Quantized TDDFT dynamics
--- Part 1: The basics of nuclear mean-field models ---

Takashi Nakatsukasa (University of Tsukuba)

- Basic properties of nuclei
  - –Saturation properties vs Single-particle motion
  - –Mean-field model vs Density functional model
- TDDFT for nuclear collective motion
  - –Linear response: High-energy giant resonances vs low-energy modes of excitation
  - –Success and failures

2017.6.19-23 @RIKEN, Wako, Japan

Different faces of nuclei

Liquid

Gas

Nuclear Saturation
“Liquid”-like property

B/A ~ 8 MeV

(B/A ~ 16 MeV for nuclear matter)

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

⇒ Liquid drop model

Bethe-Weizsäcker mass formula

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

Saturation properties of nuclear matter

- Symmetric nuclear matter w/o Coulomb
  - $N = Z = A/2$
- Constant binding energy per nucleon
  - Constant separation energy

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

- Saturation density

$$\rho \approx 0.16\,\text{fm}^{-3} \quad \Rightarrow \quad k_F \approx 1.35\,\text{fm}^{-1}$$

  - Fermi energy

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

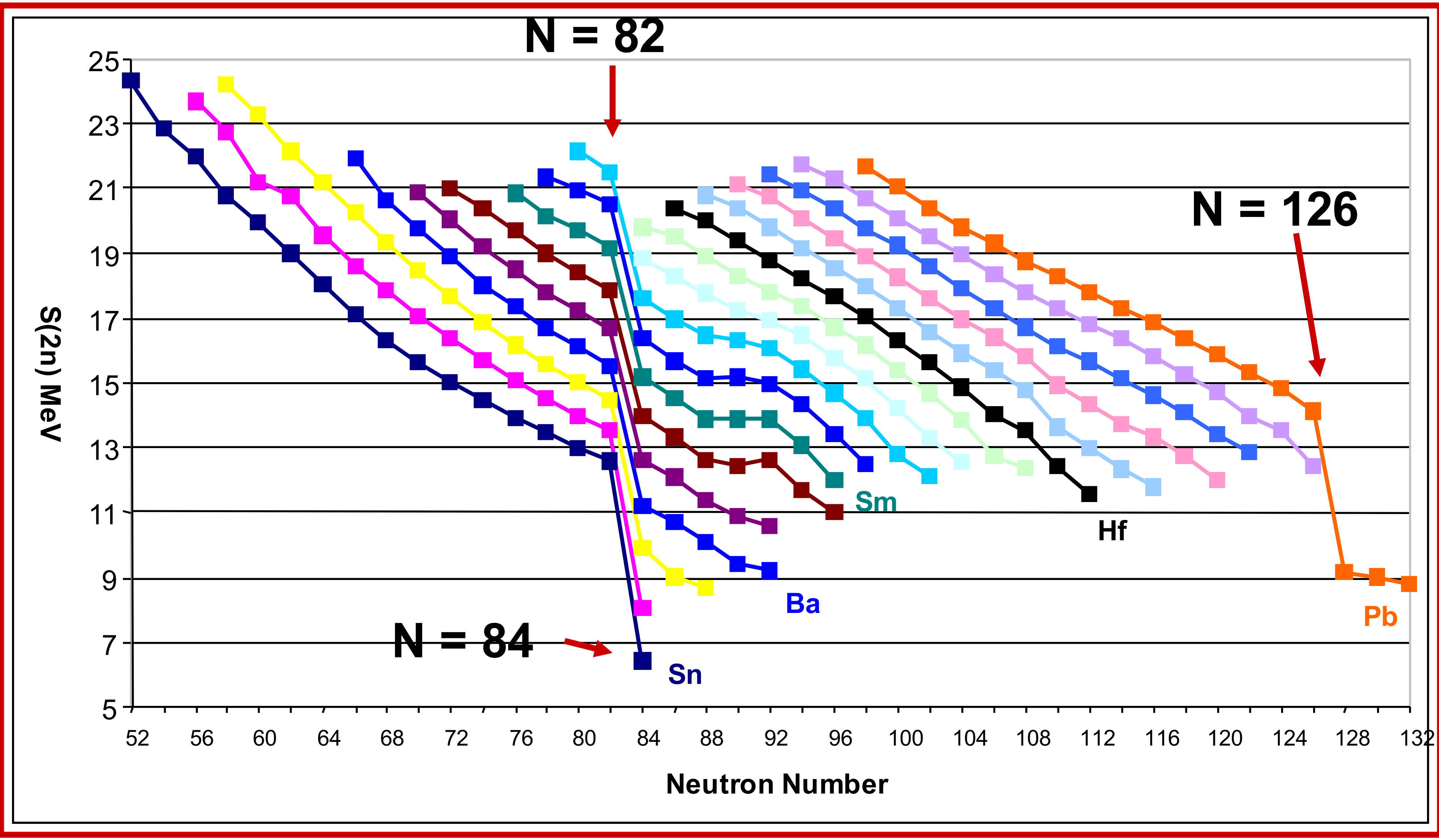
Single-particle motion
"Gas"-like picture

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

- Mean free path in nuclei
  - Neutron scattering

Energy required to remove two neutrons from nuclei

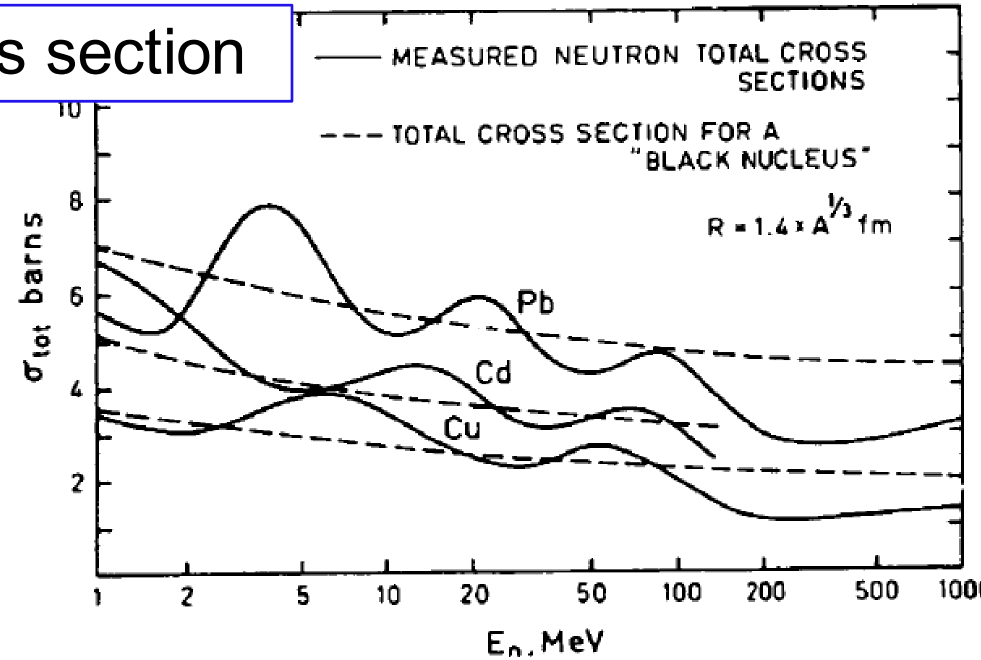
(2-neutron binding energies = 2-neutron "separation" energies)



R. Casten

Nuclear "transparency"

Neutron scattering cross section



Bohr and Mottelson, *Nuclear Structure Vol.1* (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

$$\lambda >> R$$

for *low-energy* neutrons

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

Saturated gas?

- Is the mean-field (gas or single-particle) picture consistent with the saturation property?
  - Analysis with a simple potential model for infinite nuclear matter

$$h = -\frac{\hbar^2}{2m}\nabla^2 + V$$

Saturation properties of nuclear matter

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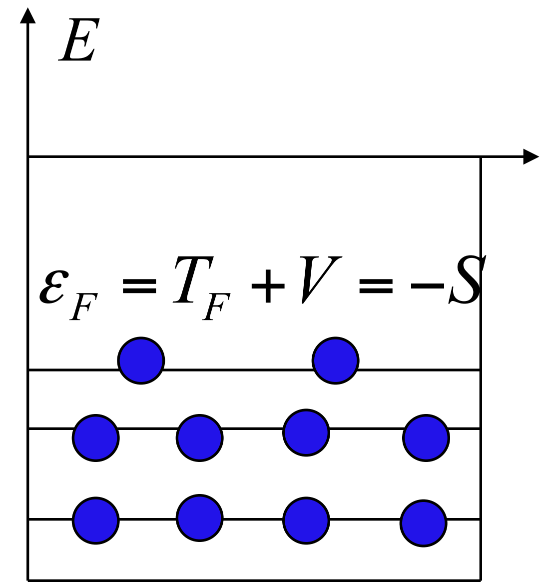
A constant mean-field potential

- Binding energy in the mean field



$$-B = \sum_{i=1}^{A}\left(T_i + \frac{V}{2}\right), \quad T_i = \frac{\hbar^2 k_i^2}{2m}$$

$$= A\left(\frac{3}{5}T_F + \frac{V}{2}\right)$$

- Saturation property

$$S = B/A \quad \Rightarrow \quad T_F = -\frac{5}{4}V$$

Inconsistent with nuclear binding

Momentum-dependent potential

- State-dependent potential
  - Momentum dependence
  - The lowest order → "Effective mass"

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

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

  - 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.

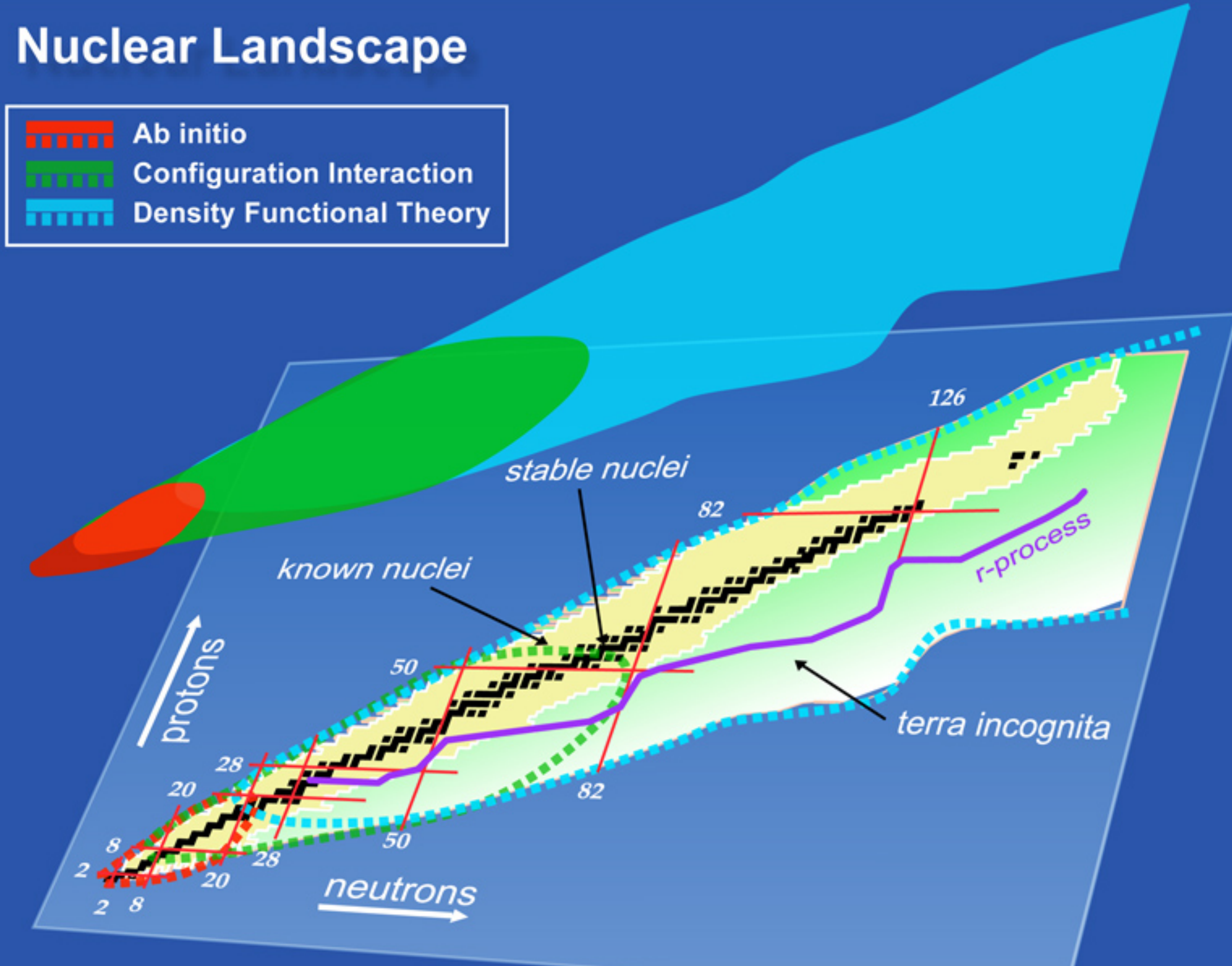
$$E\left[\rho_q, \tau_q, \overleftrightarrow{J}_q; \kappa_q\right]$$

kinetic

pair density

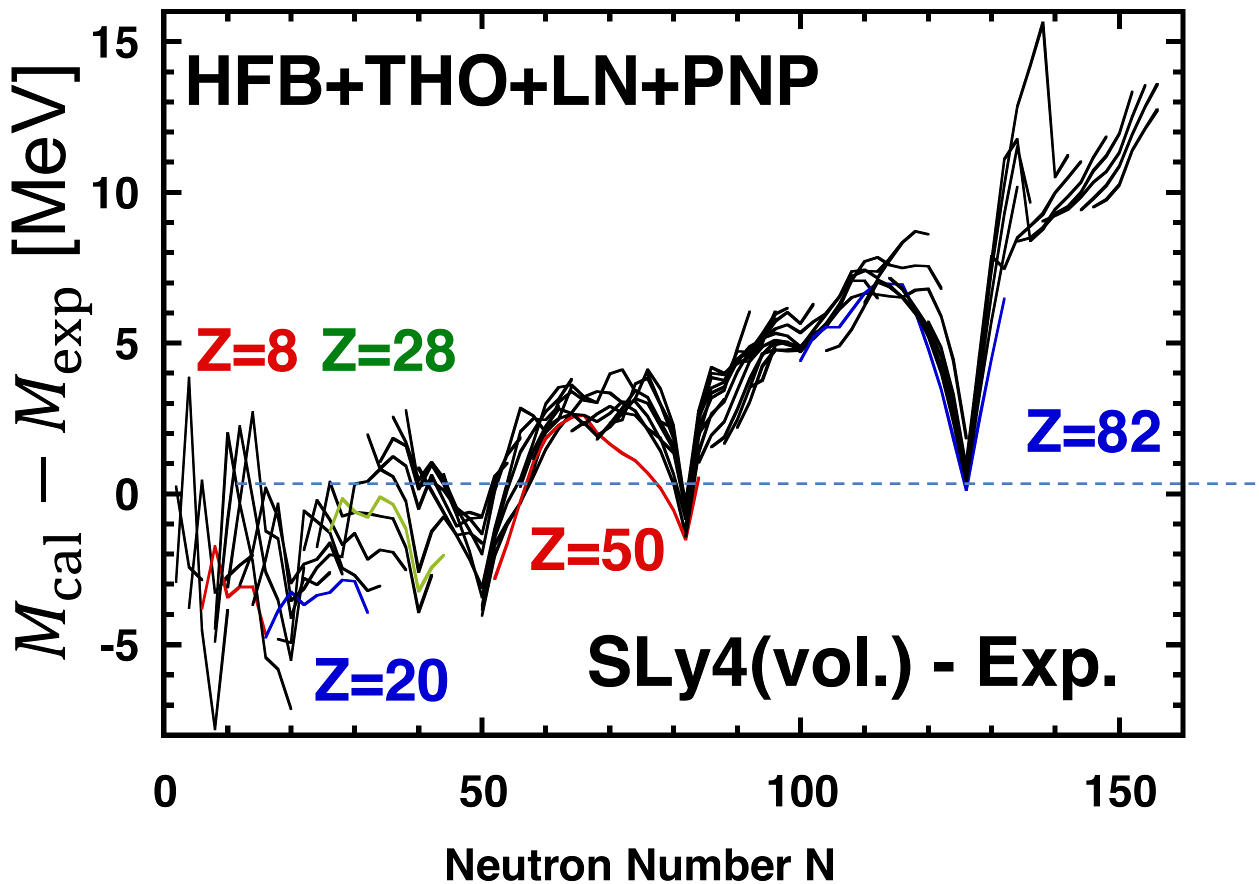
spin-current

Nuclear Landscape



From SciDAC-UNEDF project

Predicted nuclear mass



Dobaczewski et al., 2004

Missing correlations
for open-shell nuclei

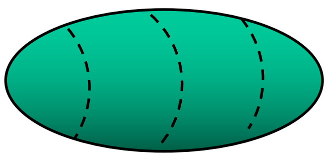
Nuclear deformation as symmetry breaking

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

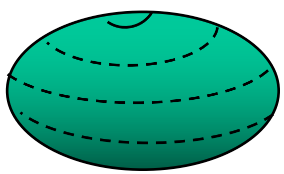
$$e^{i\phi N}|\Psi\rangle \neq |\Psi\rangle$$

Quadrupole deformation

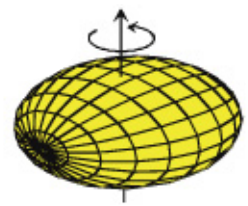
$$\beta_{2\mu} = \langle\Psi|r^2 Y_{2\mu}|\Psi\rangle$$



prolate



oblate

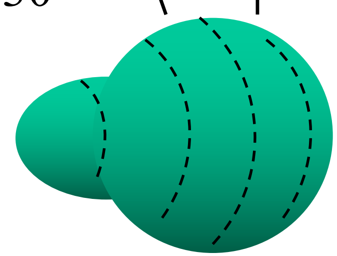


triaxial

Octupole deformation

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

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



Pear shape (μ=0)

Pairing deformation (superfluidity)

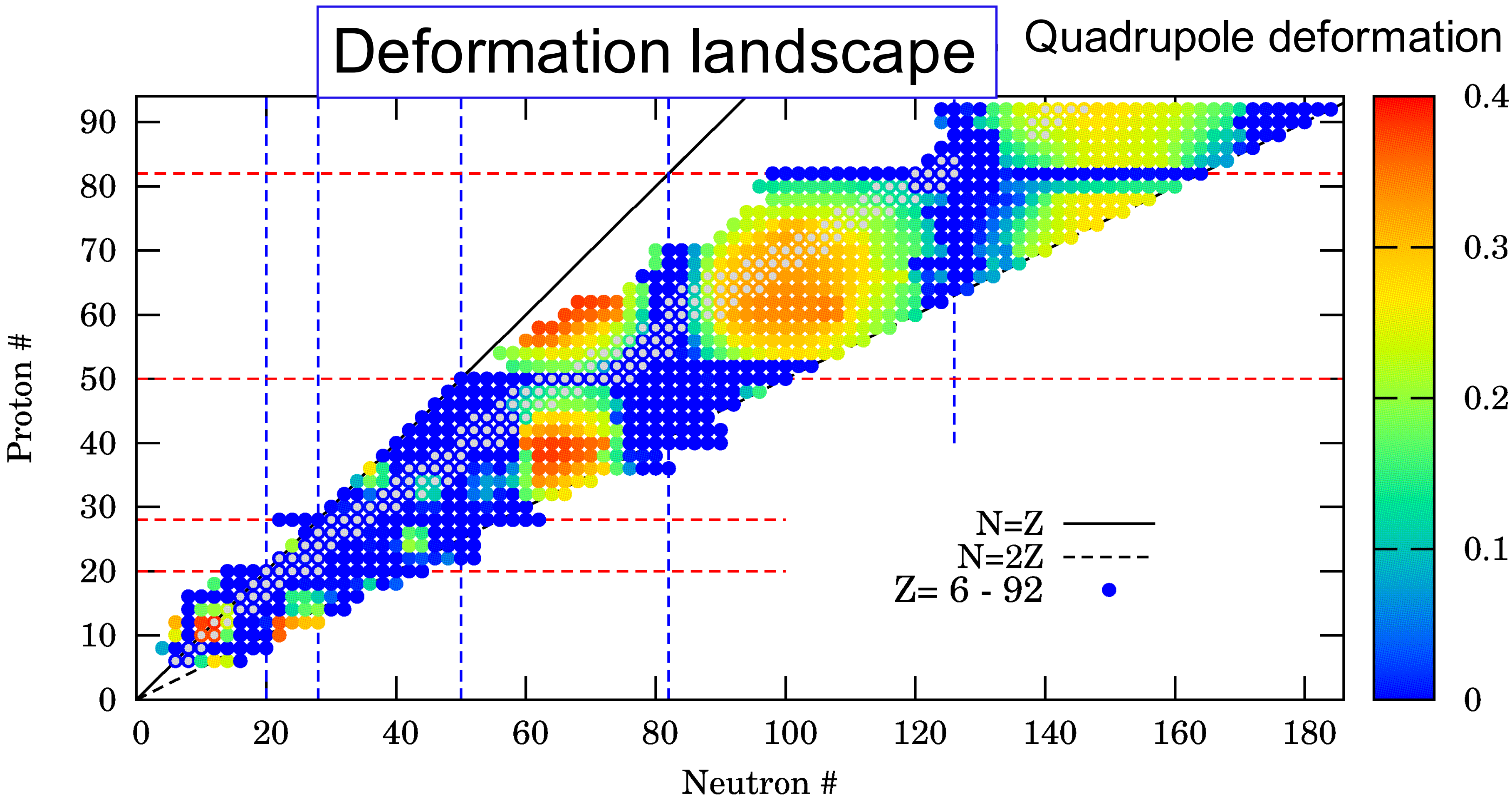
$$\Delta = \langle\Psi|\hat{\psi}\hat{\psi}|\Psi\rangle$$

Deformation in the gauge space

Nuclear Superconductivity
Nuclear Superfluidity

Nuclear deformation

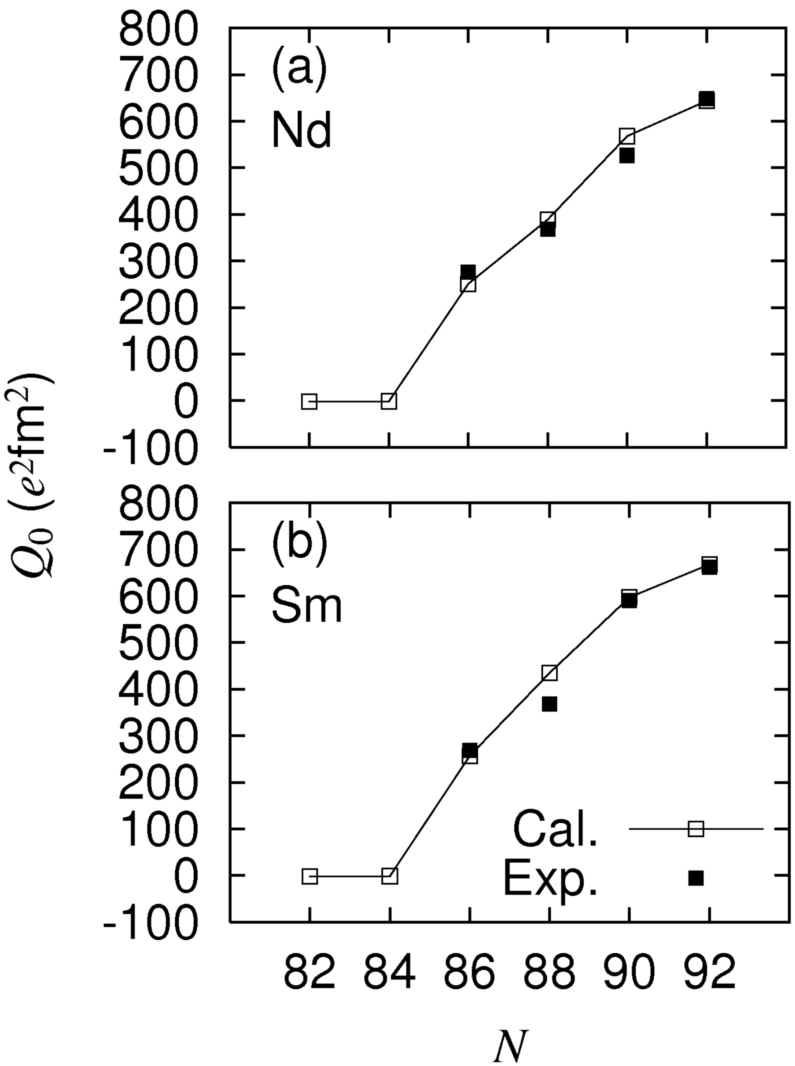
Ebata and T.N., Phys. Scr. 92 (2017) 064005



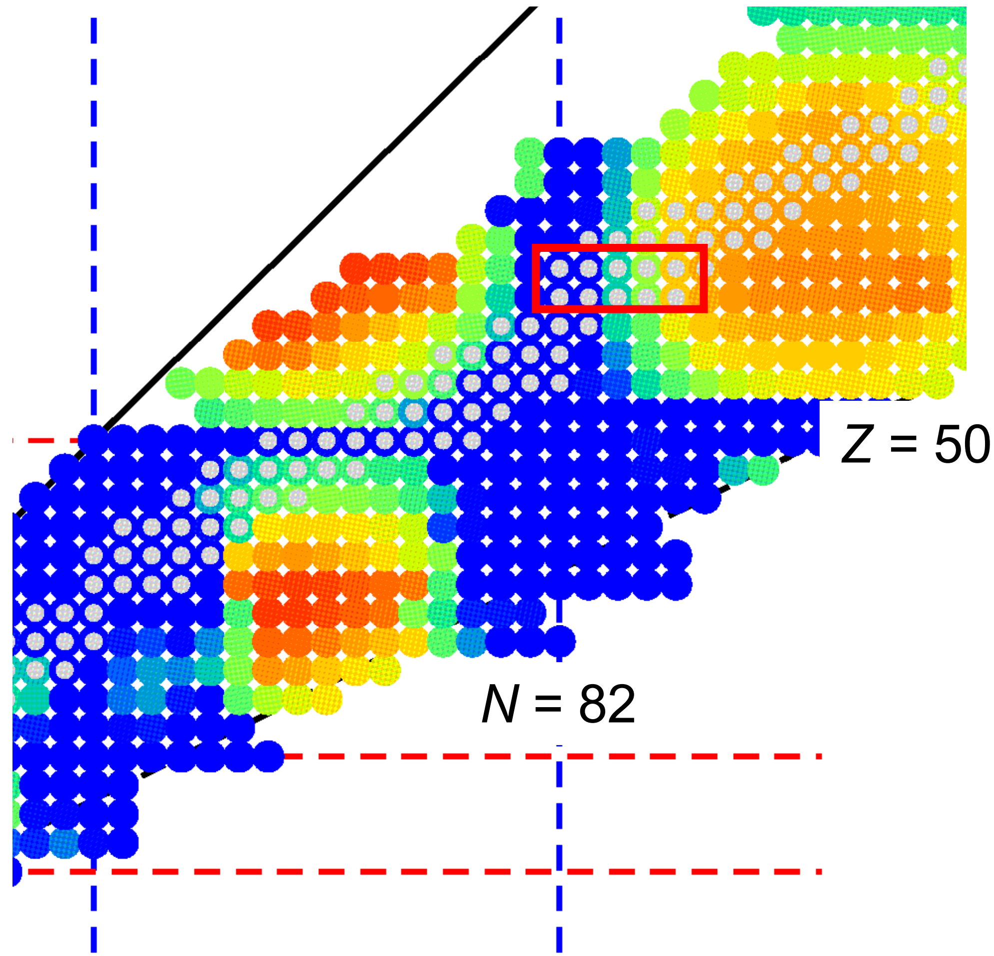
Nuclear deformation predicted by DFT

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

Linear response (RPA) equation

Assuming the external field with a fixed frequency and expanding $\delta\phi_i$ in terms of particle (unoccupied) orbitals,

$$\delta\phi_i(t) = \sum_{m>A} \phi_m^0 \left\{ X_{mi} \exp(-i\omega t) + Y_{mi}^* \exp(i\omega t) \right\}$$

$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = -\begin{pmatrix} (V_{\mathrm{ext}})_{mi} \\ (V_{\mathrm{ext}})_{im} \end{pmatrix}$$

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \left\langle \phi_m \left| \frac{\partial V}{\partial \rho_{nj}} \right|_{\rho_0} \middle| \phi_i \right\rangle$$

$$B_{mi,nj} = \left\langle \phi_m \left| \frac{\partial V}{\partial \rho_{jn}} \right|_{\rho_0} \middle| \phi_i \right\rangle$$

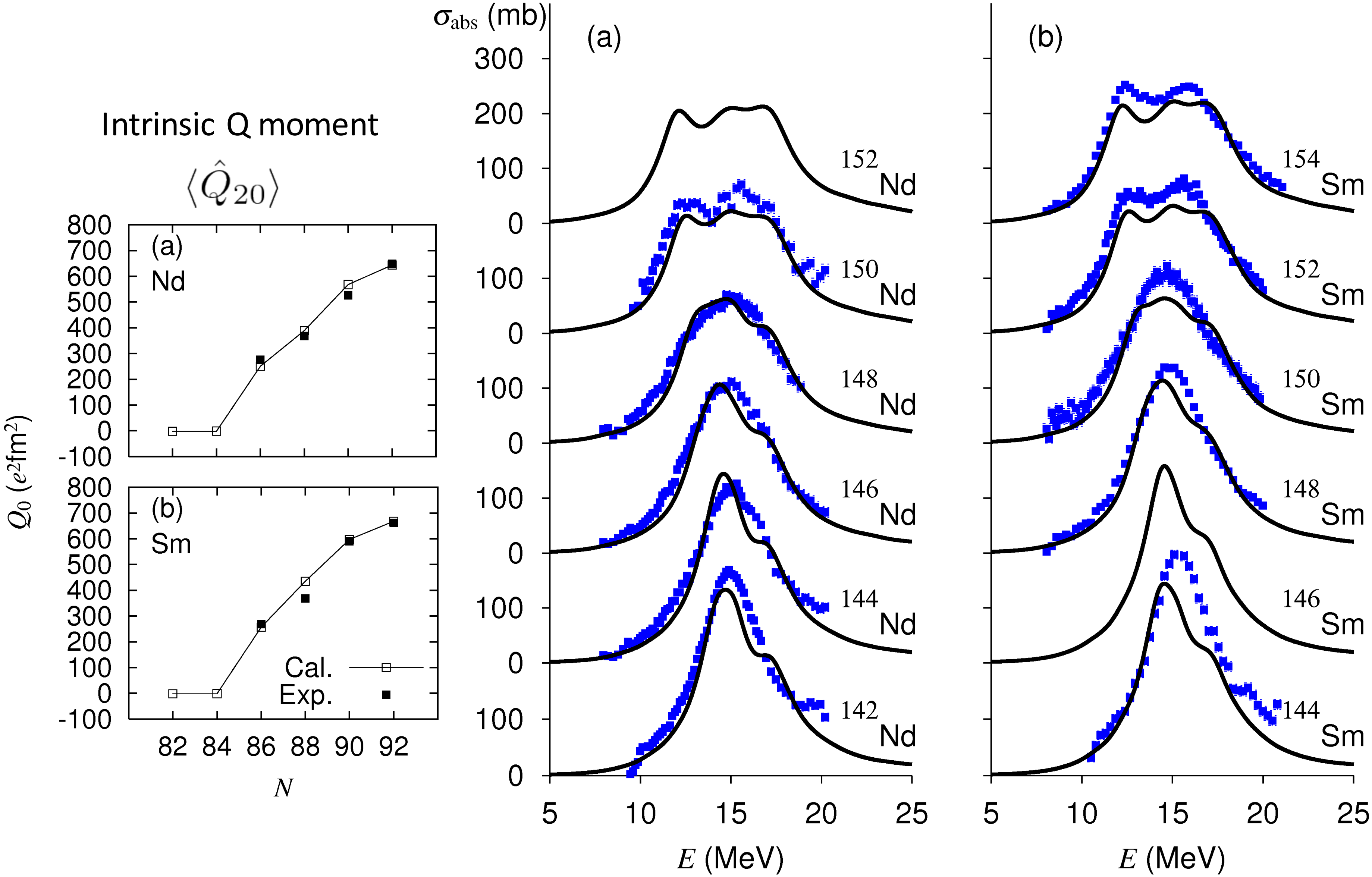
Deformation effects for photoabsorption cross section

SkM* functional

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

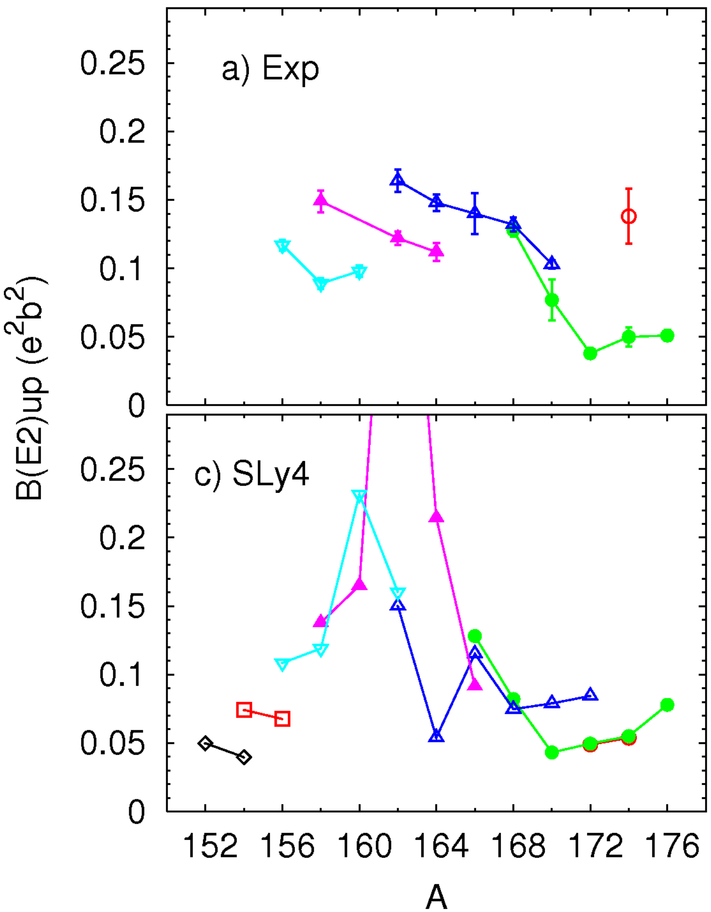
Intrinsic Q moment

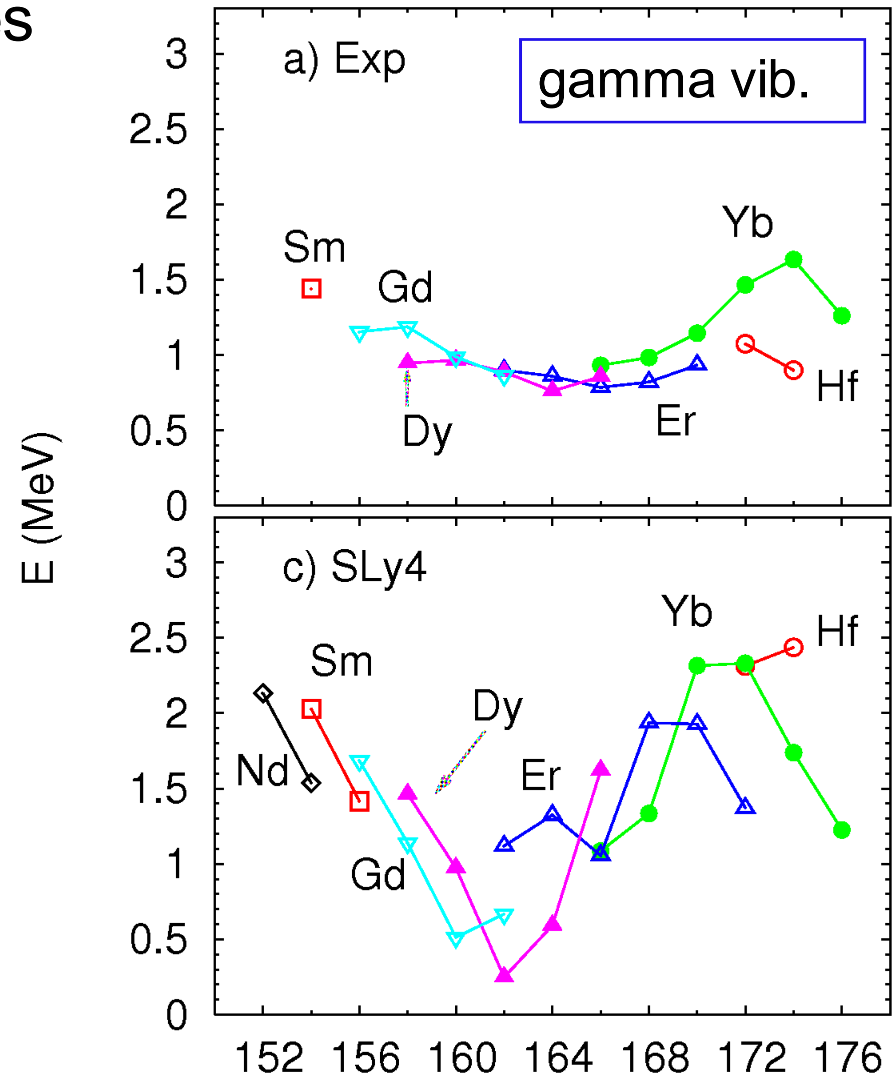
$\langle \hat{Q}_{20} \rangle$



Low-energy states

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

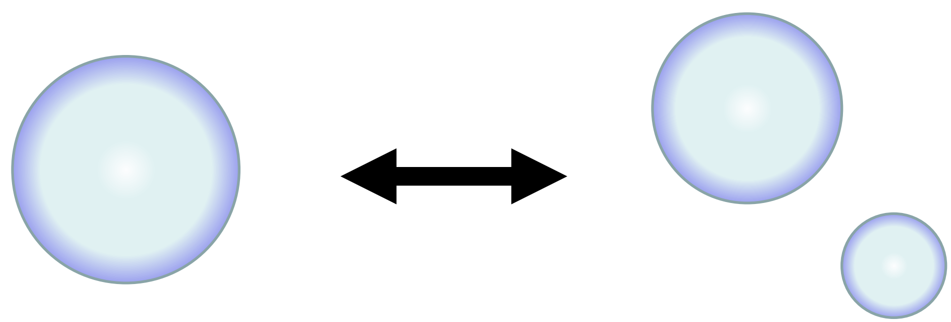




Terasaki, Engel, Phys. Rev. C 84, 014332 (2011)

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)



Summary (part 1)

- 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

Quantized TDDFT dynamics
--- Part 2: Missing correlations and quantization ---

Takashi Nakatsukasa (University of Tsukuba)

- Main origin of missing correlations
  - Quantum fluctuation associated with "slow" collective motion
  - Improving the density functional seems to be difficult
- Re-quantization of "slow" collective motion
  - Deriving a collective subspace
  - Quantization on the subspace

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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})

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

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

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

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 $[q, p] = i\hbar$

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 $[\alpha, \beta = (ph)]$

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

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

- Hamiltonian

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

Decoupled submanifold

- 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.

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

$\Gamma^\beta_{\alpha\gamma}$: Affine connection with metric $g_{\alpha\beta} \equiv \sum_\mu \frac{\partial q^\mu}{\partial \xi^\alpha}\frac{\partial q^\mu}{\partial \xi^\beta}$

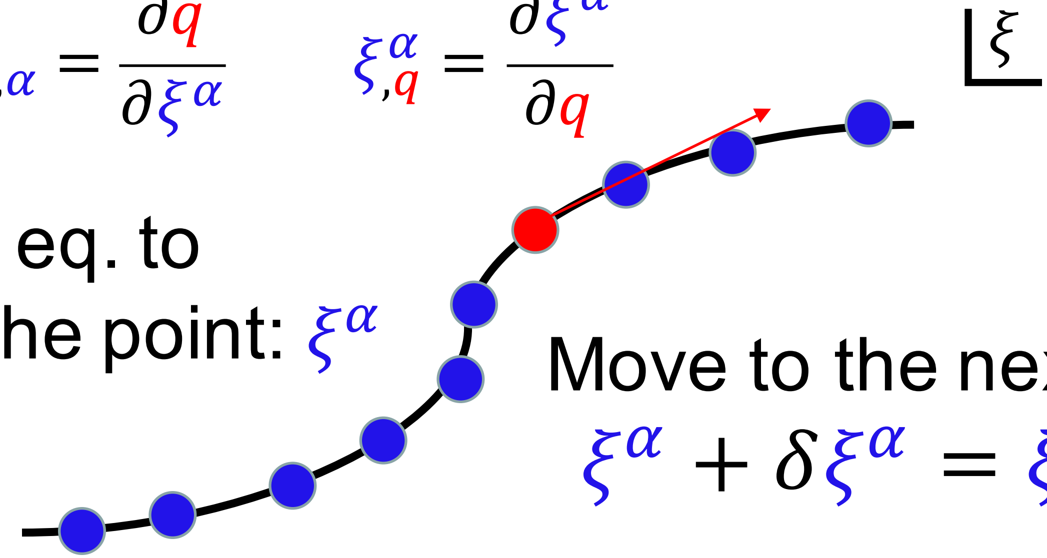
Numerical procedure

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

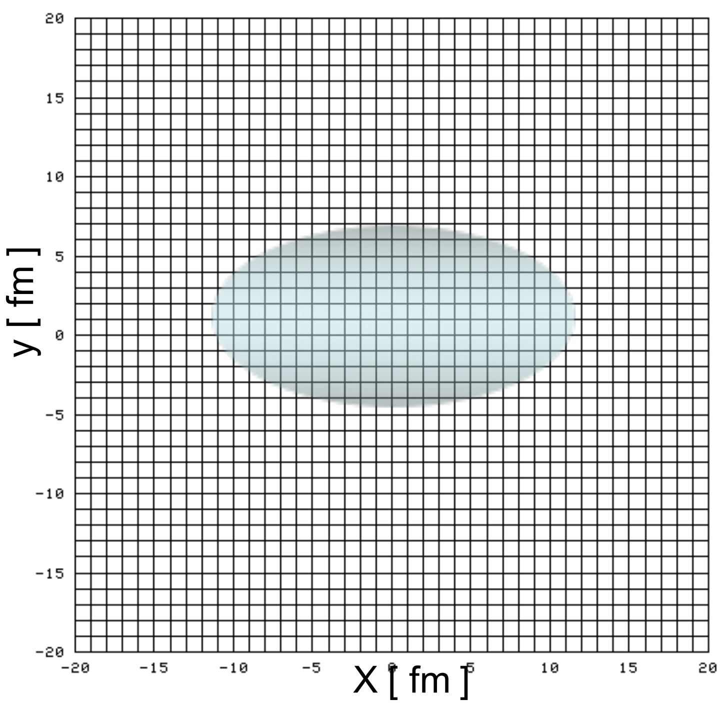
$$\xi^{\alpha} + \delta\xi^{\alpha} = \xi^{\alpha} + \varepsilon\xi^{\alpha}_{,q}$$

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
  - $\bar{H}_{\mathrm{coll}}(q,p) = \frac{1}{2}p^2 + \bar{V}(q)$, $\quad \bar{V}(q) = V(\xi(q))$
  - 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., arXiv: 1703.04319
Wen, T.N., PRC 94, 054618 (2016).
Wen, Washiyama, Ni, T.N., Acta Phys. Pol. B Proc. Suppl. 8, 637 (2015)

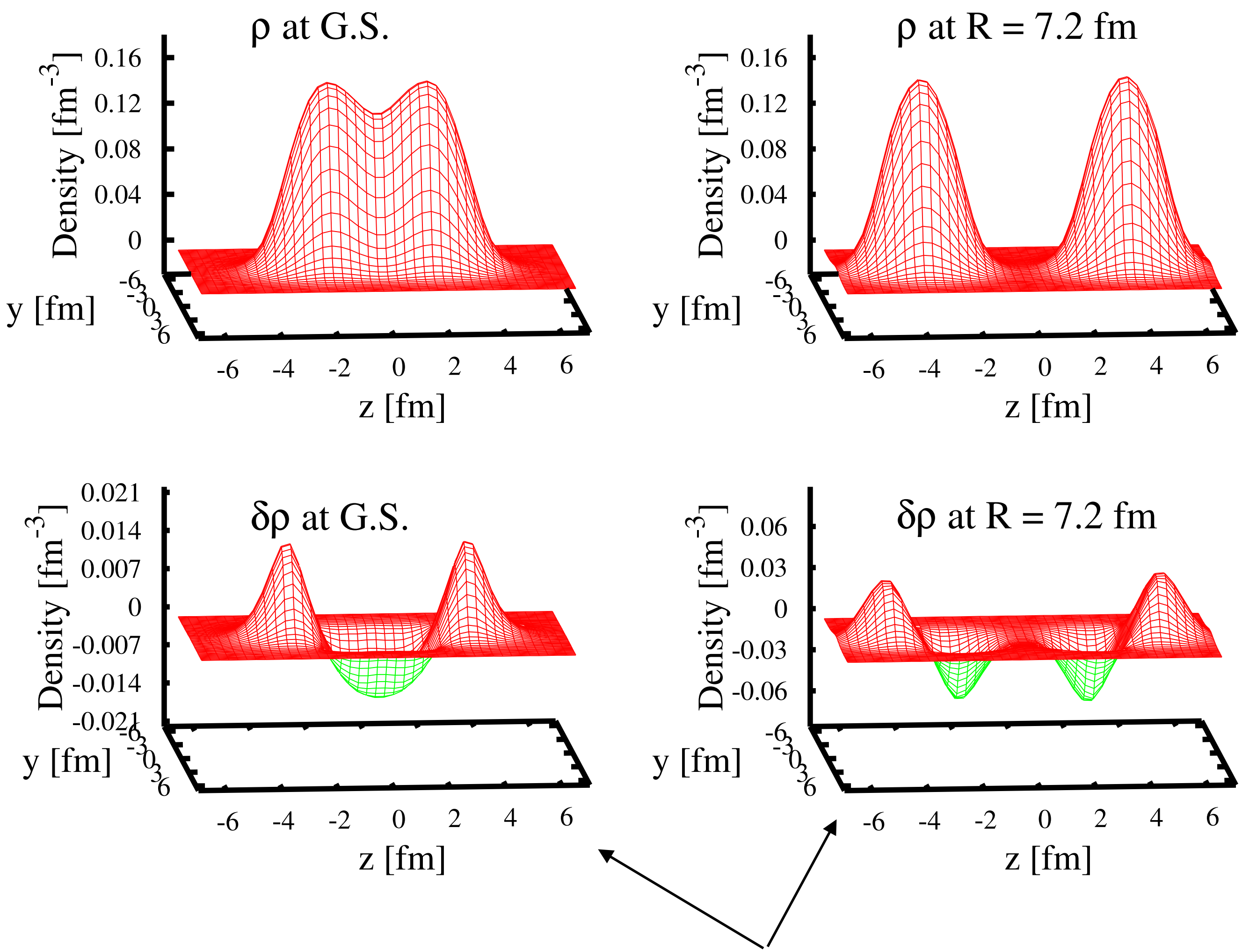
At a moment, no pairing

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)



$\rho(\vec{r})$

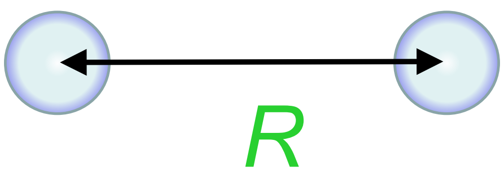
$\delta\rho(\vec{r})$

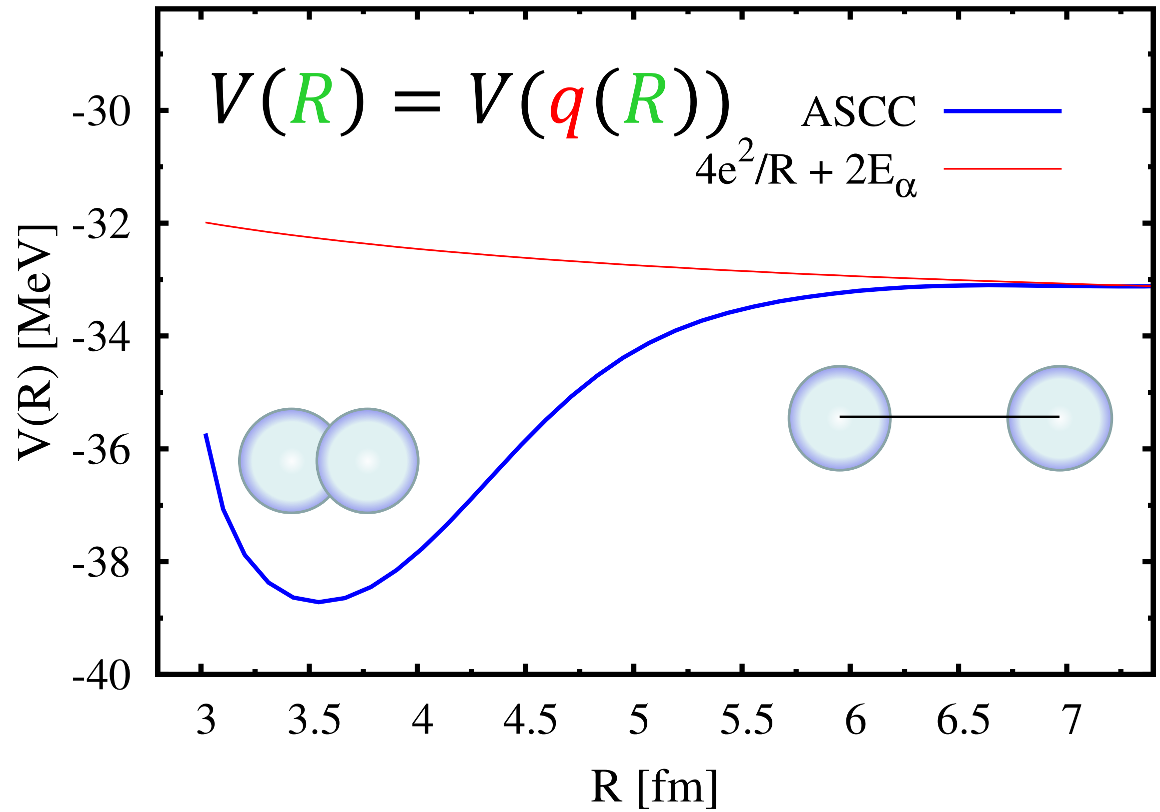
Tangent vectors (Generators)

^{8}Be: Collective potential

Represented by the relative distance R

Transformation: $q \rightarrow R$

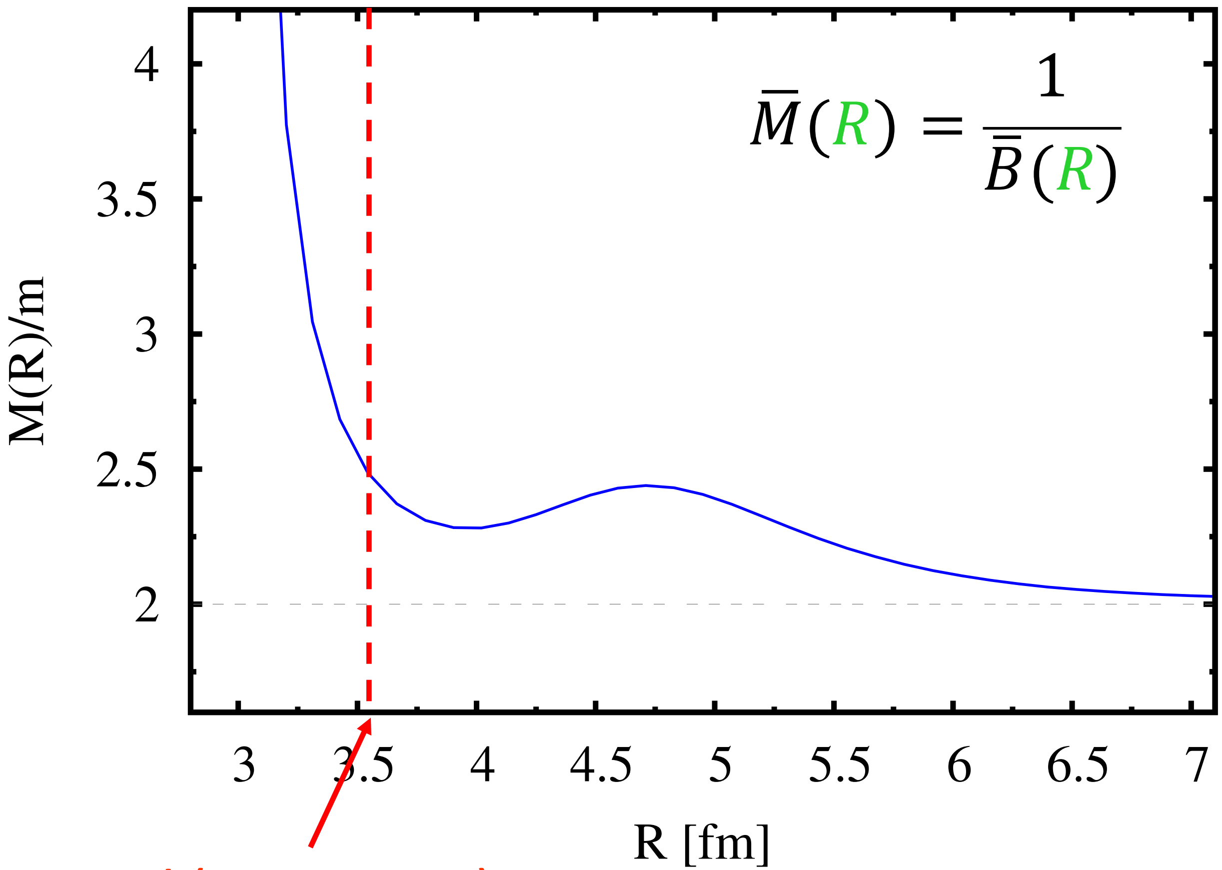




^{8}Be: Collective inertial mass

Transformation: $q \rightarrow R$

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



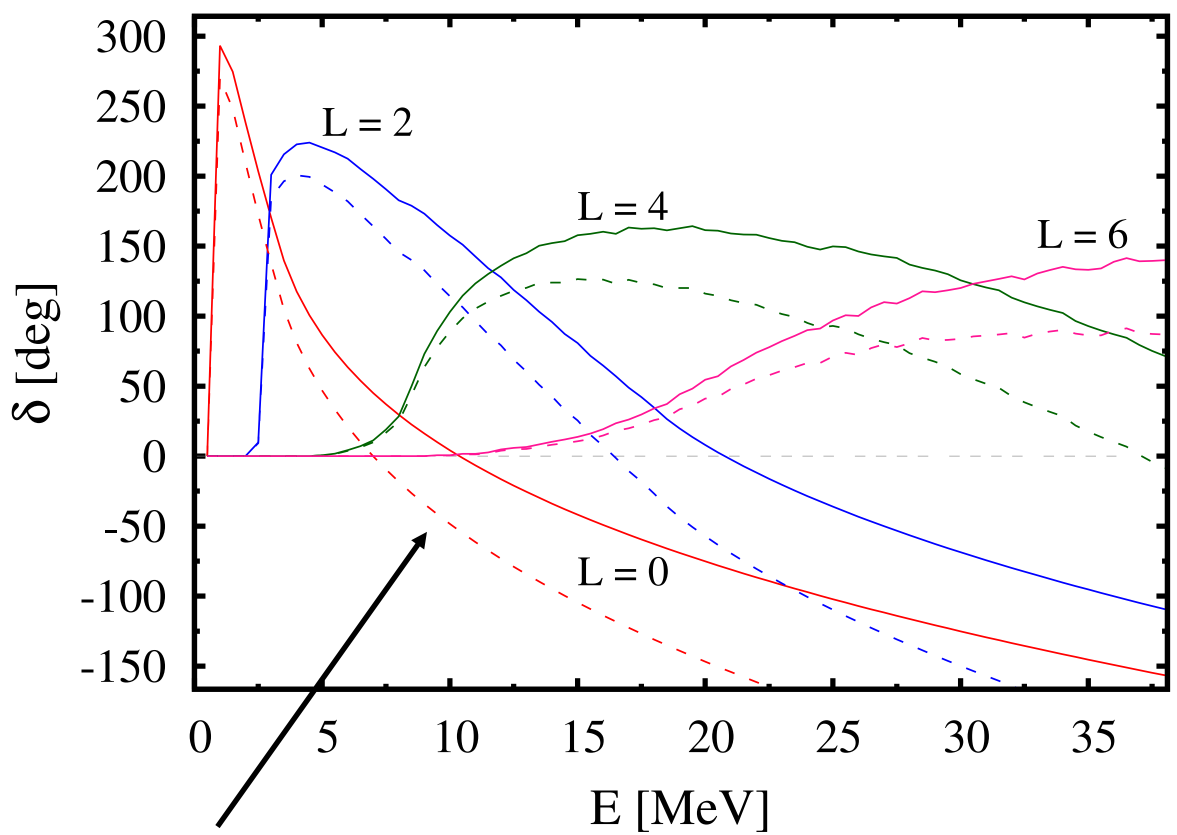
Reduced mass

$\bar{M}(R) \rightarrow 2m$

Ground (resonance) state

α + α scattering (phase shift)

Nuclear phase shift

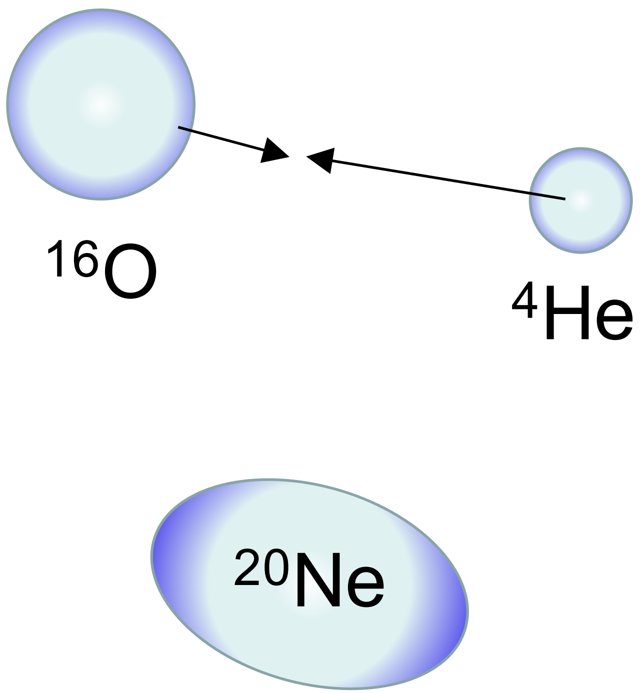


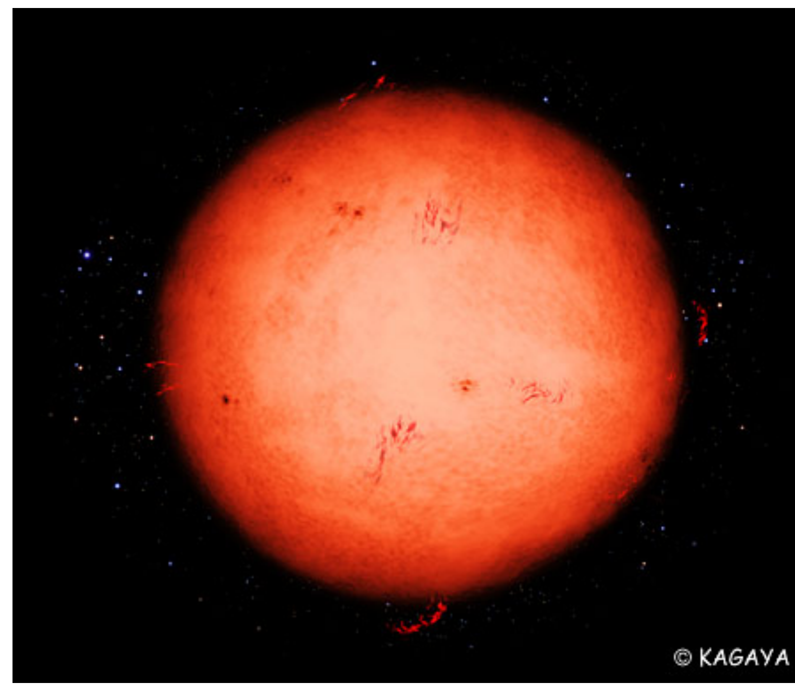
Effect of dynamical change of the inertial mass

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

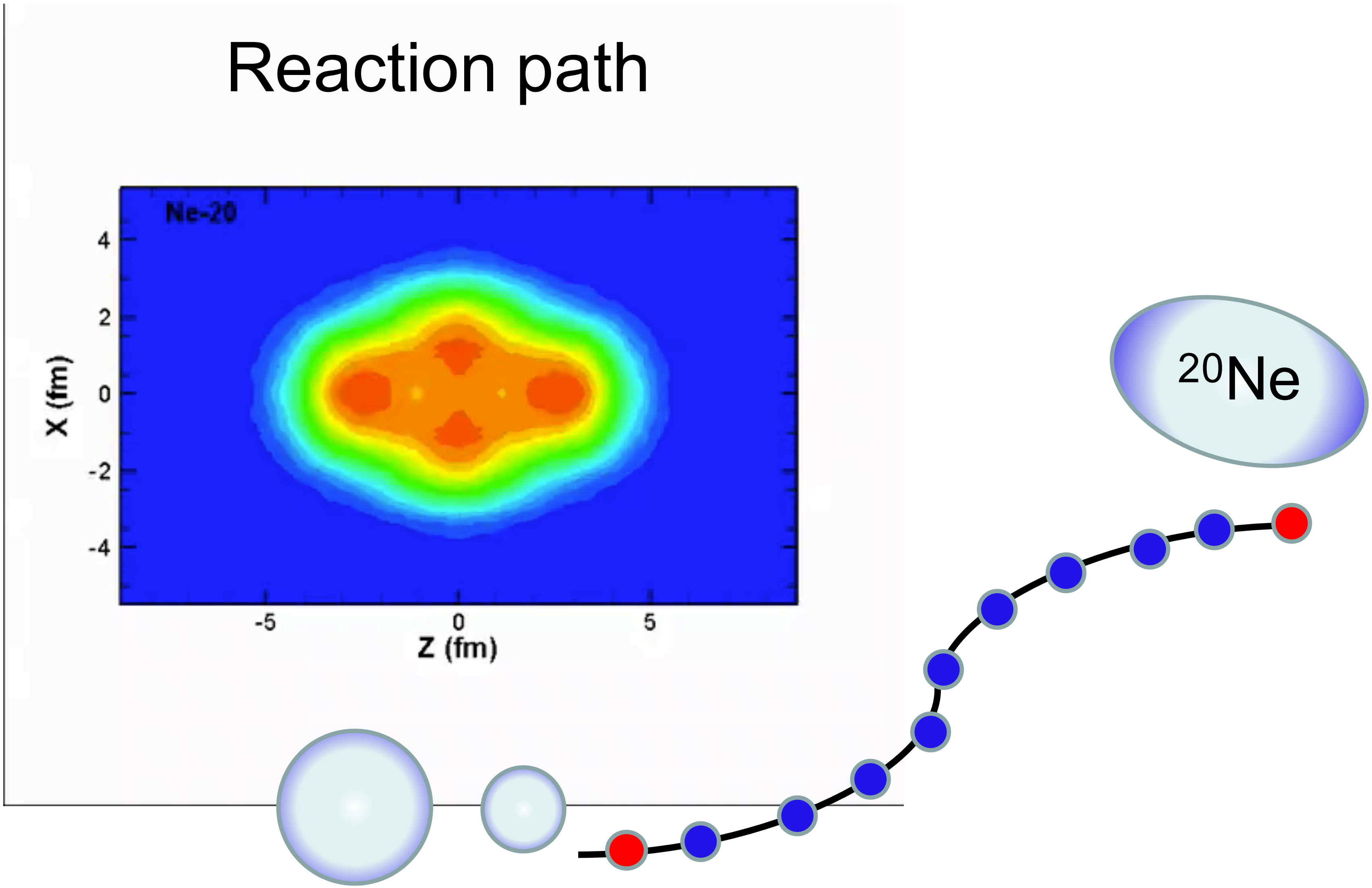
$^{16}O + \alpha$ scattering

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

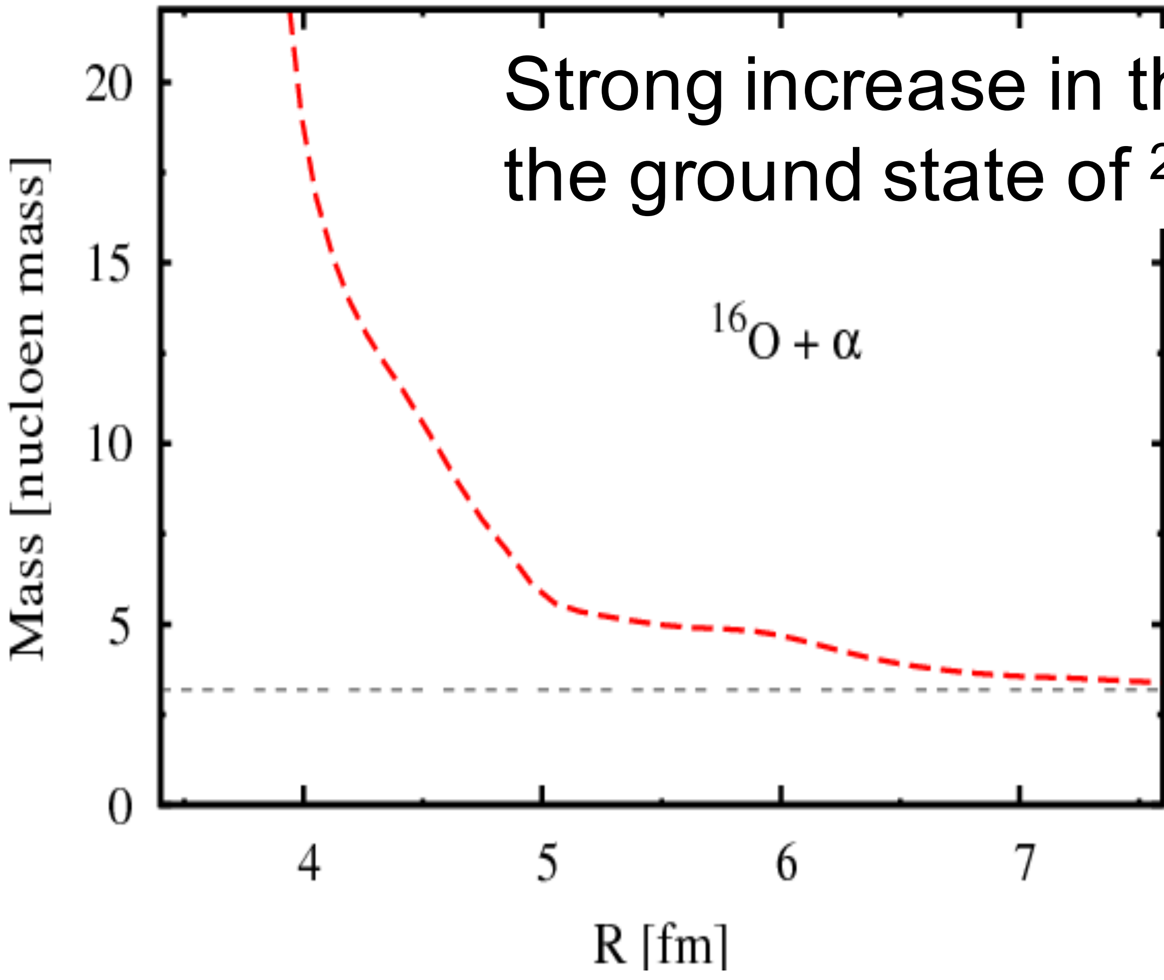




$^{16}O + \alpha$ to/from ^{20}Ne



^{20}Ne: Inertial mass

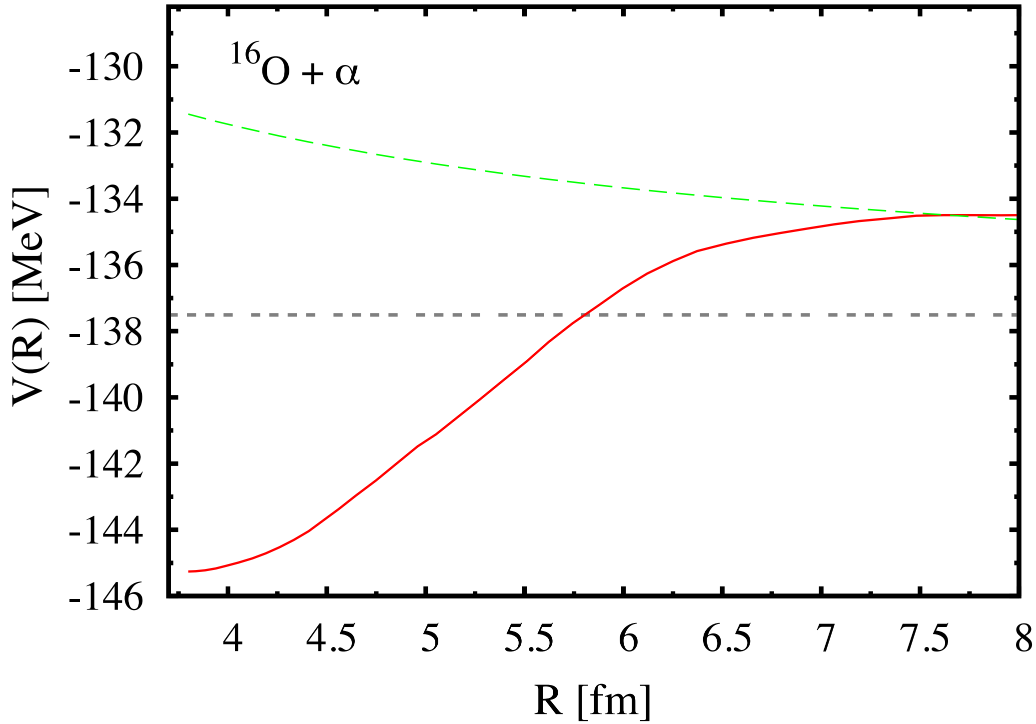


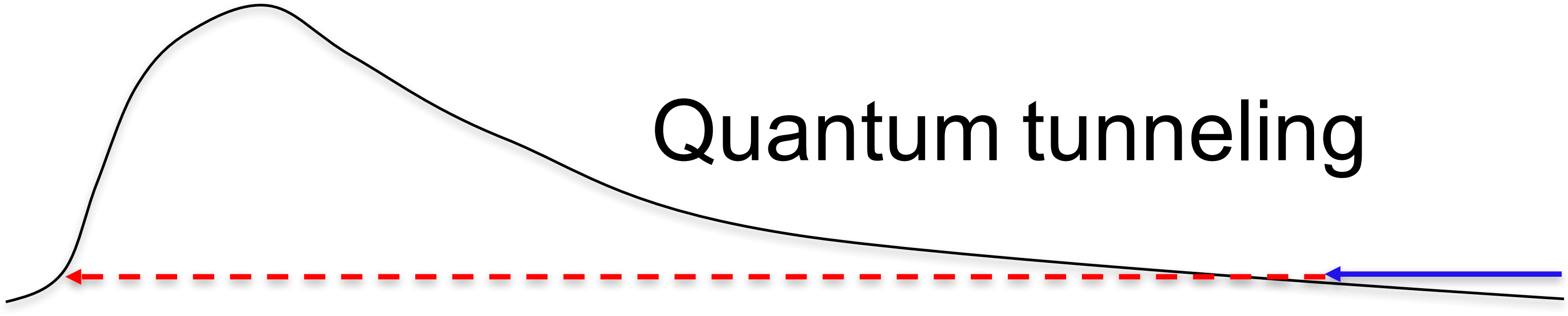
Strong increase in the mass near the ground state of ^{20}Ne

Reduced mass

$M(R) \to 3.2m$

^{20}Ne: Collective potential

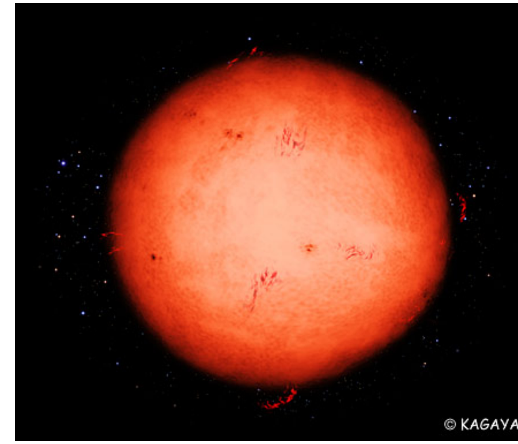




Quantum tunneling

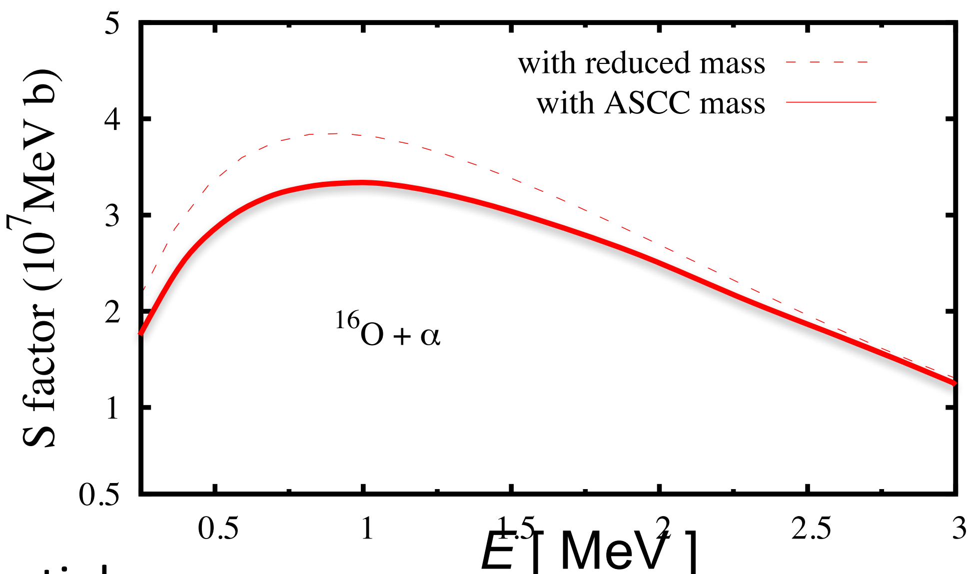
Alpha reaction：$^{16}O + \alpha$

Nuclear reaction to produce ^{20}Ne



Fusion reaction:
Astrophysical S-factor

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



Effect of dynamical change of the inertial mass

Dashed line: Constant reduced mass ($M(R) \to 3.2m$)

Summary (Part-2)

- 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

Summary (Part-2)

- Review articles
  - T.N., Prog. Theor. Exp. Phys. 2012, 01A207 (2012)
  - T.N. et al., Rev. Mod. Phys. 88, 045004 (2016)

- Collaborators
  - Shuichiro Ebata (Hokkaido Univ.)
  - Kai Wen (Univ. Surrey)
  - Kenichi Yoshida (Kyoto Univ.)