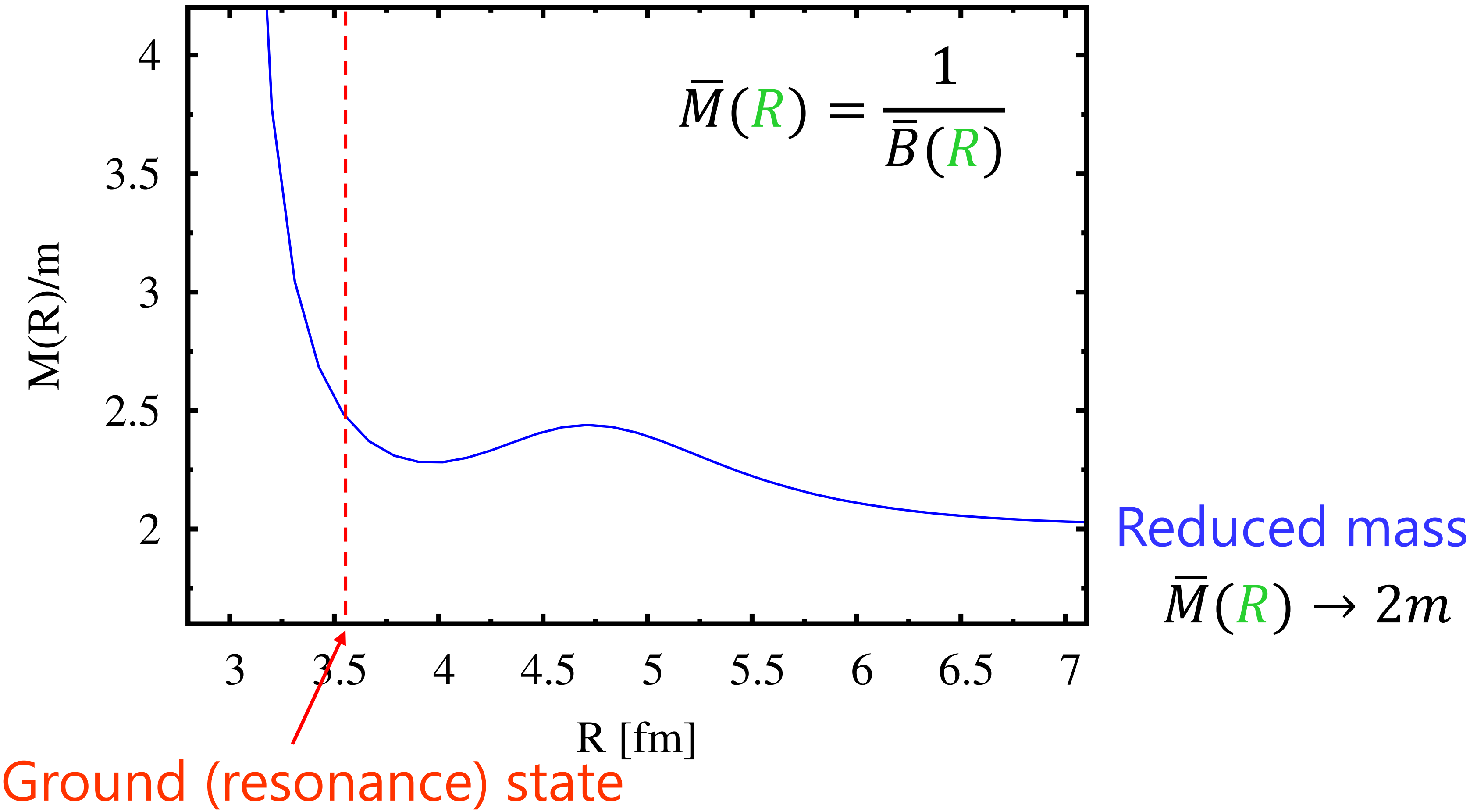


$M(R)$ for relative motion



Transformation: $q \to R$

$$\bar{B}(R) = \frac{\partial R}{\partial q}\bar{B}\frac{\partial R}{\partial q} = \left(\frac{\partial R}{\partial q}\right)^2$$



Introduction of effective mass

$$E[\rho] = \int \frac{1}{2m}\tau(\mathbf{r})d\mathbf{r} + \int d\mathbf{r}\left\{\frac{3}{8}t_0\rho^2(\mathbf{r}) + \frac{1}{16}t_3\rho^3(\mathbf{r})\right\}$$

$$+ \iint d\mathbf{r}d\mathbf{r}'\rho(\mathbf{r})v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}')$$

$$+ B_3 \int d\mathbf{r}\{\rho(\mathbf{r})\tau(\mathbf{r}) - \mathbf{j}^2(\mathbf{r})\},$$

$$\hat{h}_{\mathrm{HF}}(\mathbf{r}) = -\nabla\frac{1}{2m^*(\mathbf{r})}\nabla + \frac{3}{4}t_0\rho(\mathbf{r}) + \frac{3}{16}t_3\rho^2(\mathbf{r})$$

$$+ \int d\mathbf{r}'v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}') + B_3[\tau(\mathbf{r}) + i\nabla\cdot\mathbf{j}(\mathbf{r})]$$

$$+ 2iB_3\mathbf{j}(\mathbf{r})\cdot\nabla,$$

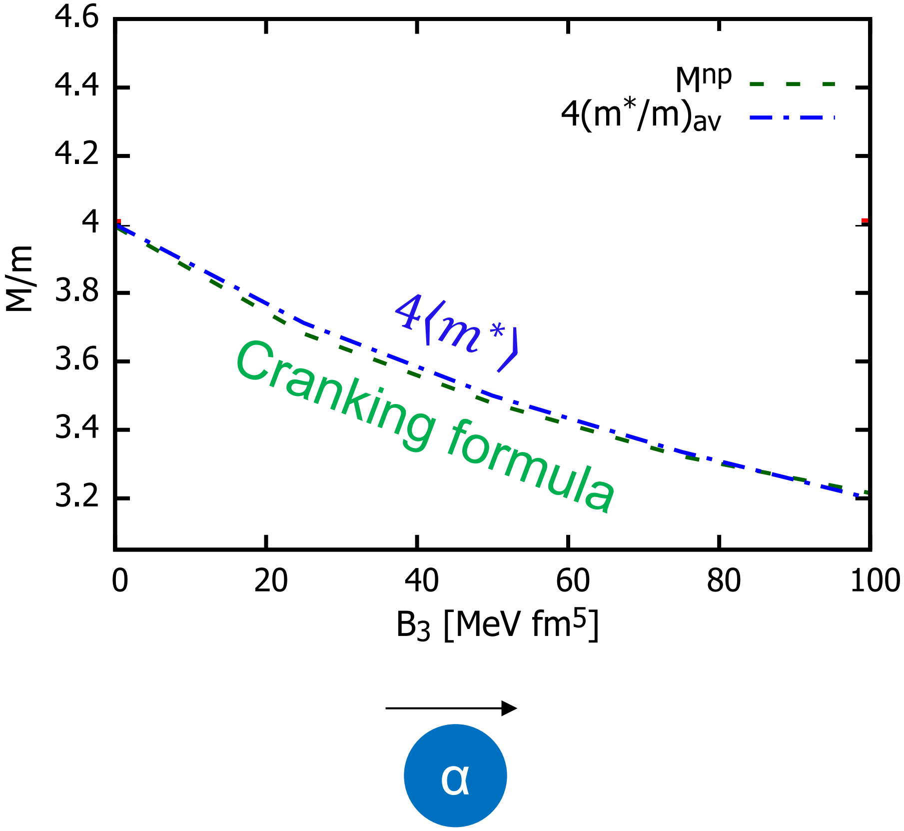
$B_3 = 0 \quad \rightarrow \quad m^* = m$

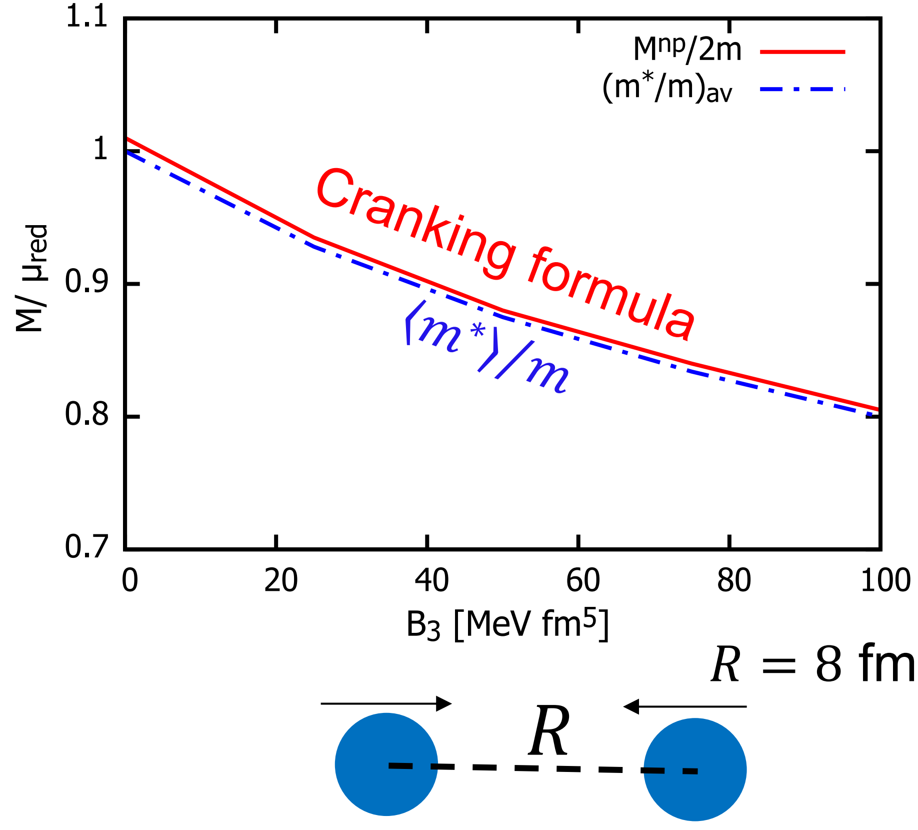
$B_3 > 0 \quad \rightarrow \quad m^* < m$

Failure of cranking formula

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

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



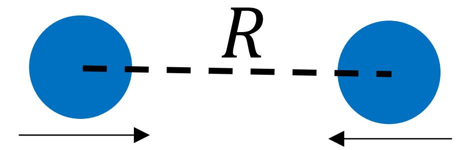


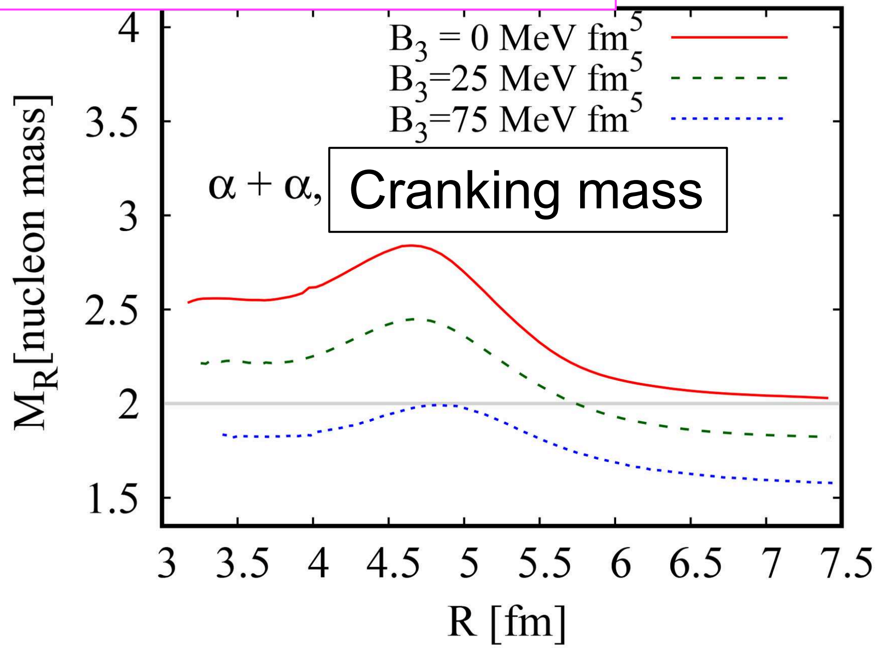
$R = 8$ fm

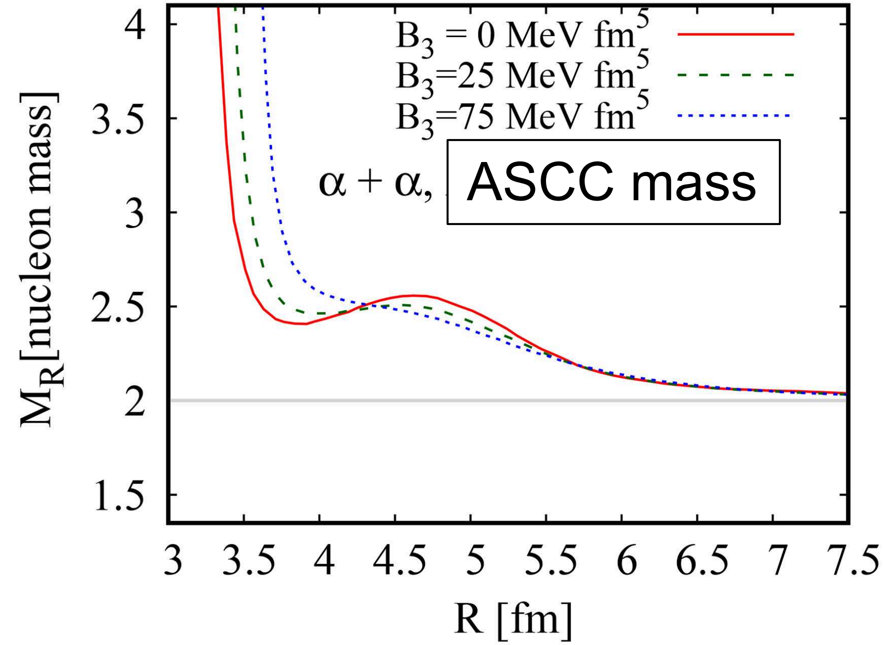
$M(R) \quad (m^*/m \leq 1)$

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

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







Cranking mass

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

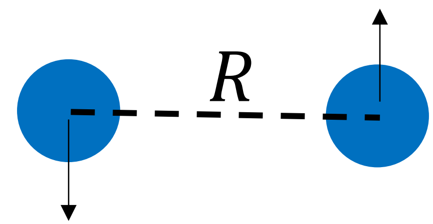
ASCC mass

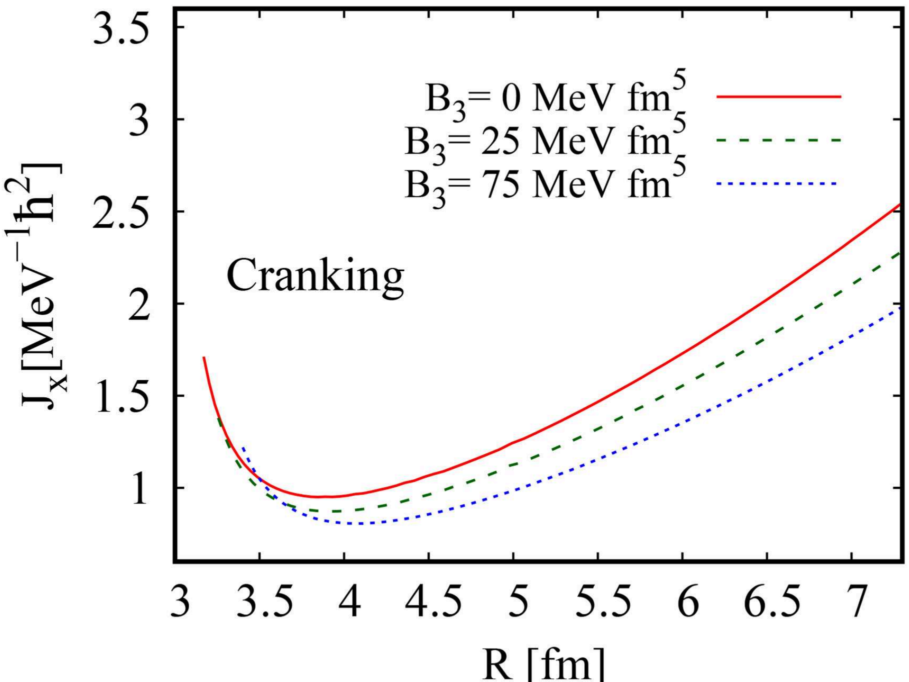
$$M(R) = \mu_R \quad (R \to \infty)$$

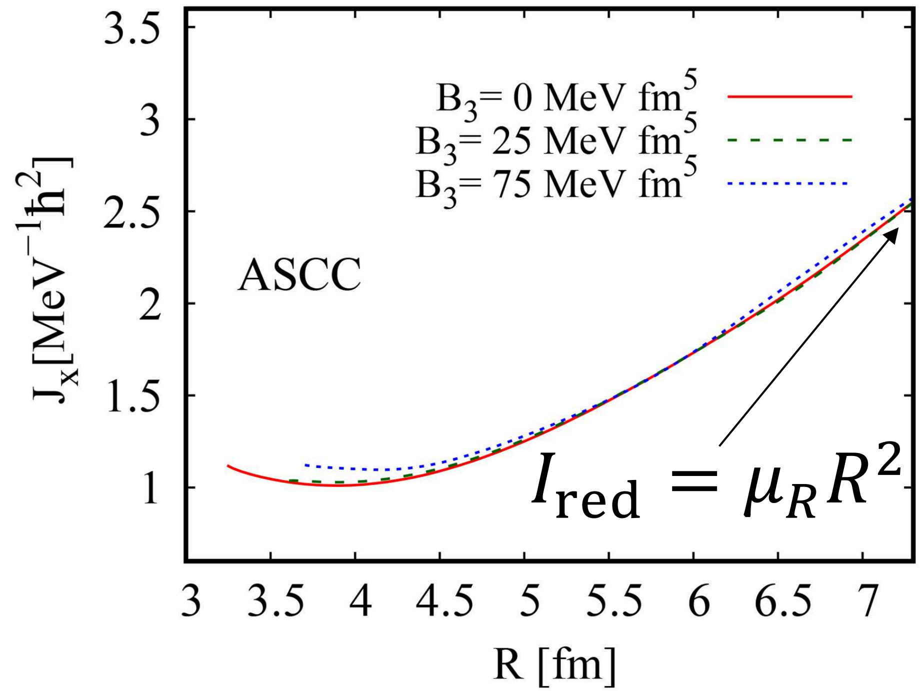
$I(R) \quad (m^*/m \leq 1)$

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

$\alpha + \alpha$







Cranking MoI

$I(R) \neq \mu_R R^2 \quad (R \to \infty)$

ASCC MoI

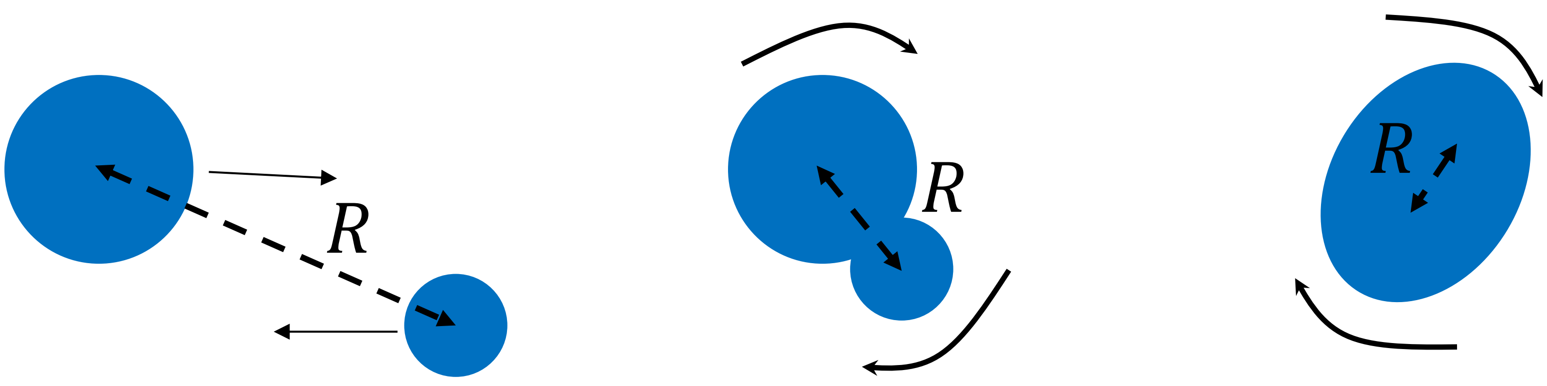
$I(R) = \mu_R R^2 \quad (R \to \infty)$

Microscopic construction of nuclear reaction model

Model Hamiltonian

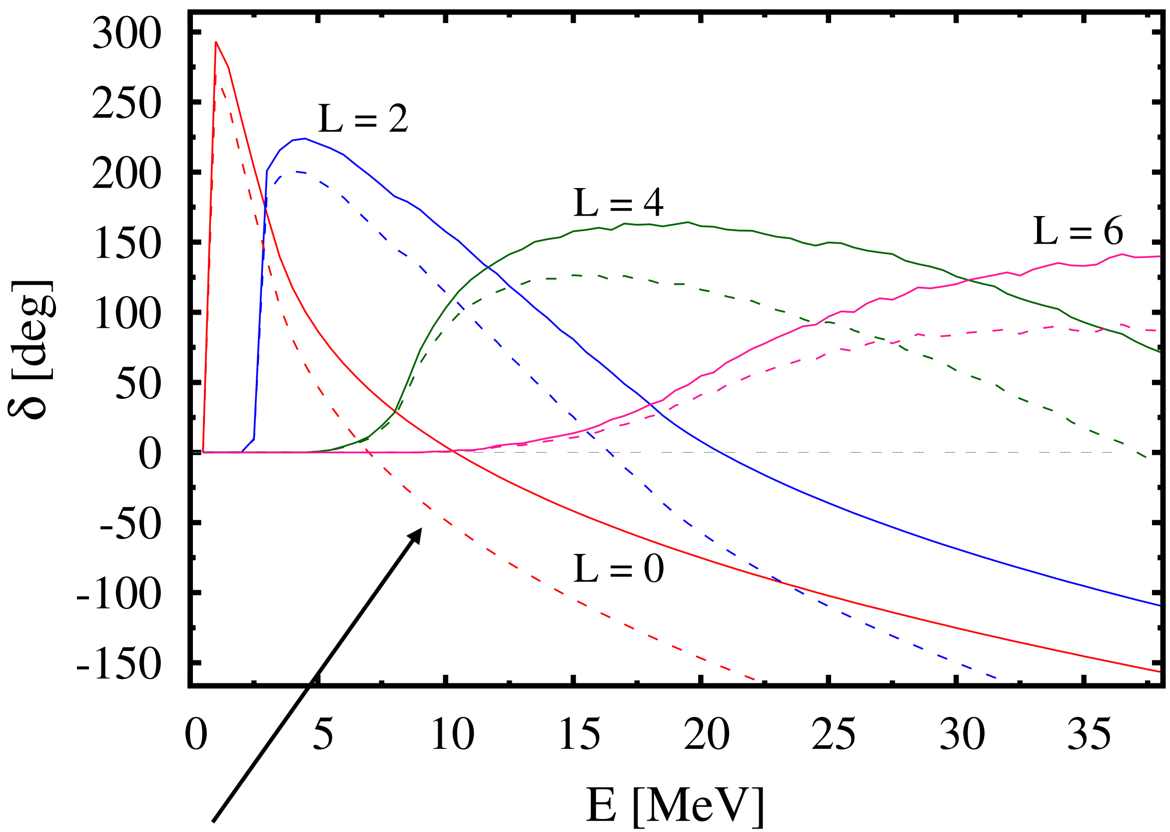
$$\left\{-\frac{d}{dR}\frac{1}{2M(R)}\frac{d}{dR}+\frac{L(L+1)}{2I(R)}+V(R)\right\}\psi_L(R)=E_L\psi_L(R)$$

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



α + α scattering (phase shift)

Nuclear phase shift

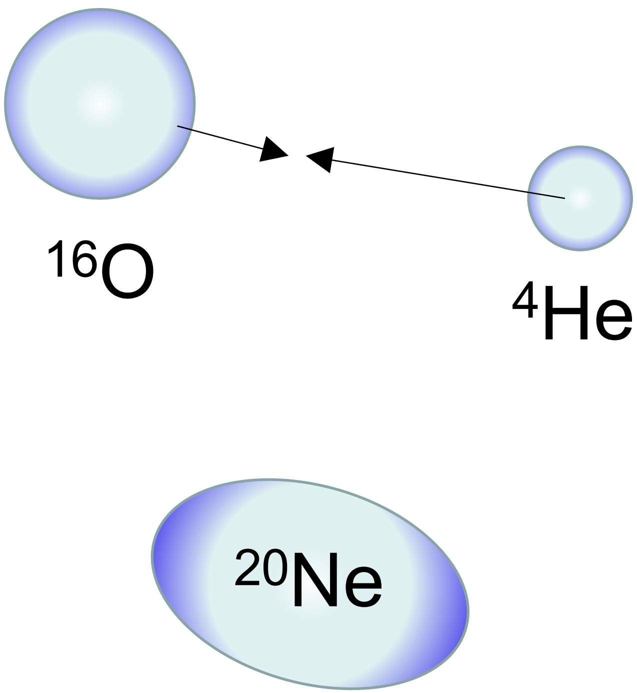


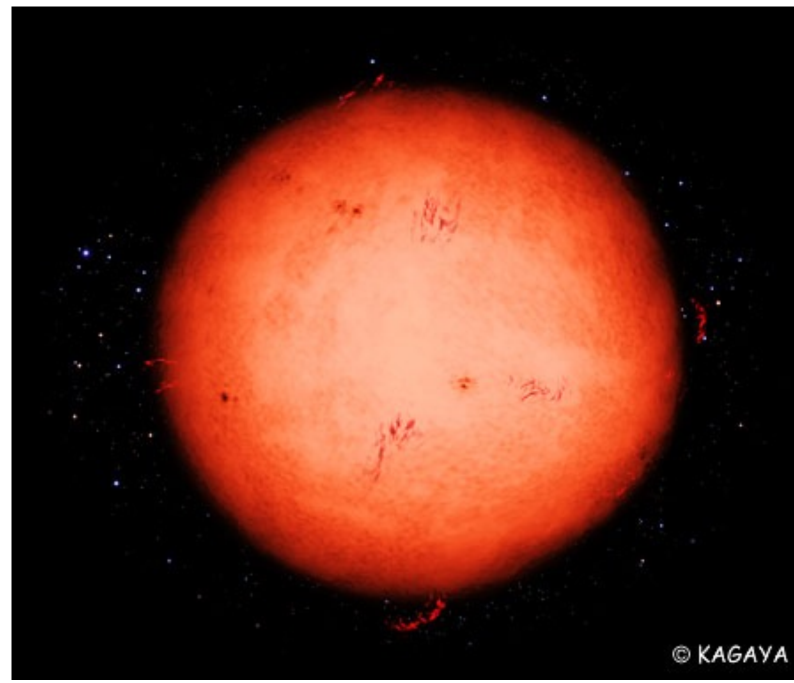
Effect of dynamical change of the inertial mass

Dashed line: Constant reduced mass ($M(R) \to 2m$)

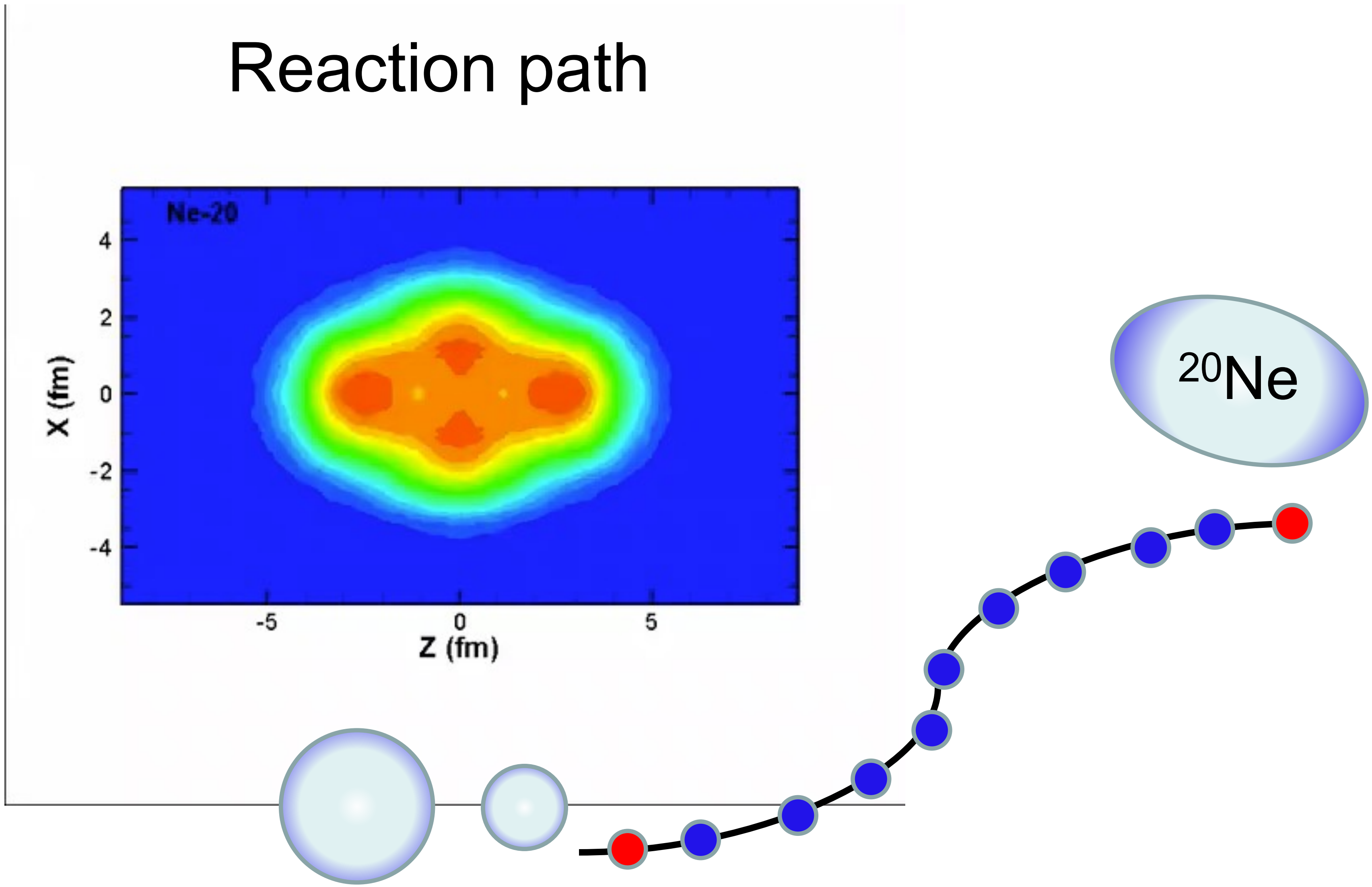
$^{16}O + \alpha$ scattering

- Important reaction to synthesize heavy elements in giant stars
  - Alpha reaction

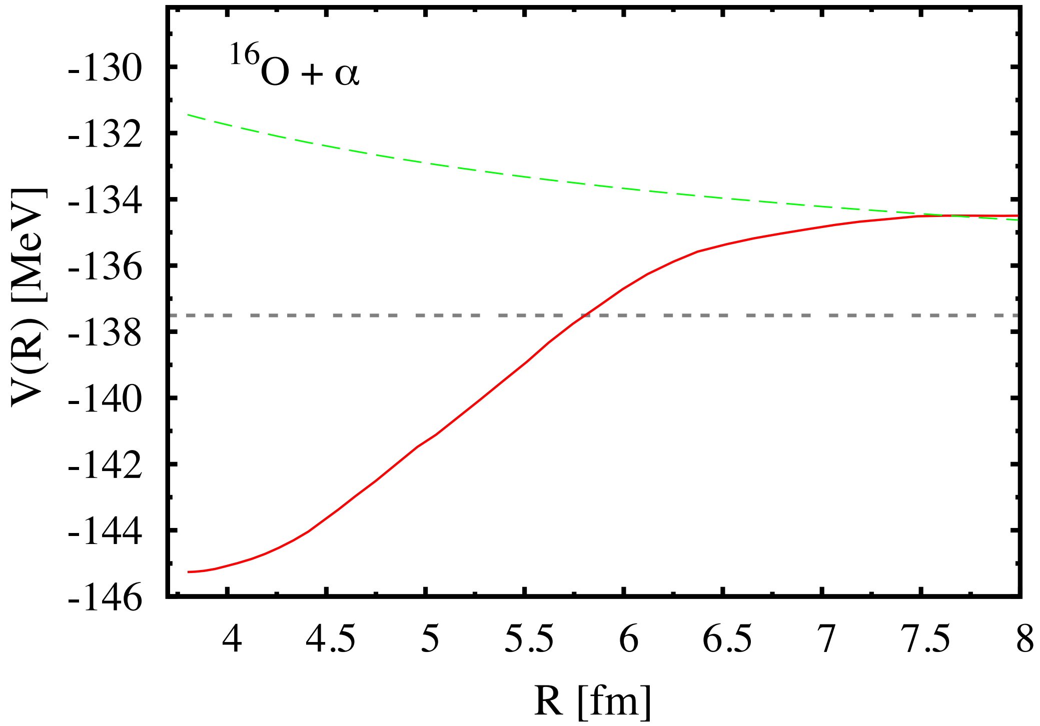


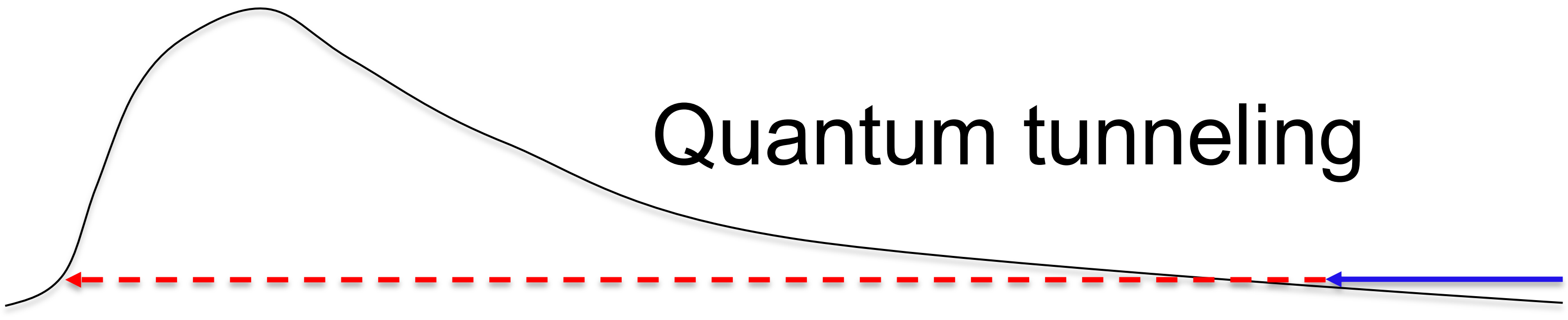


$^{16}O + \alpha$ to/from ^{20}Ne



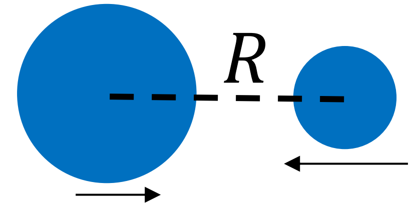
^{20}Ne: Collective potential



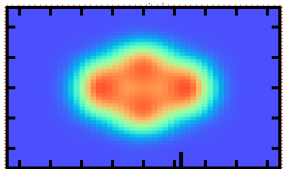


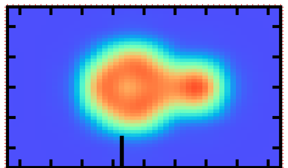
Quantum tunneling

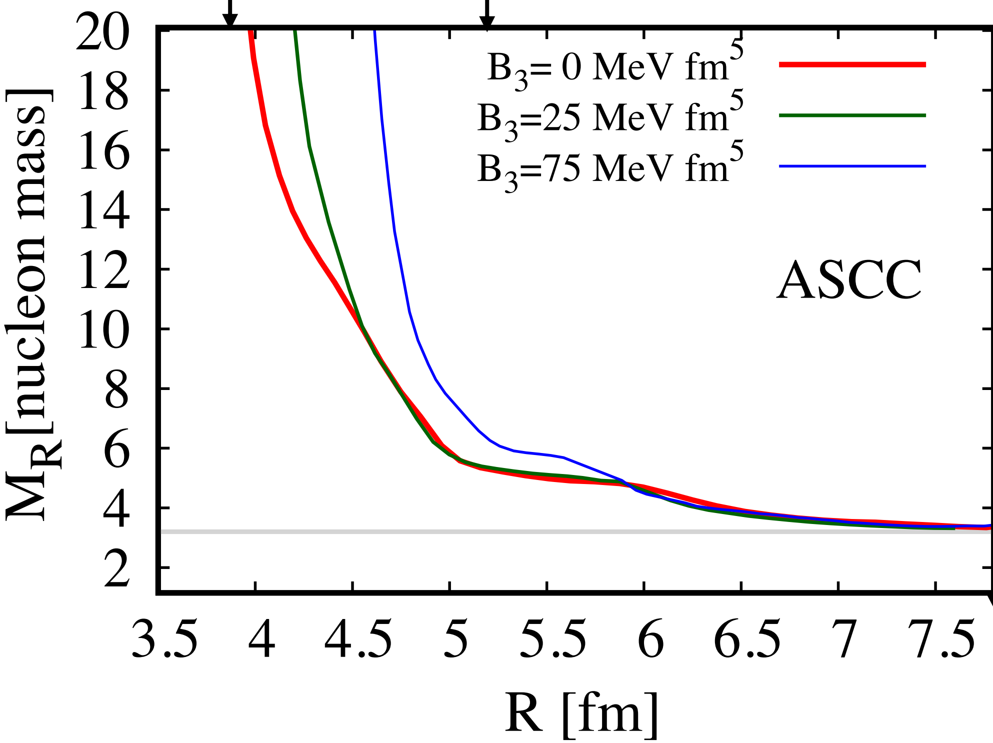
$M(R)$ $(m^*/m \leq 1)$



$\alpha + {}^{16}O$

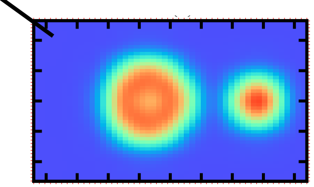




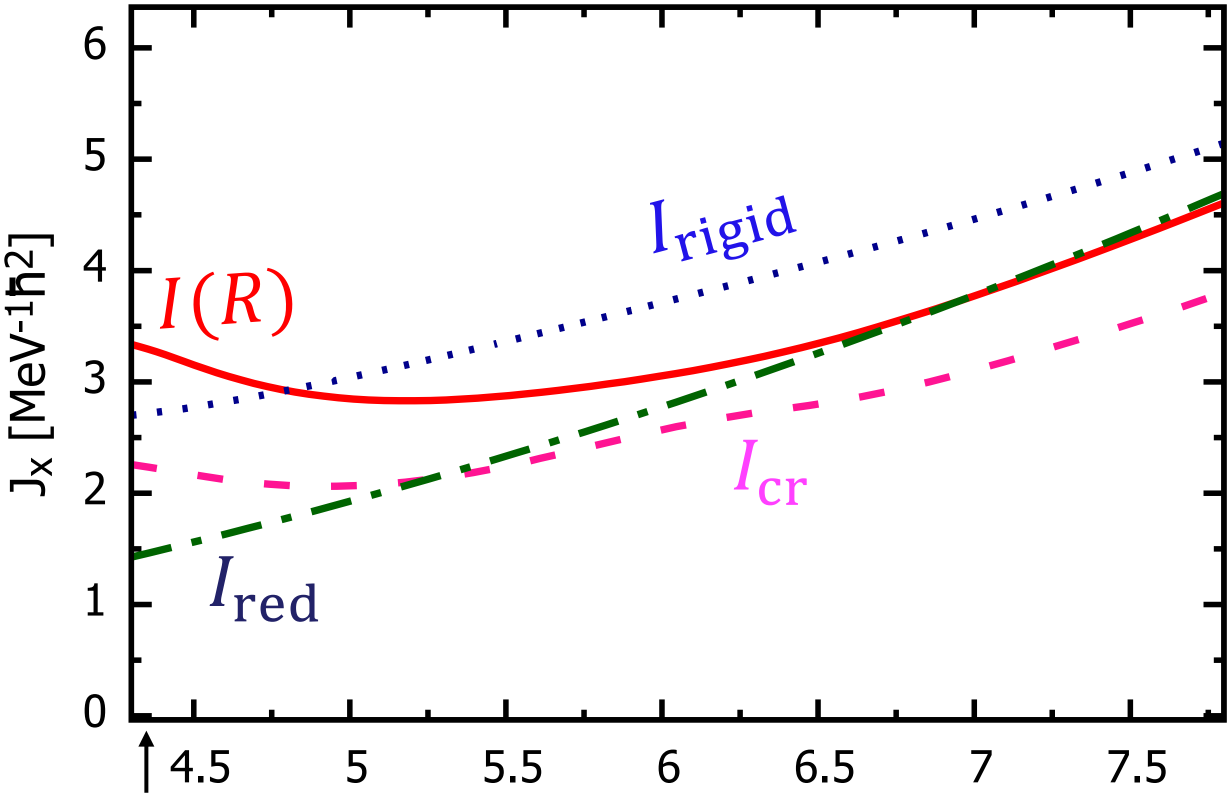


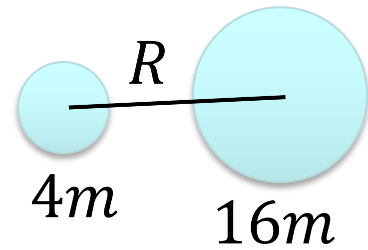
$m^* < m^* < m^* = m$

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

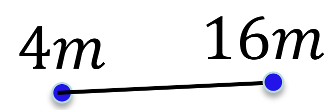


$I(R)$ $(m^*/m < 1)$

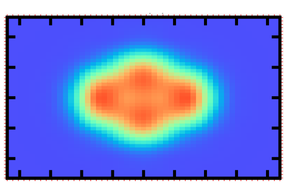




"Point-particle approx."



Ground state of ^{20}Ne



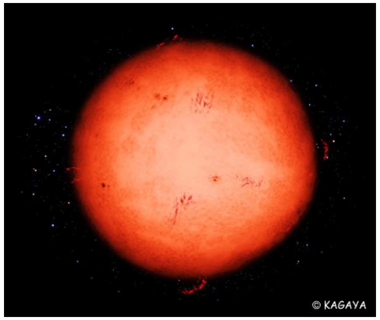
$I(R) = I_{\mathrm{red}}$ at large R

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

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

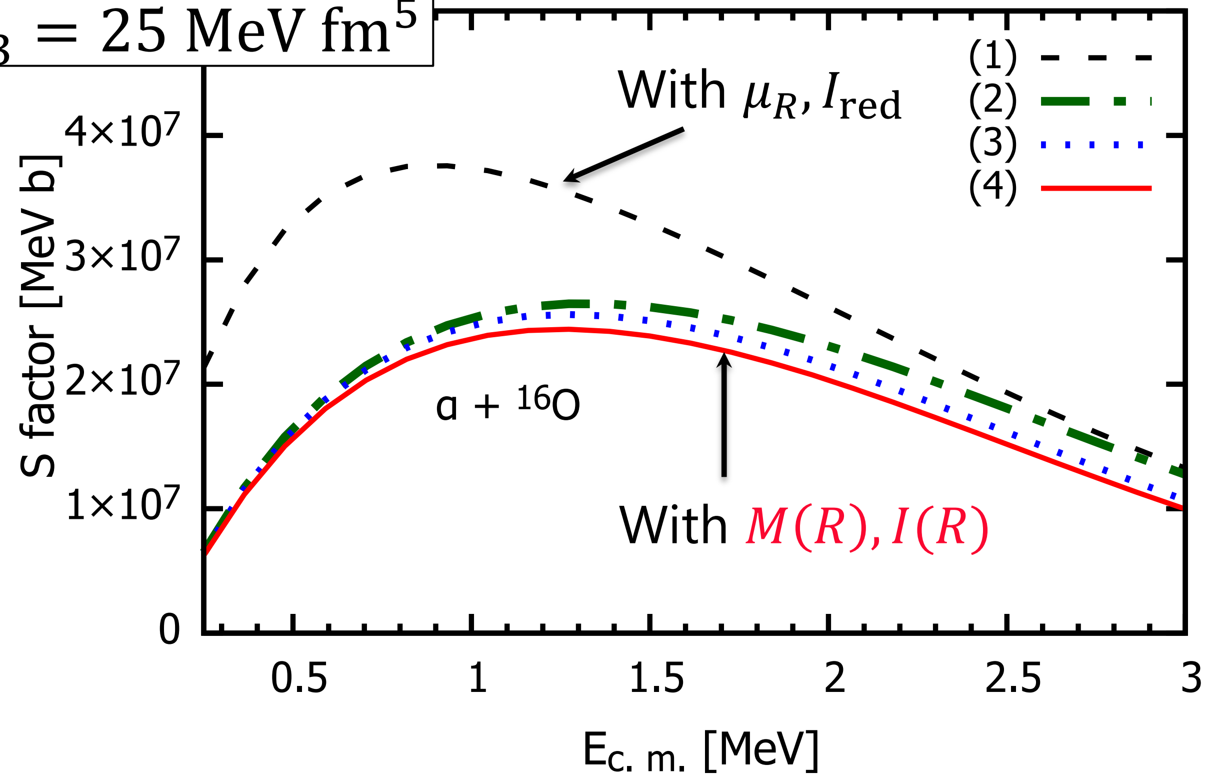
Fusion reaction:
Astrophysical S-factor

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



Synthesis of ^{20}Ne

$B_3 = 25$ MeV fm^5



Summary

- Missing correlations in nuclear density functional
  - Correlations associated with low-energy collective motion
- Re-quantize a specific mode of collective motion
  - Derive the slow collective motion
  - Quantize the collective Hamiltonian
  - Applicable to nuclear structure and reaction

Recent progress: Talk by K. Wen on Dec. 12