Theories of nuclear large amplitude collective motion

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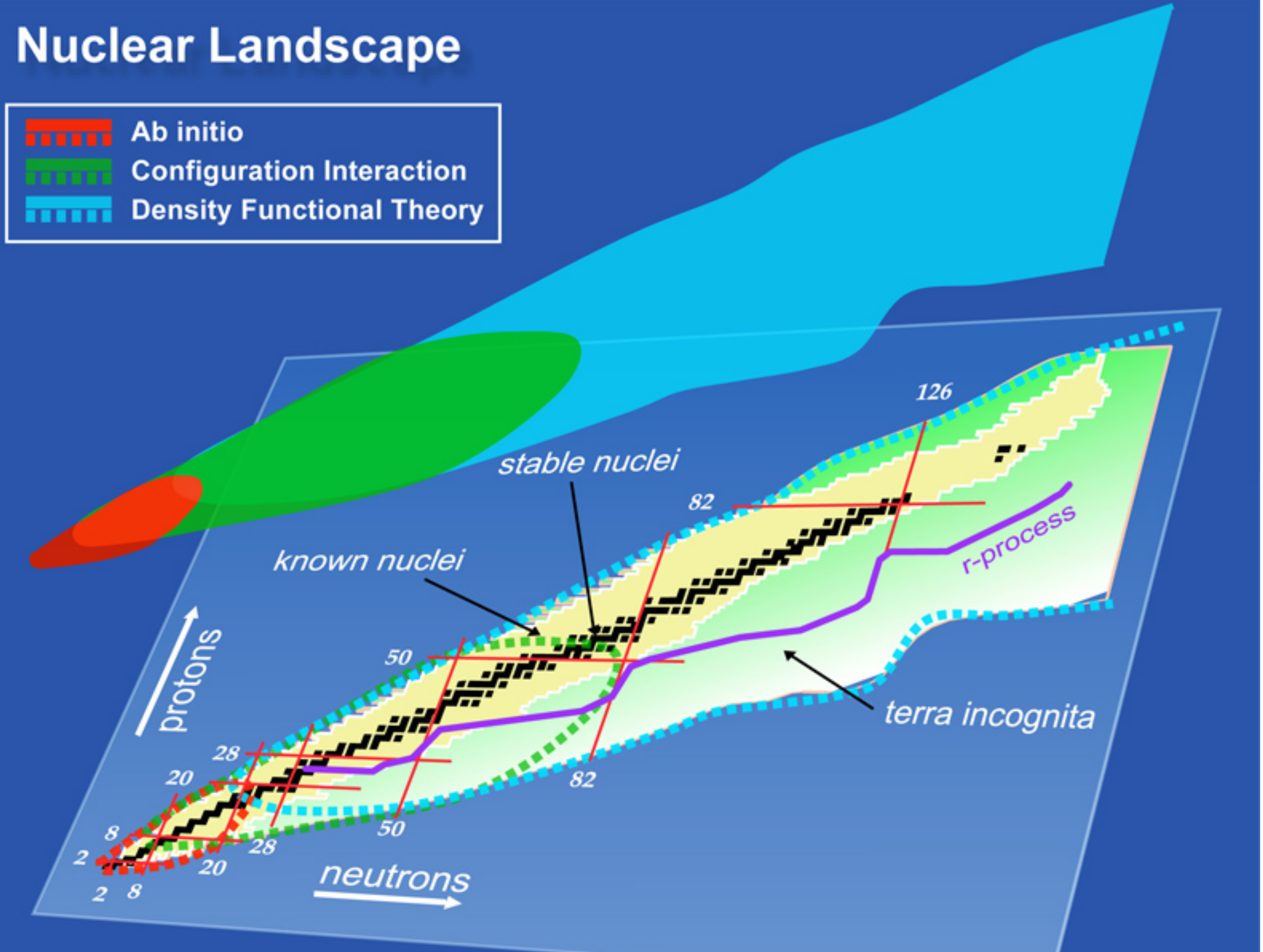
- Nuclear collective motion
  - Small amplitude & fast collective motion
    - TDDFT simulation and linear response calculation
  - Large amplitude "slow" collective motion
    - Problems in direct application of TDDFT
    - Re-quantization of collective subspace
    - Application to alpha reaction, subbarrier fusion

2018.9.14-19 1st APCTP-TRIUMF joint workshop on "Understanding Nuclei from Different Theoretical Approaches" @APCTP, Pohang, Korea

Nuclear Landscape



From SciDAC-UNEDF project

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

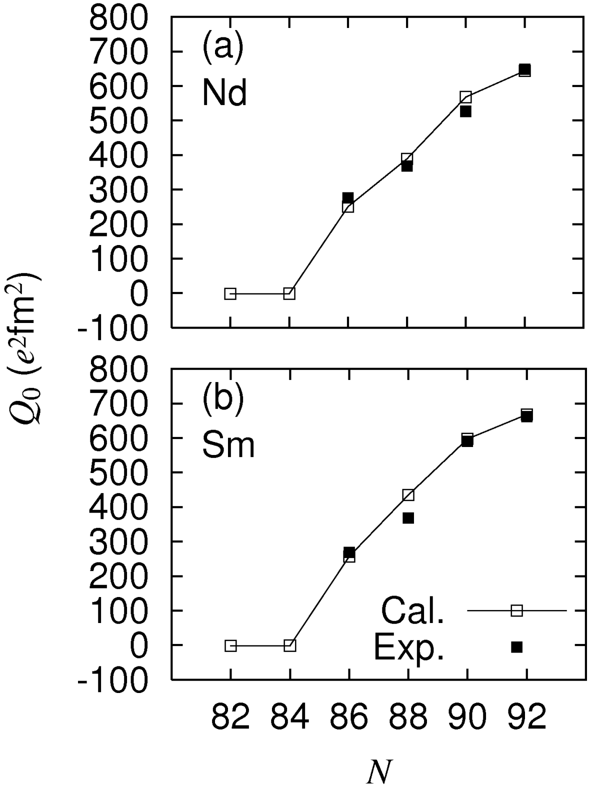
Success: Giant resonances

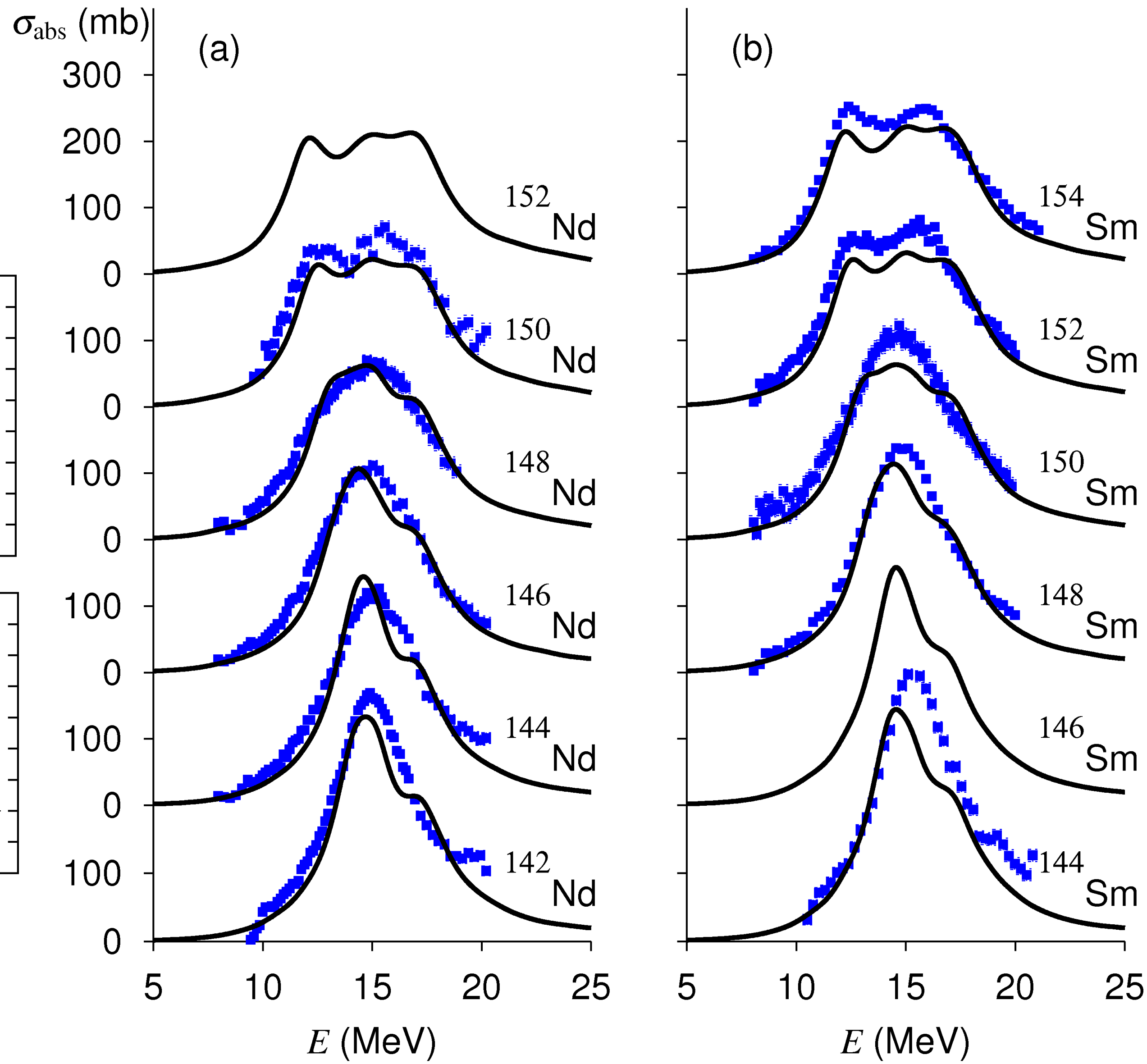
SkM* functional

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

Intrinsic Q moment

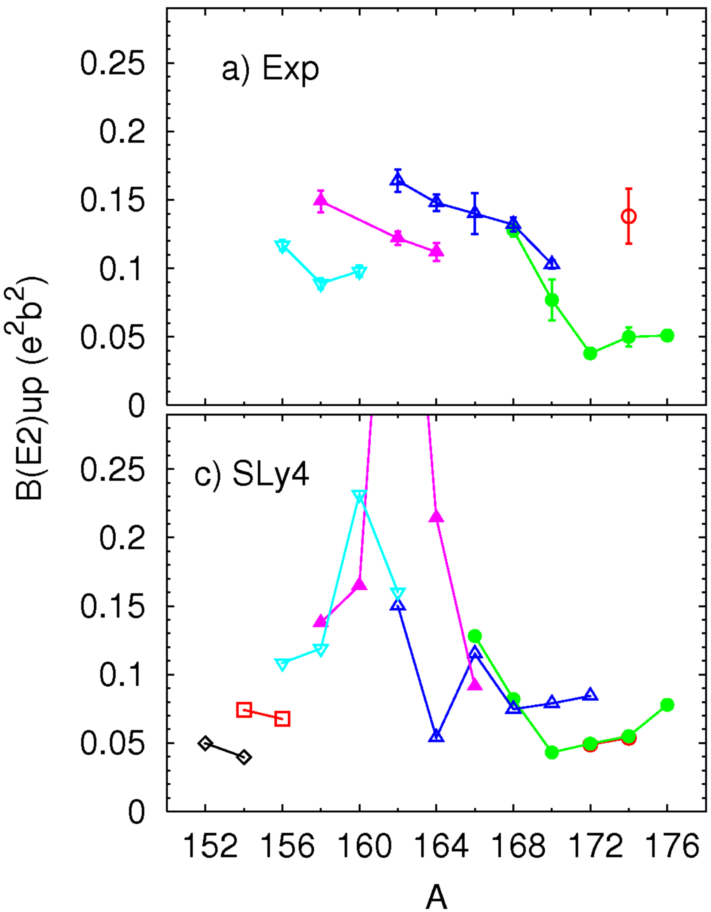
$\langle \hat{Q}_{20} \rangle$

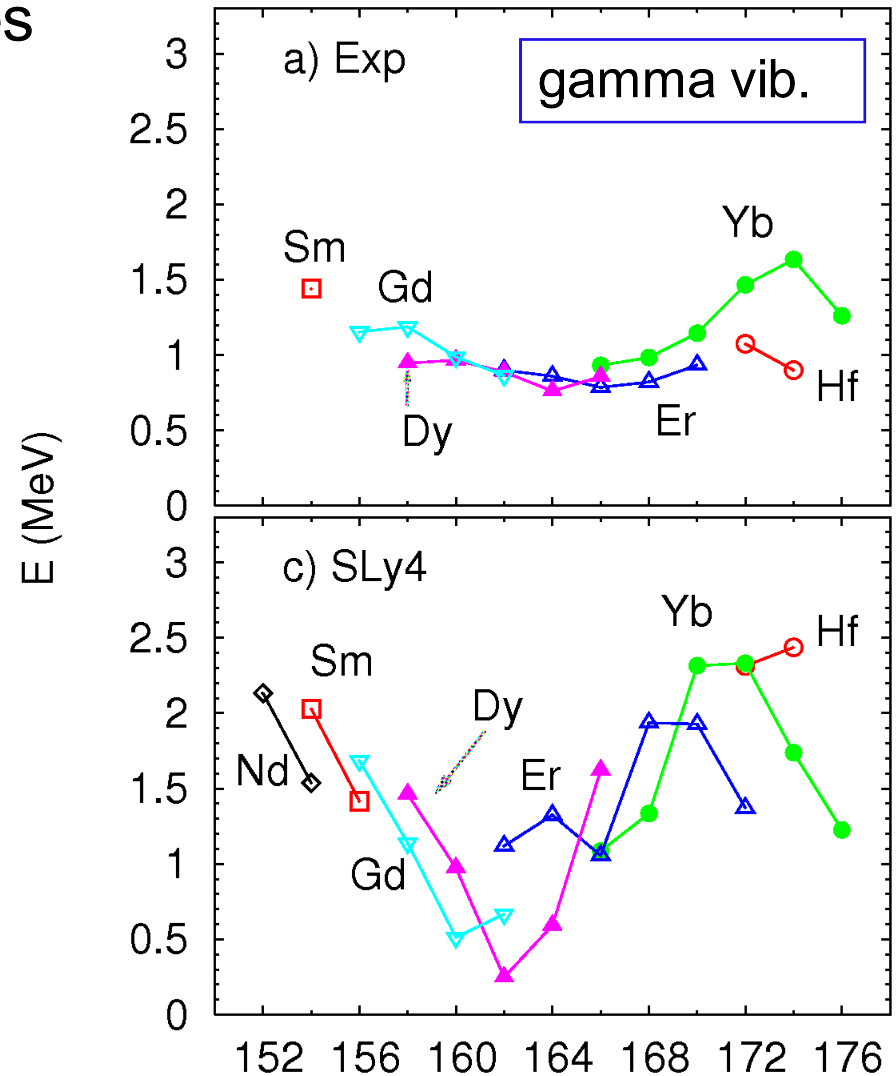




Problem: Low-energy states

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





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

Time-dependent density functional theory (TDDFT) without pairing

- 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

- Time-dependent Kohn-Sham equation

$$i \frac{\partial \psi_i(t)}{\partial t} = h[\rho(t)]\psi_i(t)$$

Heavy-ion collision simulation

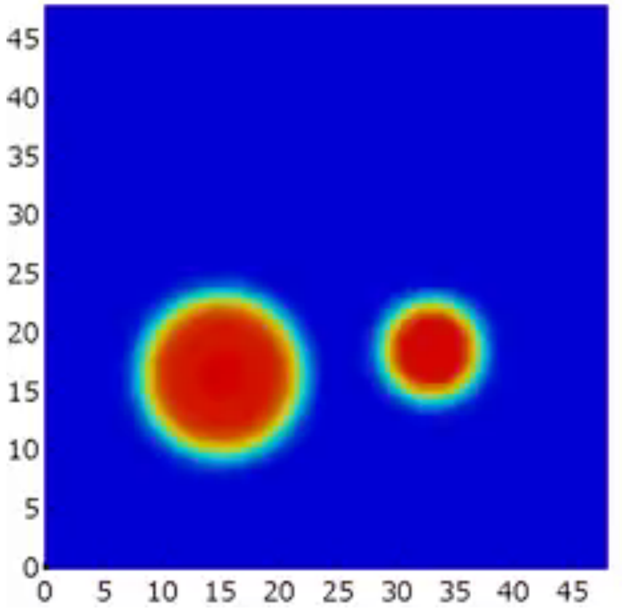
Success: Reaction above the Coulomb barrier

“Partial”-space particle-number projection

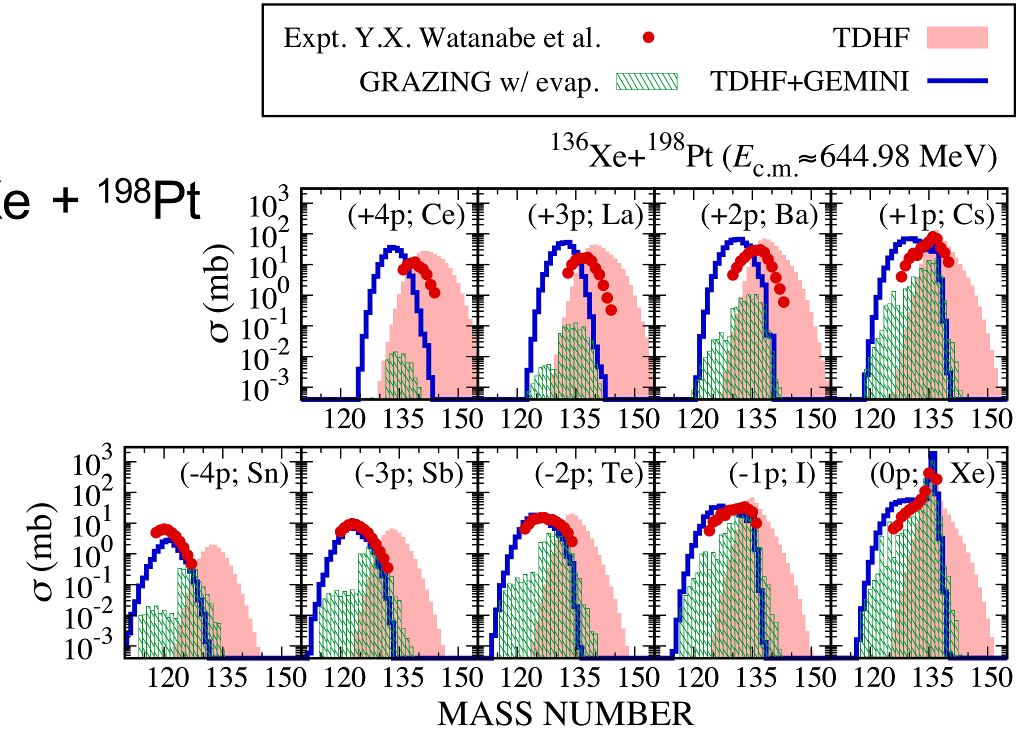
Simenel, C., 2010, Phys. Rev. Lett. 105, 192701.

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

Real-time simulation



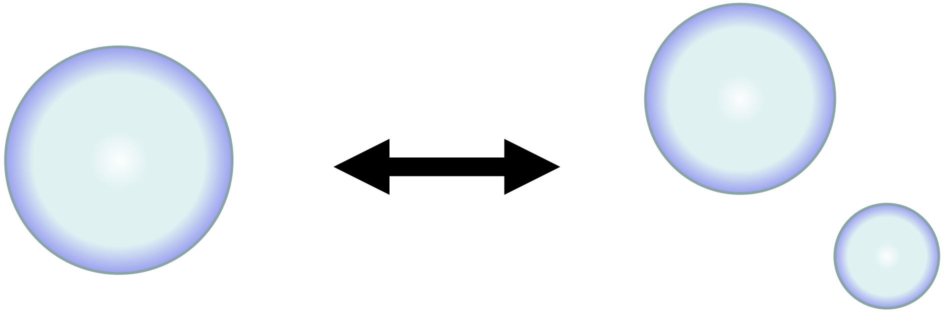
$^{136}Xe + ^{198}Pt$



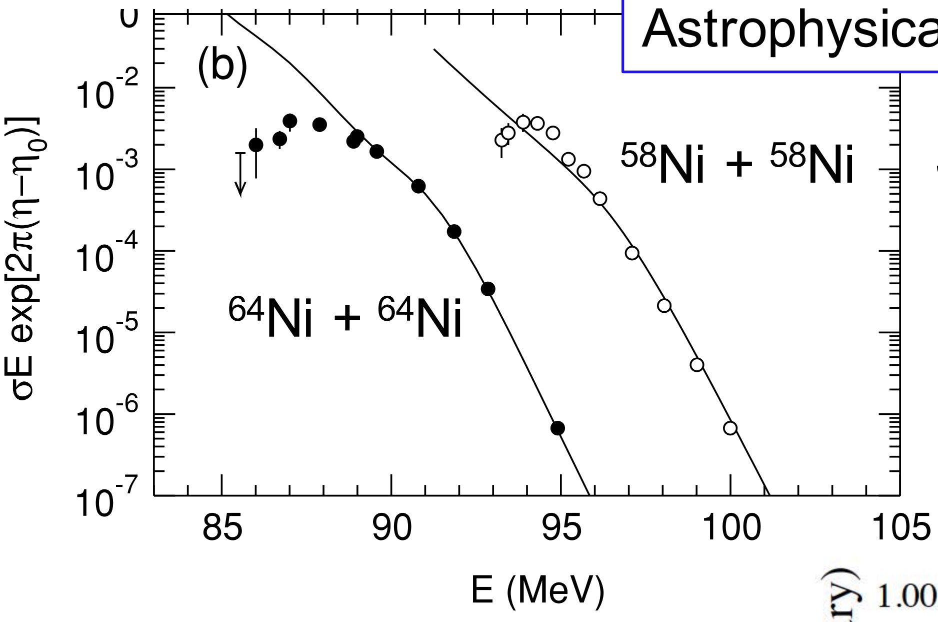
Sekizawa, Phys. Rev. C **96**, 014615 (2017)

Problem: Reaction below the Coulomb barrier

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

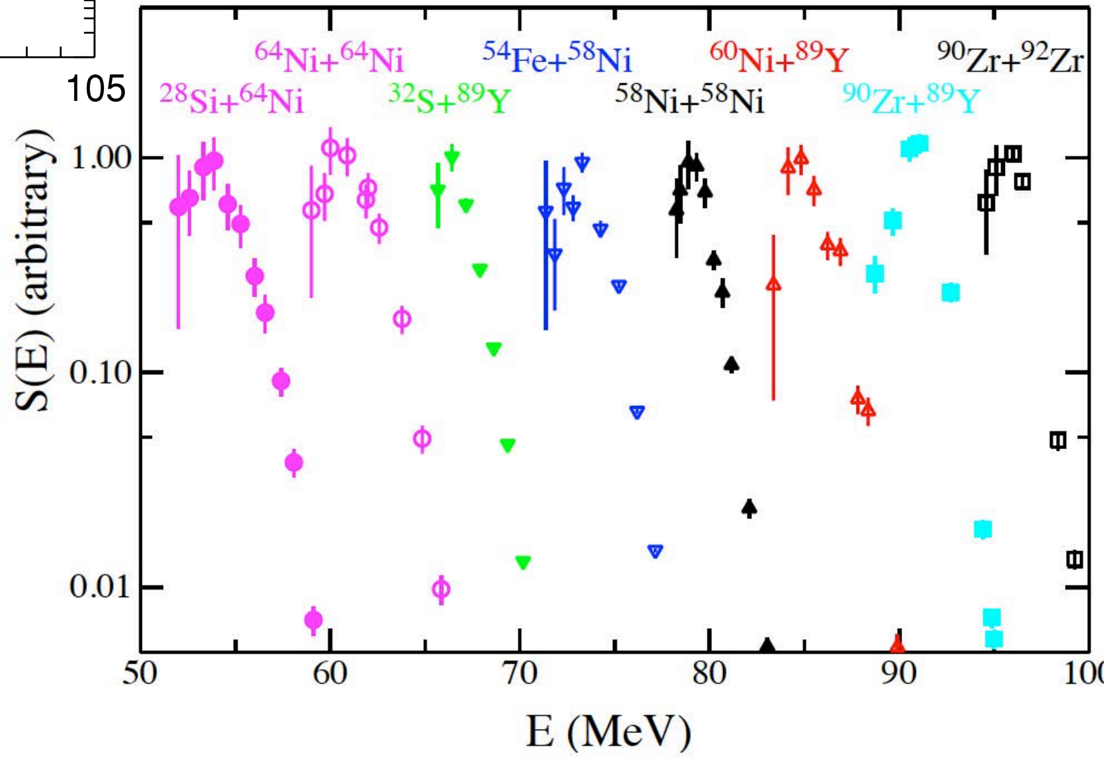


Deep-subbarrier fusion hindrance



Astrophysical S-factor

Jiang et al, PRC 73, 014613 (2006)



Systematic investigation for Fusion hindrance at extreme sub-barrier energies

(Jiang, private comm.)

Summary (Part-1)

- Success of nuclear TDDFT
  - Giant resonances (*linearized TDDFT*)
  - Heavy-ion reaction at above-barrier energy
- Problems
  - Low-energy collective motion
  - Many-body tunneling (spontaneous fission, sub-barrier fusion, astrophysical reaction)
- Possible solutions
  - Improving DF (ω-dep., beyond LDA, etc.)
  - Identification & re-quantization of collective subspace

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
  - Take into account “missing” quantum fluctuation 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 $[\alpha, \beta = (ph)]$

- Point 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)
  - $\{\xi^\alpha, \pi_\alpha\} \rightarrow \{q, p;\ q^a, p_a;\quad a = 2, \cdots, N_{ph}\}$
- 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 $g_{\alpha\beta} \equiv \sum_\mu \frac{\partial q^\mu}{\partial \xi^\alpha}\frac{\partial q^\mu}{\partial \xi^\beta}$

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

Numerical procedure

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

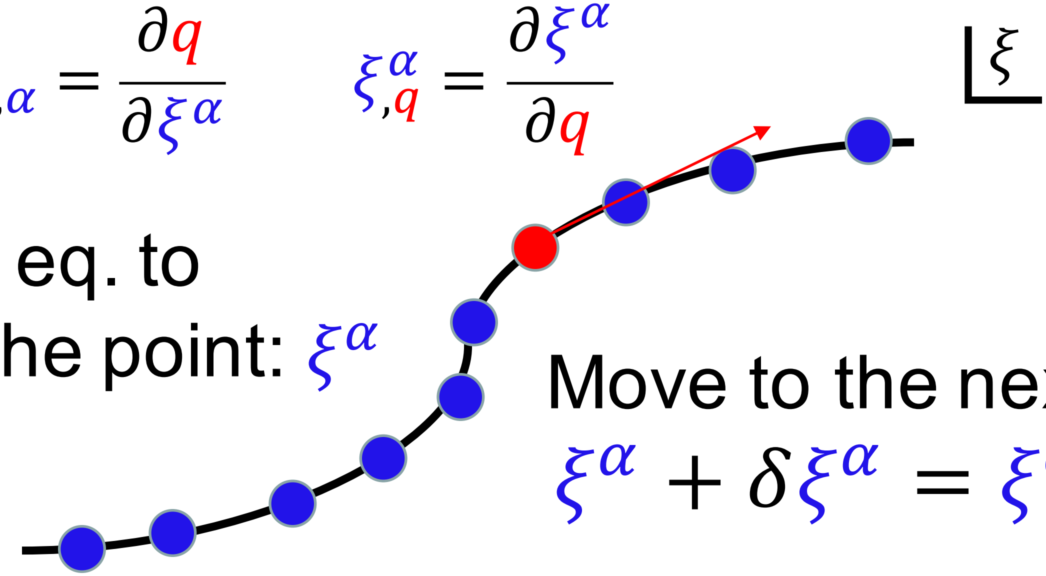
Moving mean-field eq.

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

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

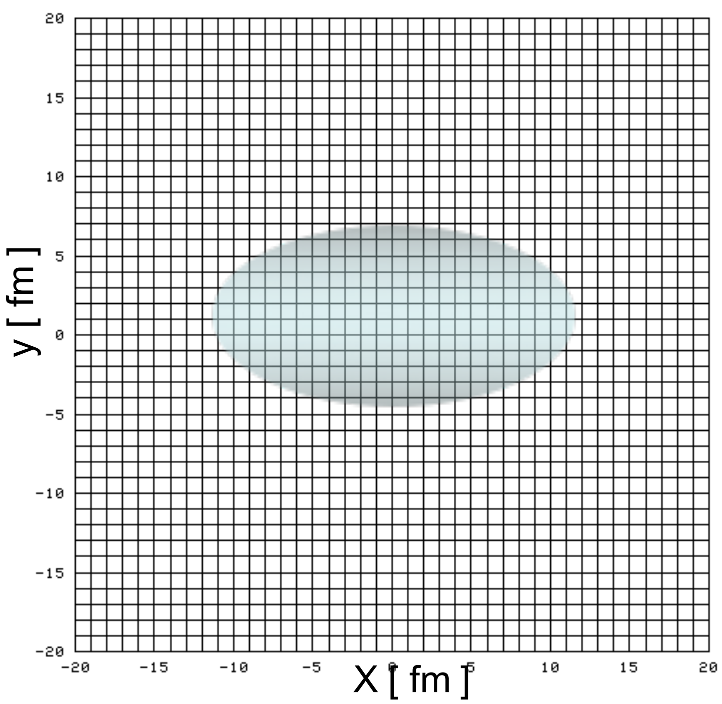
$$\xi^\alpha + \delta\xi^\alpha = \xi^\alpha + \delta q\, \xi^\alpha_{,q}$$

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
  - $\bar{H}_{\text{coll}}(q, p) = \frac{1}{2}p^2 + \bar{V}(q), \qquad \bar{V}(q) = V(\xi(q))$
  - 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))



At a moment, no pairing

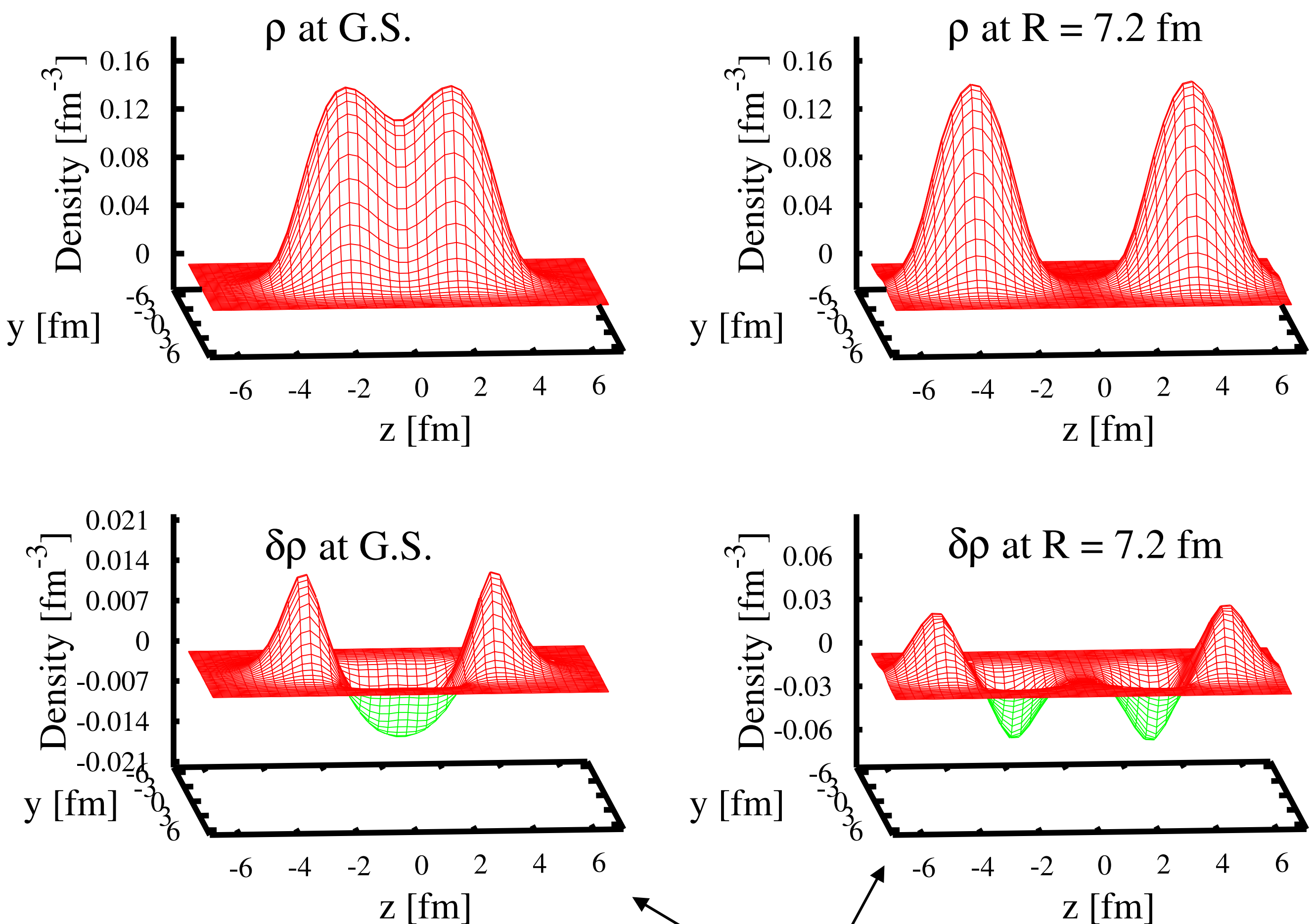
1-dimensional reaction path extracted from the Hilbert space of dimension of $10^4 \sim 10^5$.

Wen, T.N., PRC 94, 054618 (2016);
PRC 96, 014610 (2017)

Simple case: α + α scattering

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

^{8}Be: Tangent vectors (generators)



$\rho(\vec{r})$

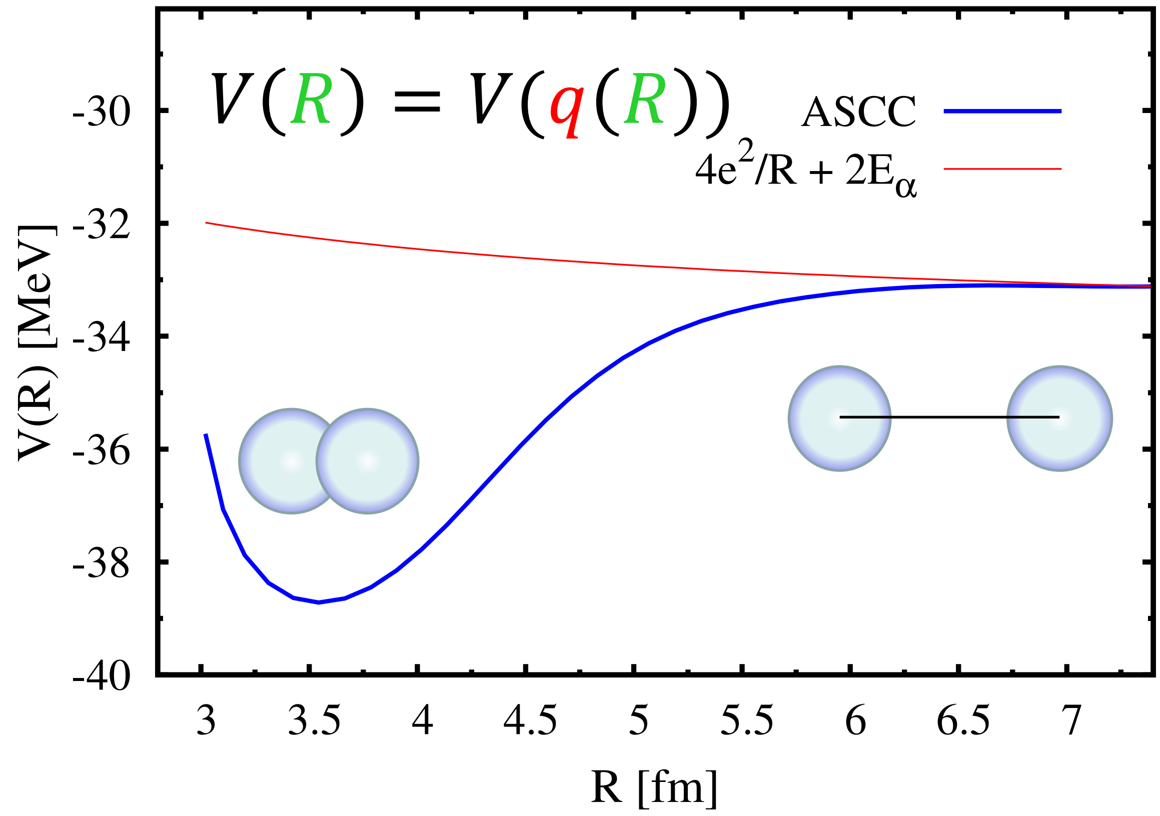
$\delta\rho(\vec{r})$

Tangent vectors (Generators)

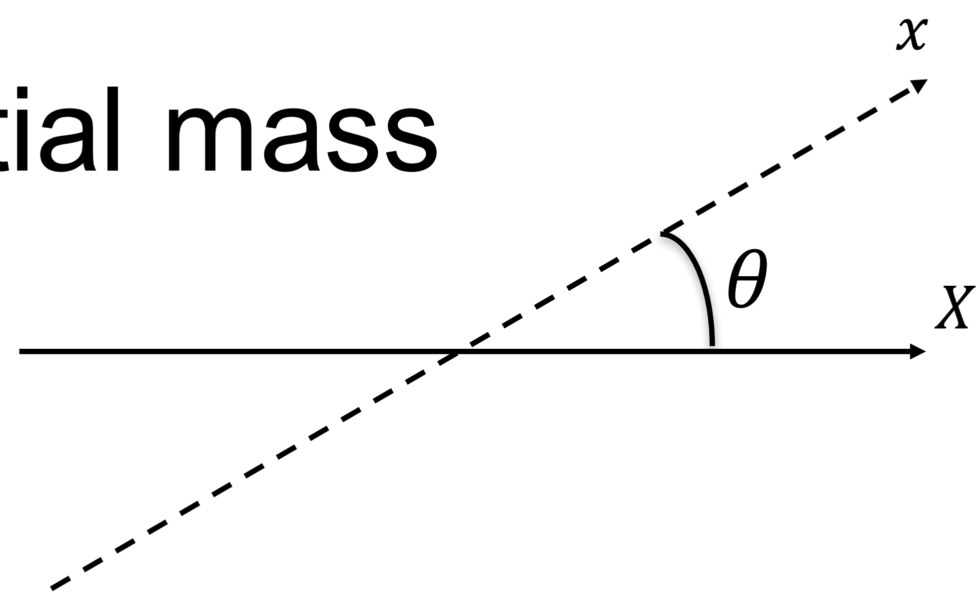
^{8}Be: Collective potential

Represented by the relative distance R

Transformation: $q \rightarrow R$



Inertial mass

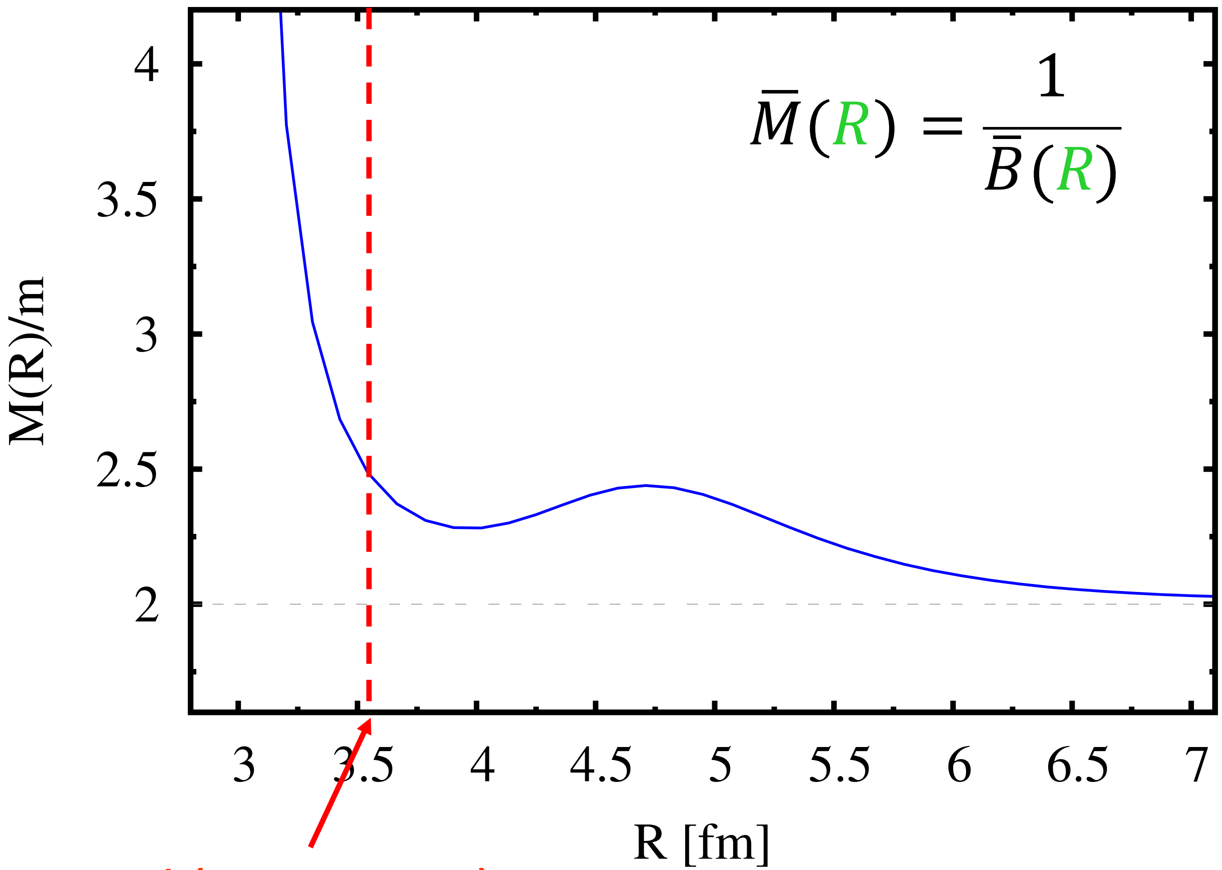


- A particle moving along the x axis
  - $H = \frac{1}{2} m \dot{x}^2$
- Assuming the motion along the X axis
  - $H = \frac{1}{2} m \dot{X}^2$ (Wrong dynamics)
- Representing in the X axis ($x = f(X)$)
  - $H = \frac{1}{2} m_{eff} \dot{X}^2$ (Correct dynamics)
  - $m_{eff} = \frac{m}{(\cos\theta)^2}$

^{8}Be: Collective inertial mass

Transformation: $q \rightarrow R$

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



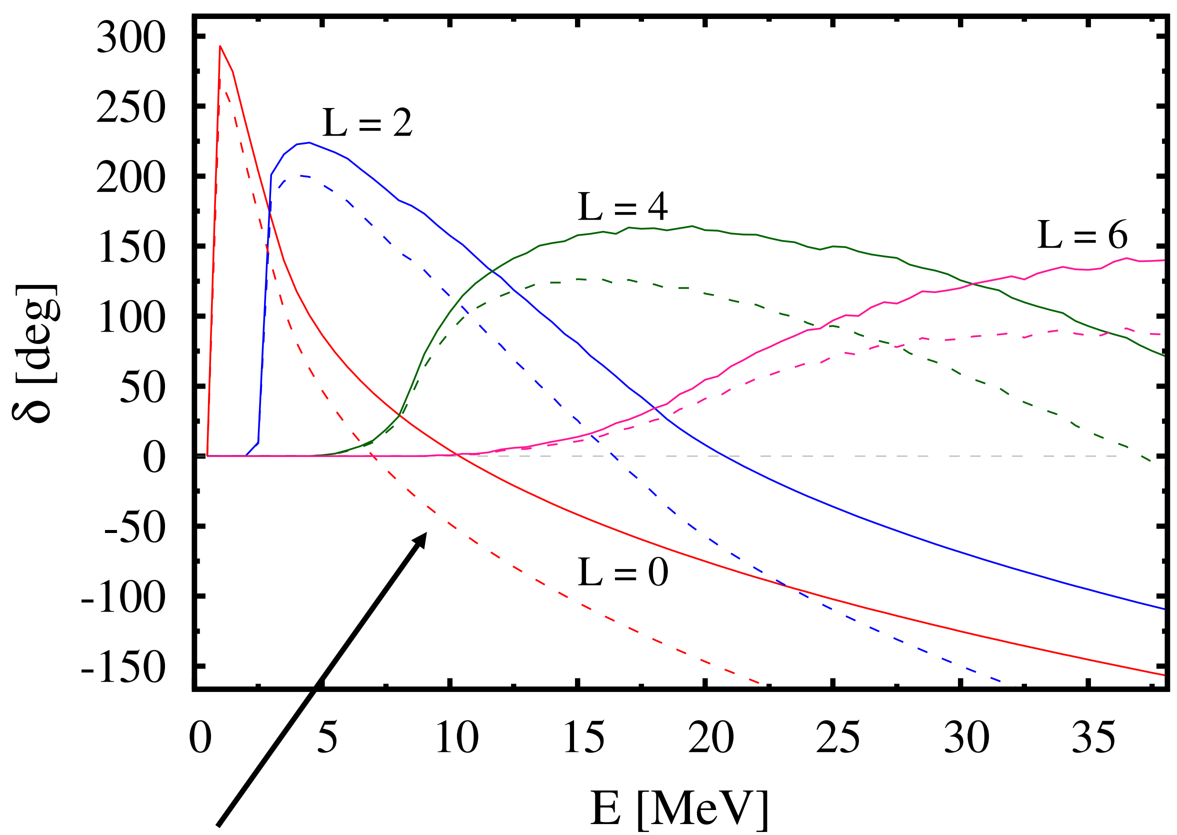
Reduced mass

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

Ground (resonance) state

α + α scattering (phase shift)

Nuclear phase shift

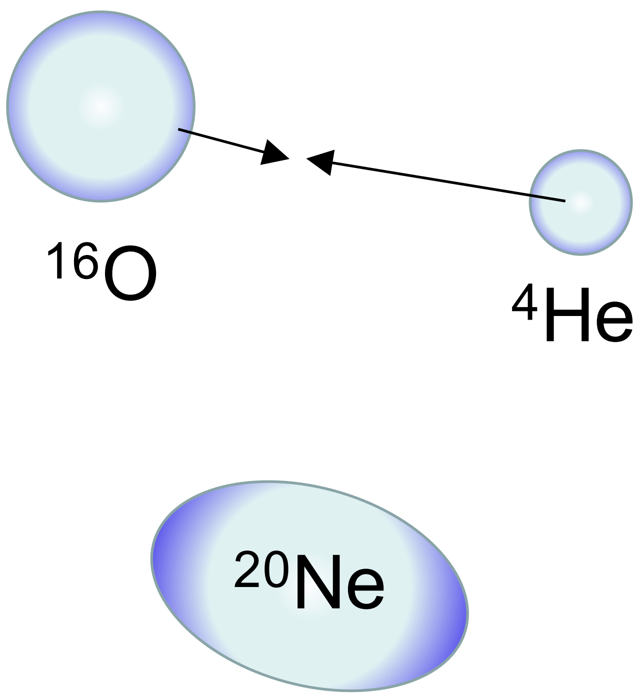


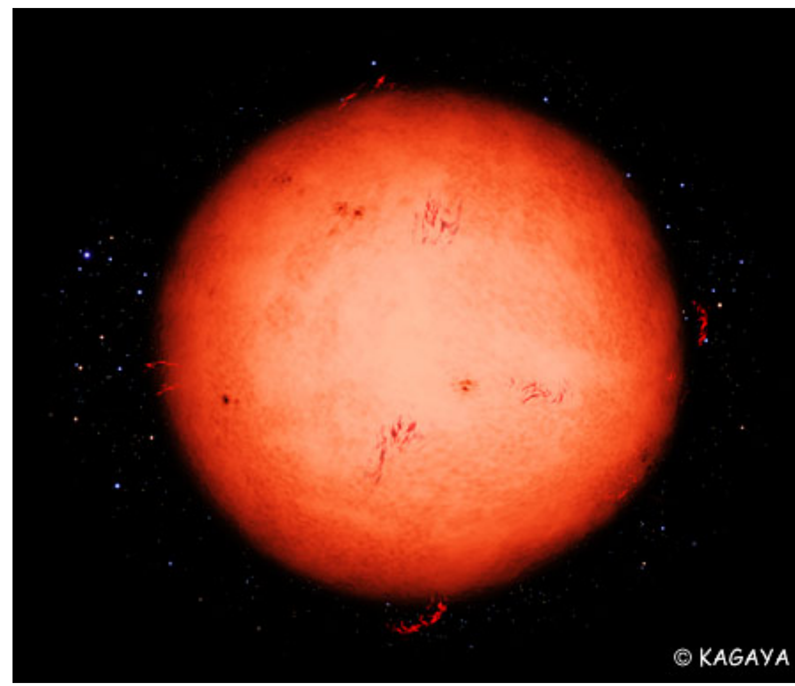
Effect of dynamical change of the inertial mass

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

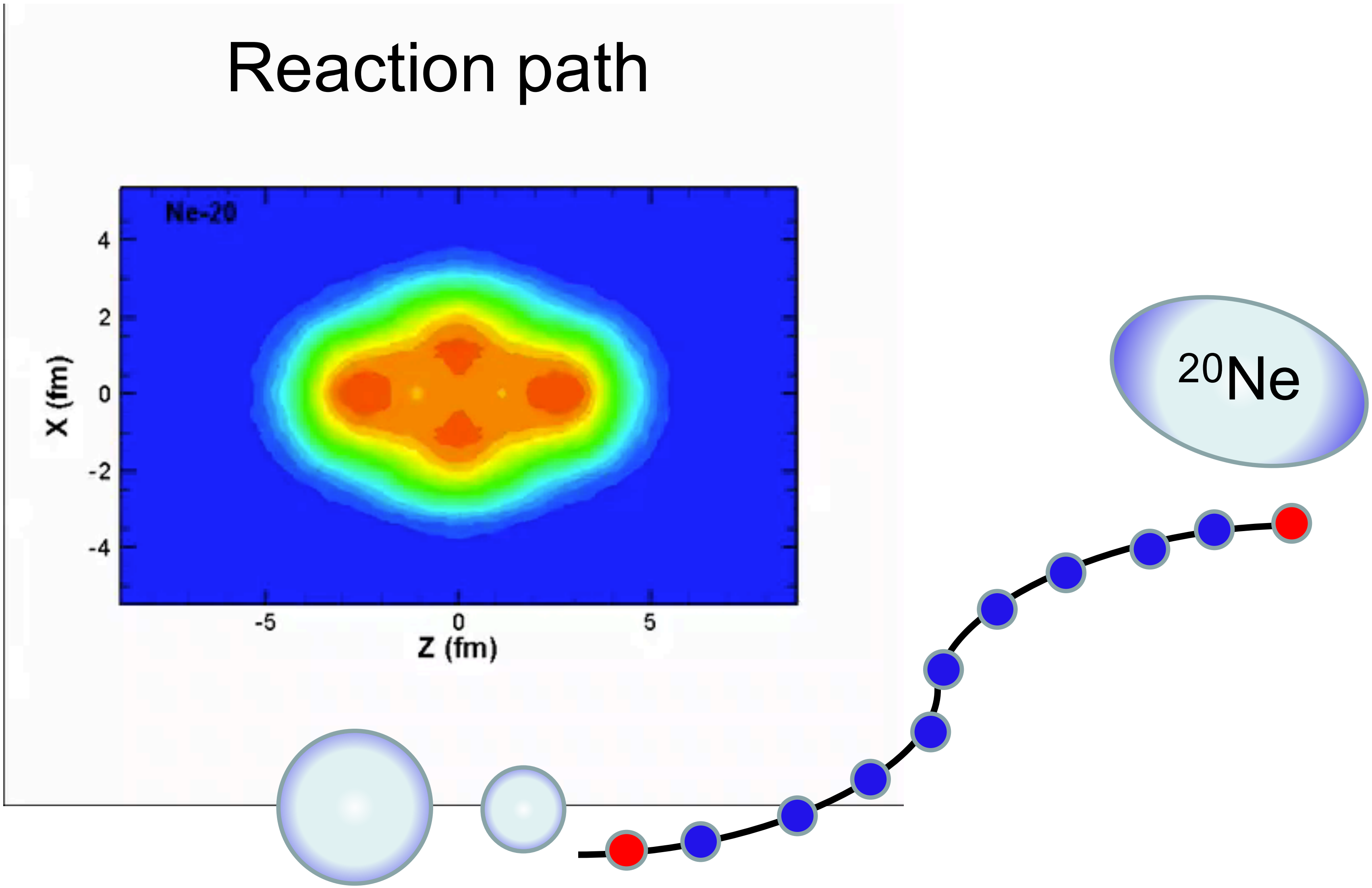
$^{16}O + \alpha$ scattering

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



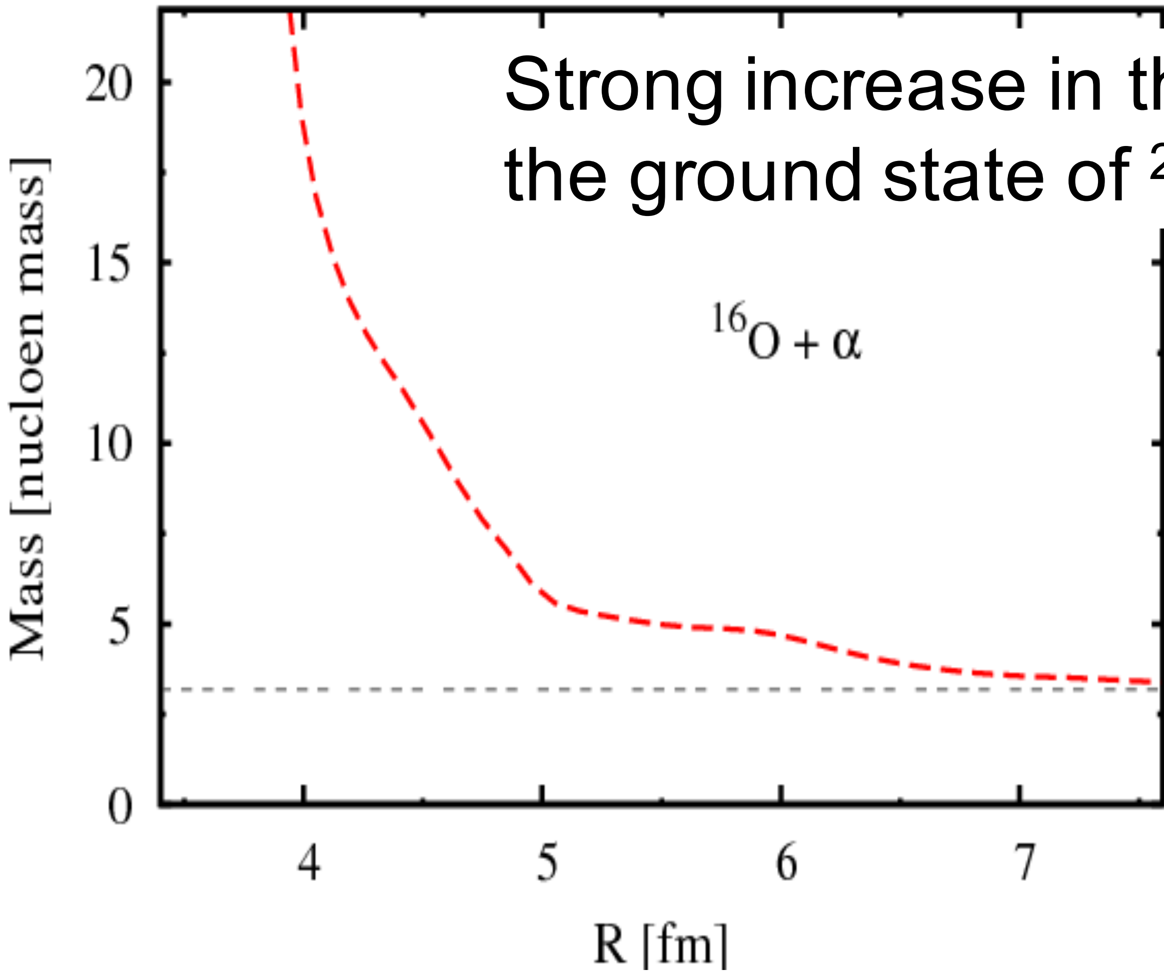


$^{16}O + \alpha$ to/from ^{20}Ne



^{20}Ne: Inertial mass

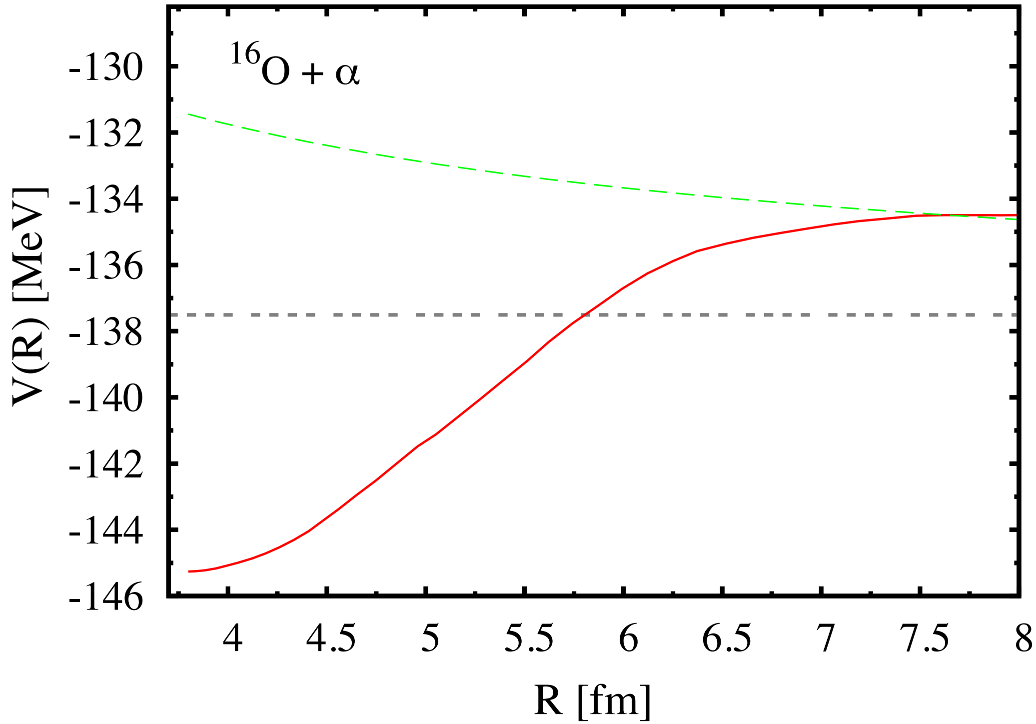
Strong increase in the mass near the ground state of ^{20}Ne

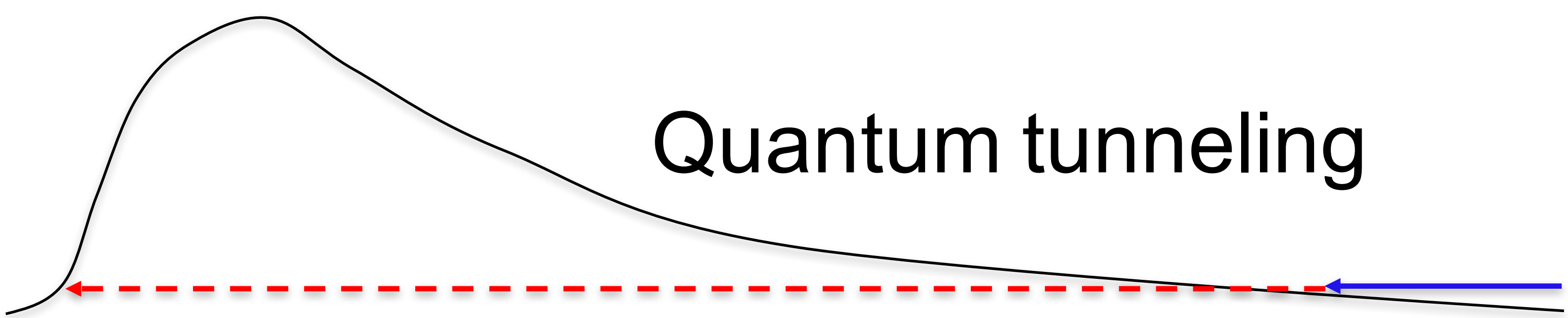


Reduced mass

$M(R) \to 3.2m$

^{20}Ne: Collective potential

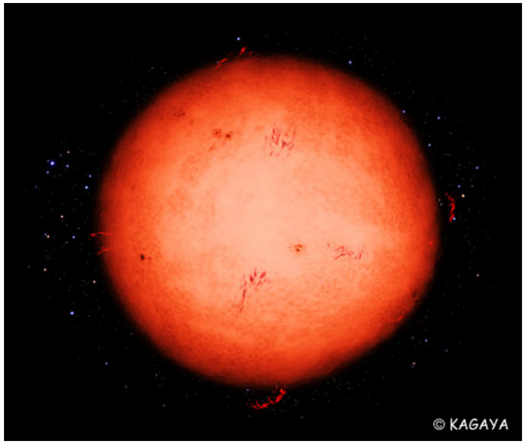




Quantum tunneling

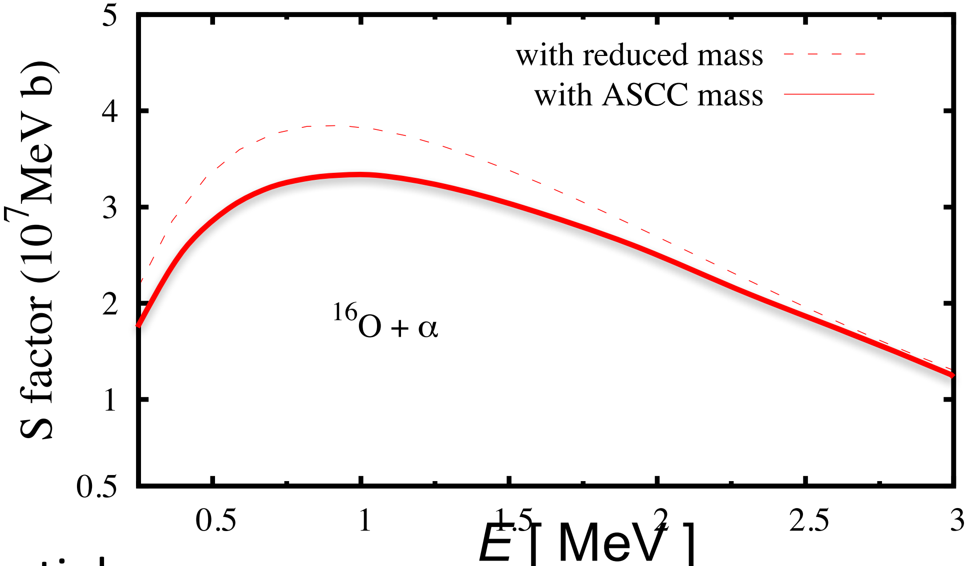
Alpha reaction : ^{16}O + α

Nuclear reaction to produce ^{20}Ne



Fusion reaction:
Astrophysical S-factor

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

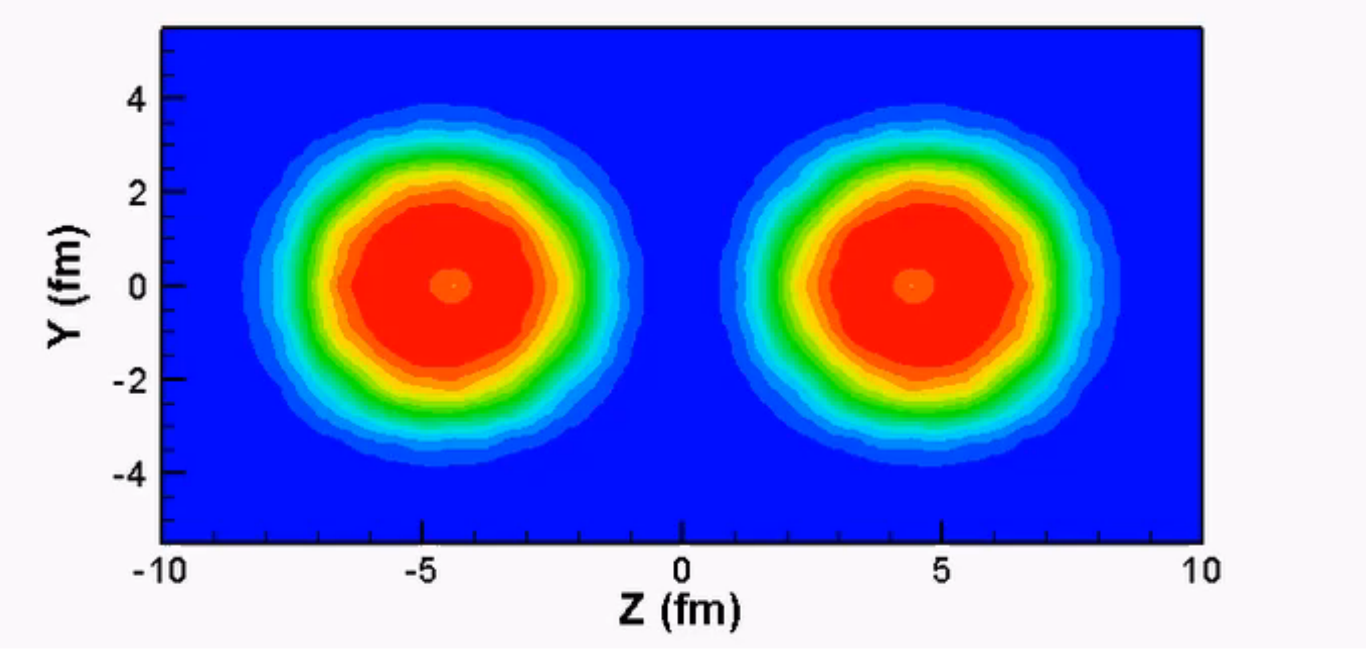


Effect of dynamical change of the inertial mass

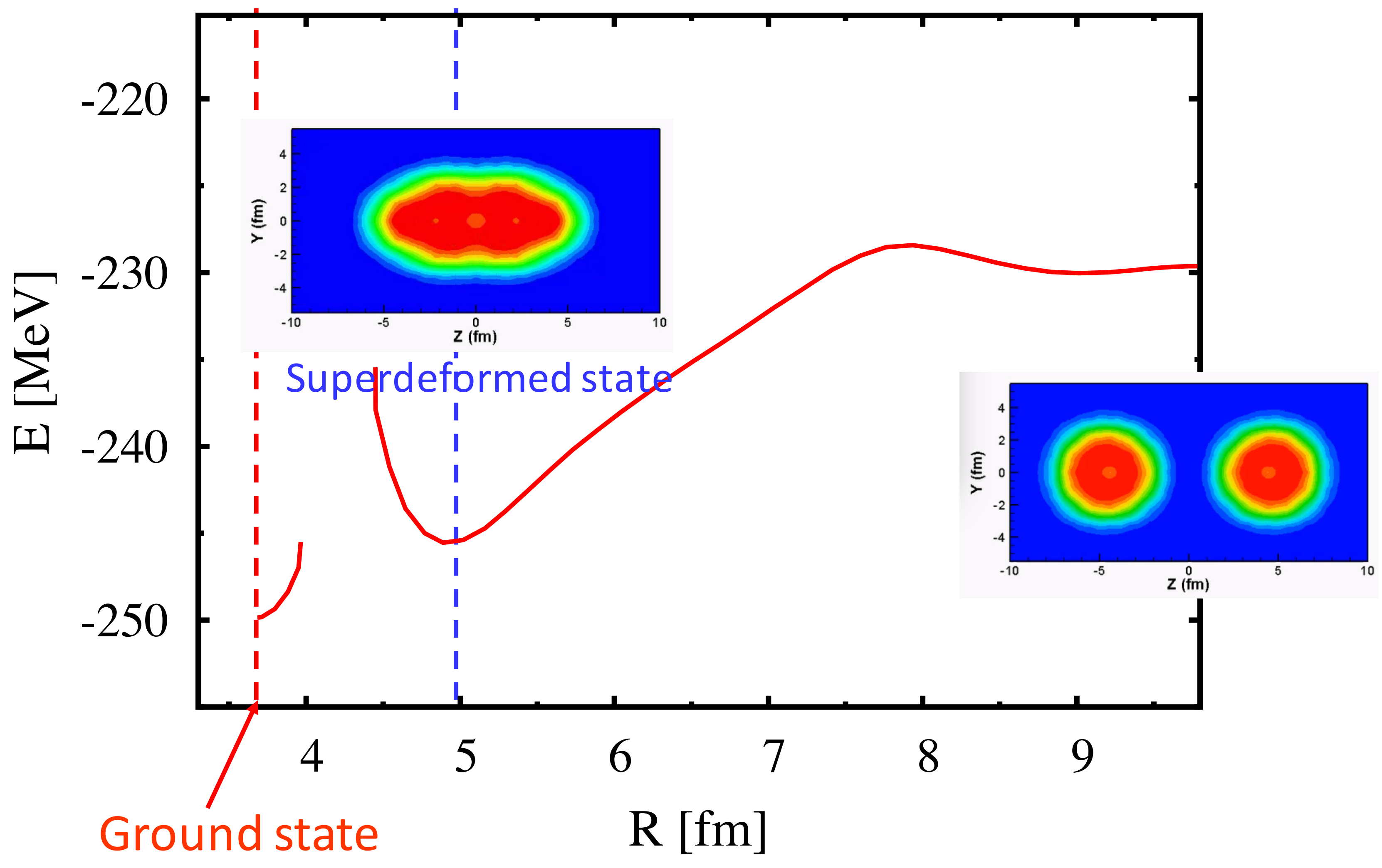
Dashed line: Constant reduced mass ($M(R) \rightarrow 3.2m$)

$^{16}O+^{16}O \rightarrow ^{32}S$: Reaction path

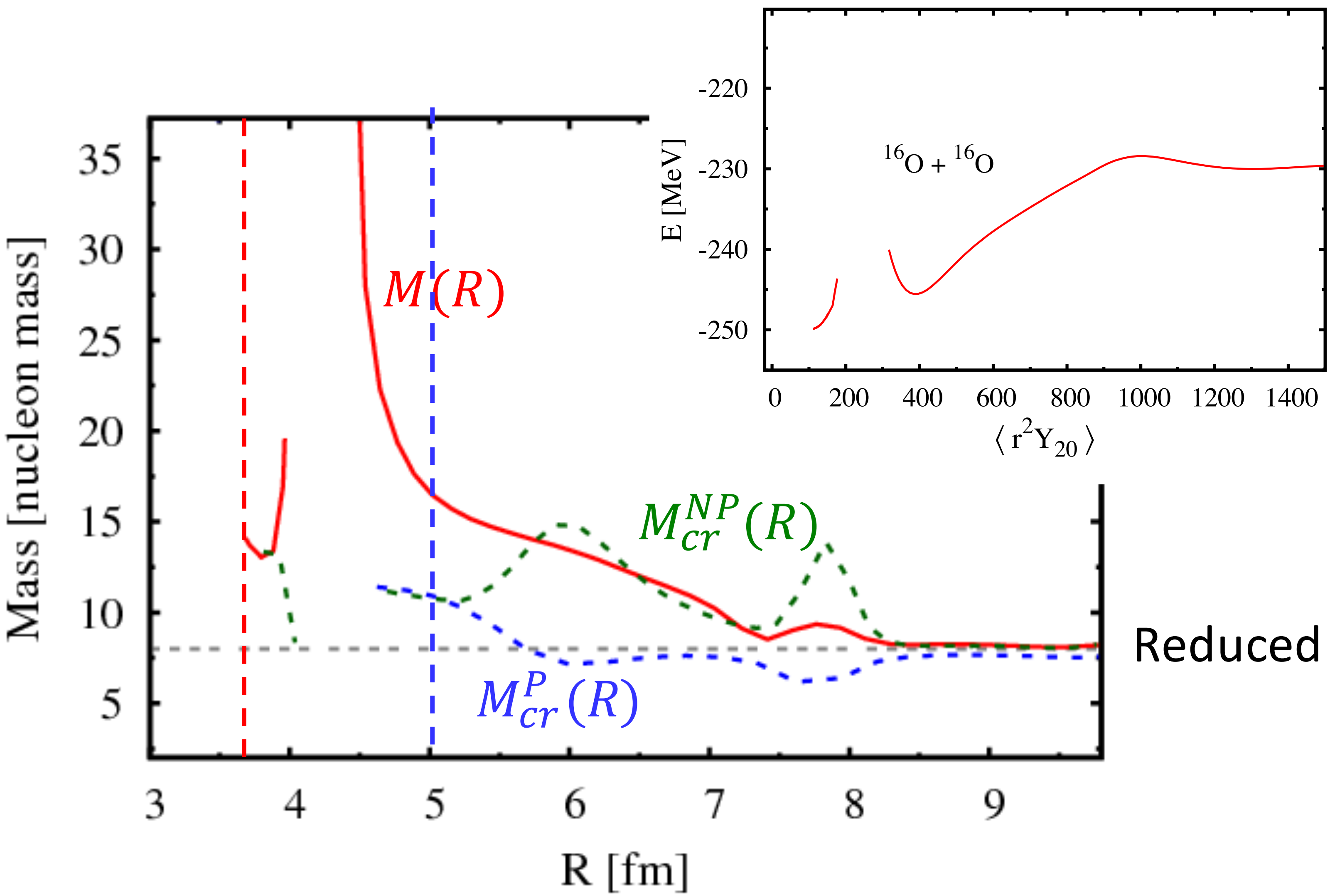
Starting from two ^{16}O configuration



$^{16}O+^{16}O \rightarrow ^{32}S$: Collective potential



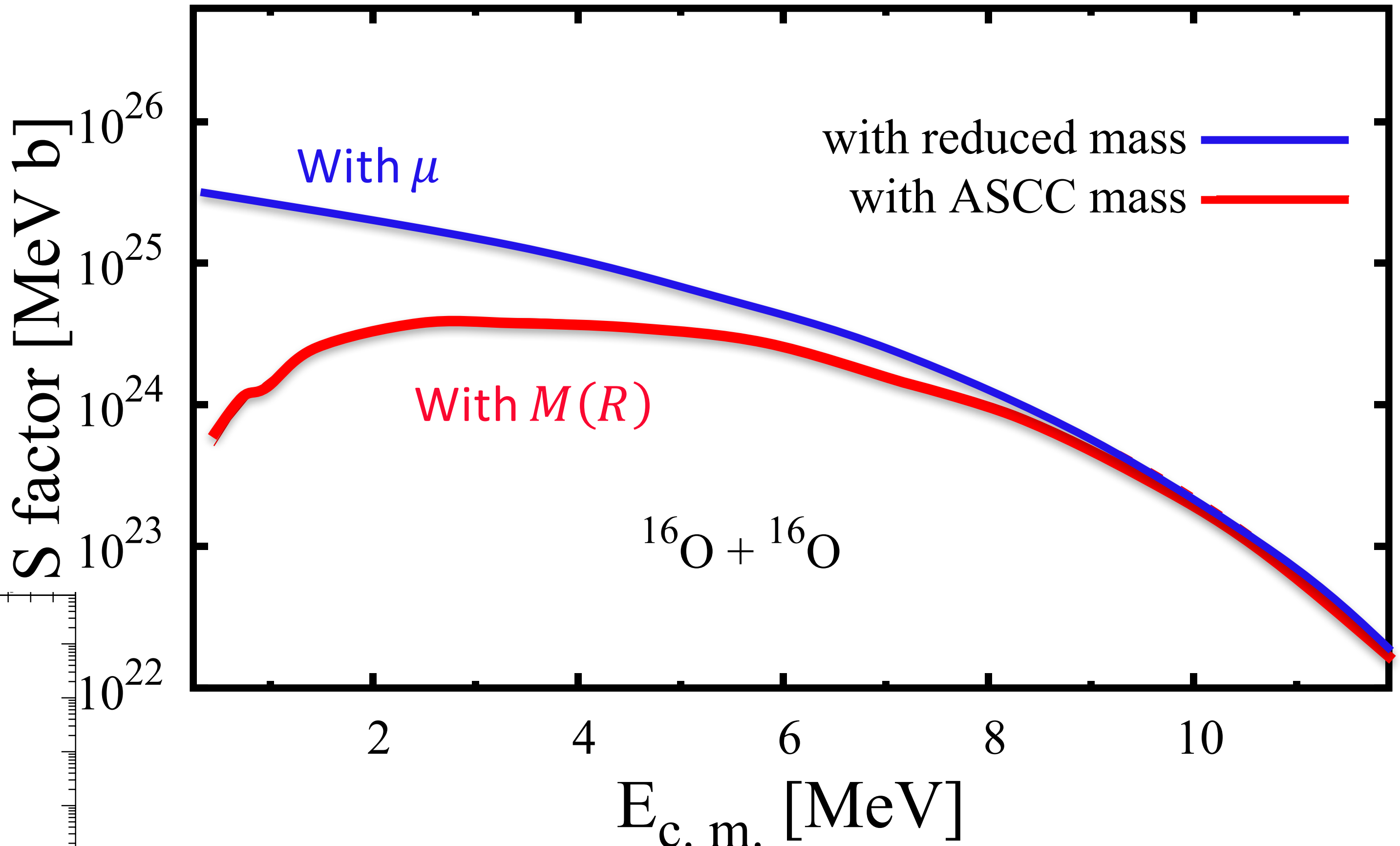
$^{16}O+^{16}O \rightarrow ^{32}S$: Collective mass



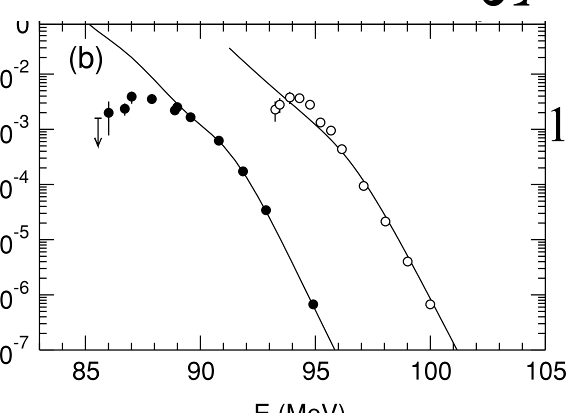
Reduced mass

Fusion reaction : ^{16}O + ^{16}O

Effect of dynamical change of the inertial mass *hinders the fusion cross section by 2 orders of magnitude*.



Exp (Ni+Ni)



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.)
  - Fang Ni (Univ. Tsukuba)
  - Kai Wen (Univ. Surrey)
  - Kenichi Yoshida (Kyoto Univ.)

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

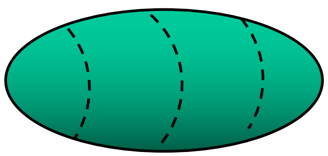
Nuclear deformation as symmetry breaking

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

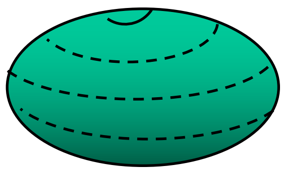
$$e^{i\phi N}|\Psi\rangle \neq |\Psi\rangle$$

Quadrupole deformation

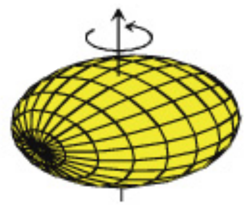
$$\beta_{2\mu} = \langle\Psi|r^2 Y_{2\mu}|\Psi\rangle$$



prolate



oblate

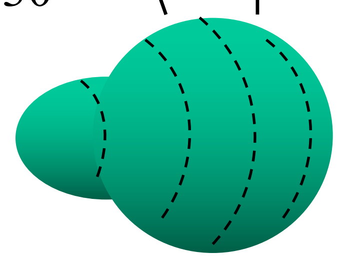


triaxial

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)

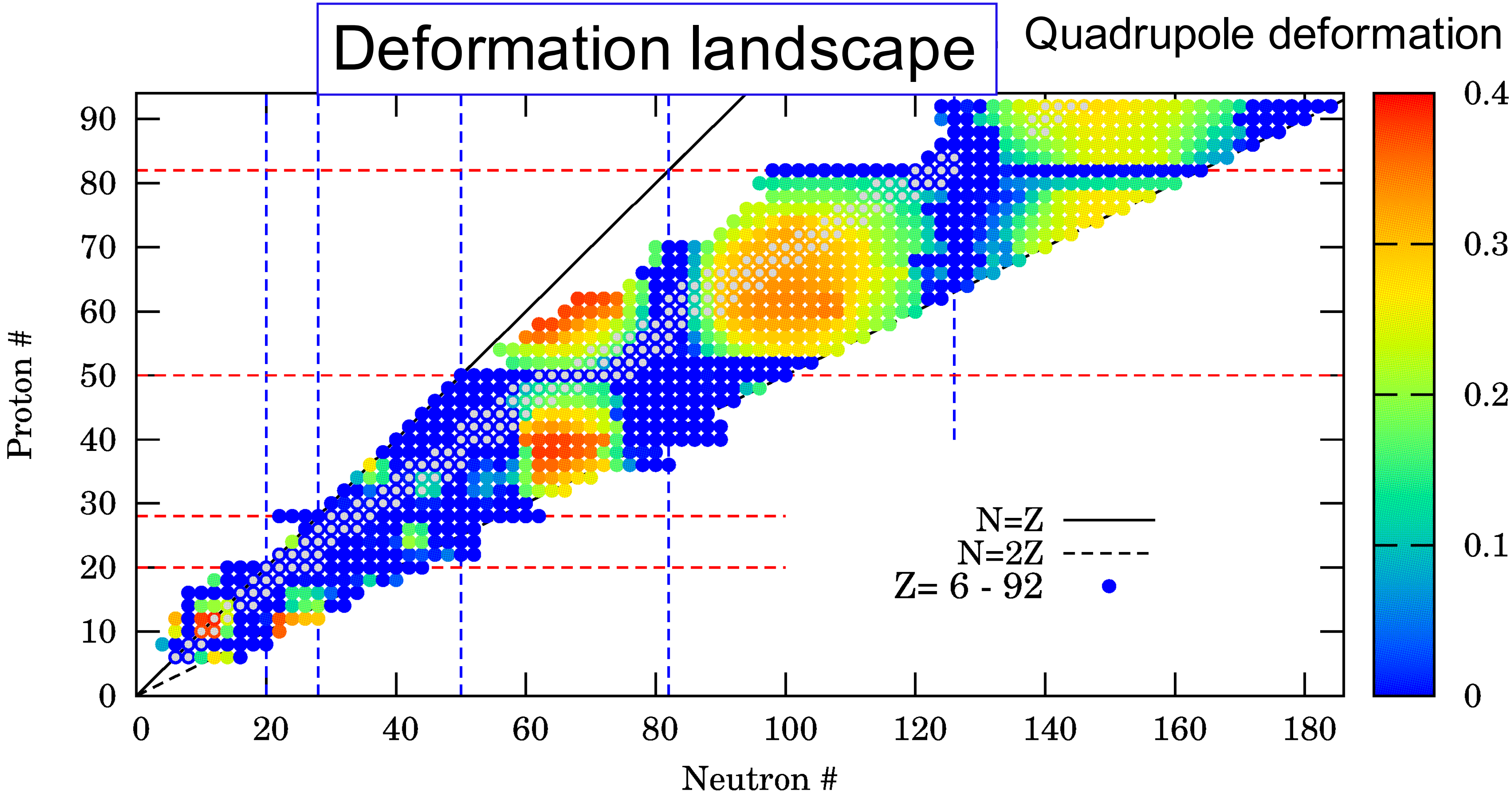
$$\Delta = \langle\Psi|\hat{\psi}\hat{\psi}|\Psi\rangle$$

Deformation in the gauge space

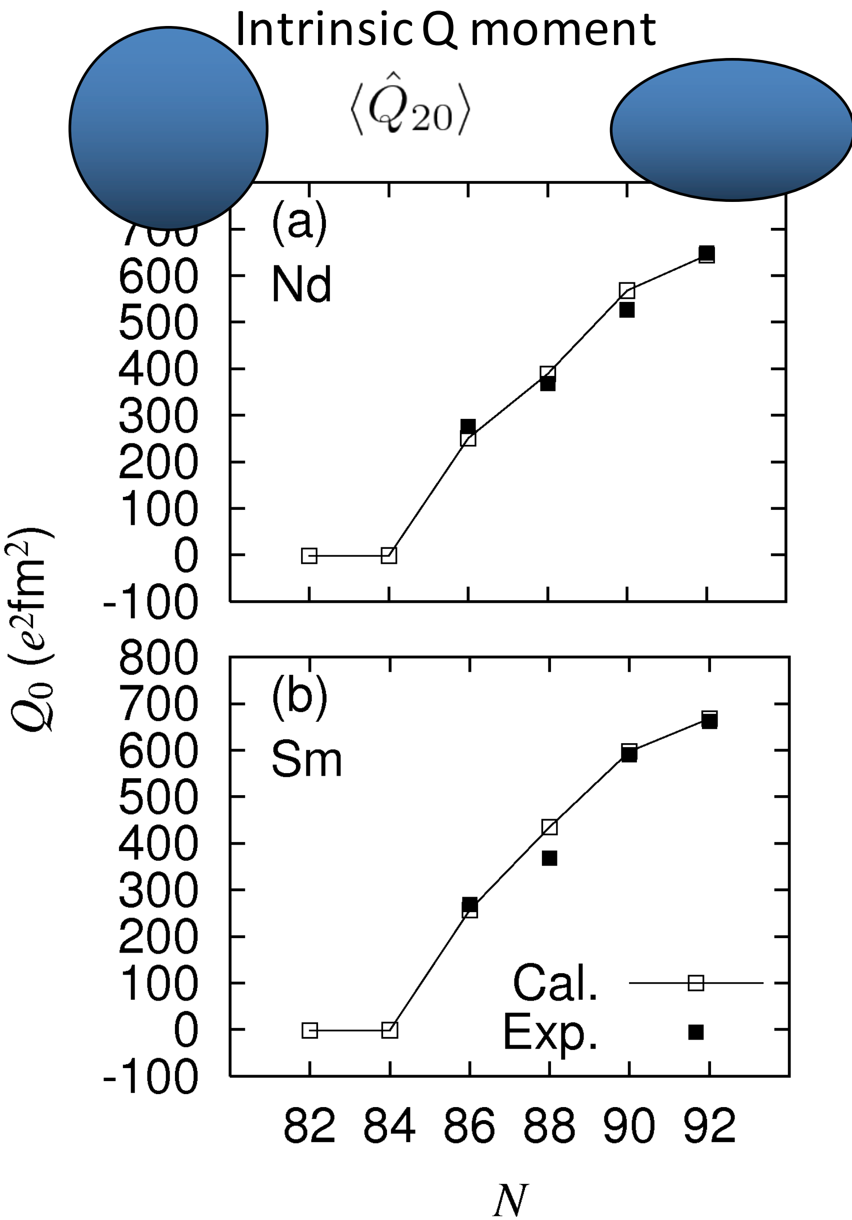
Nuclear Superconductivity
Nuclear Superfluidity

Nuclear deformation

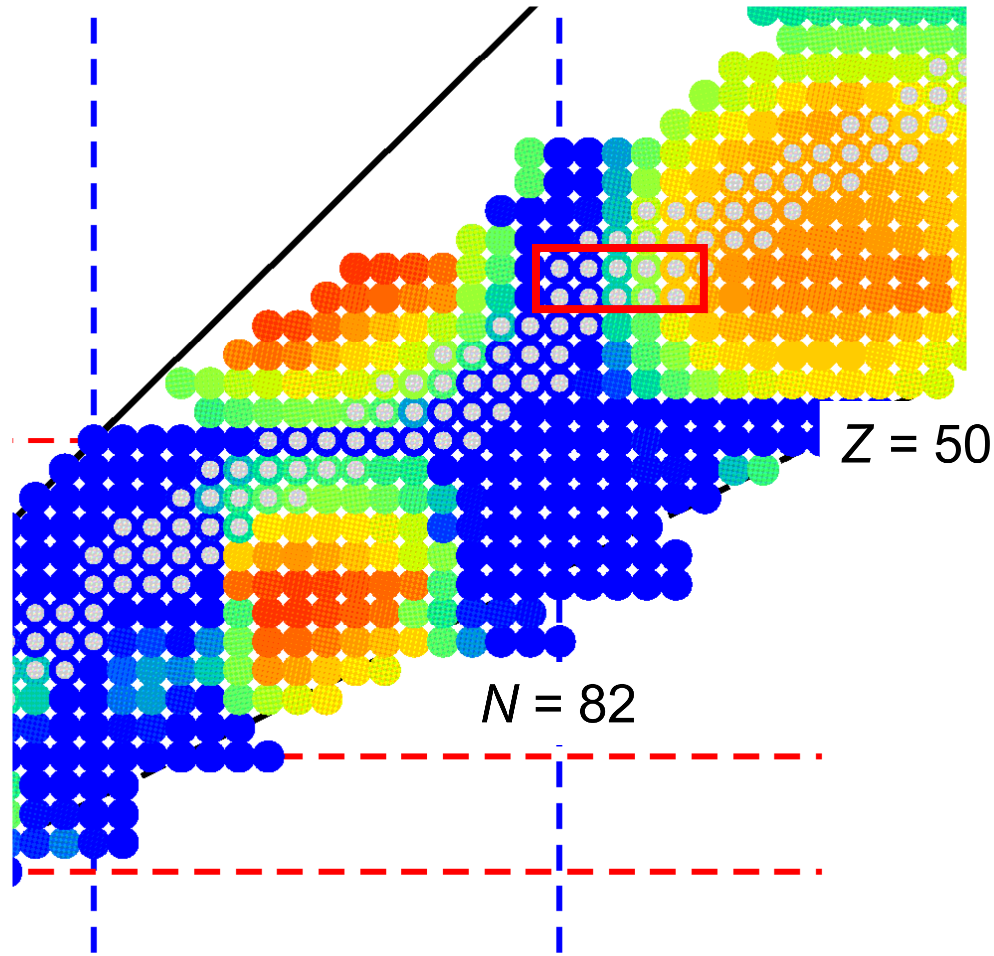
Ebata and T.N., Phys. Scr. 92 (2017) 064005



Nuclear deformation predicted by DFT



Deformation landscape



Linear response (RPA) equation

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

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

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

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

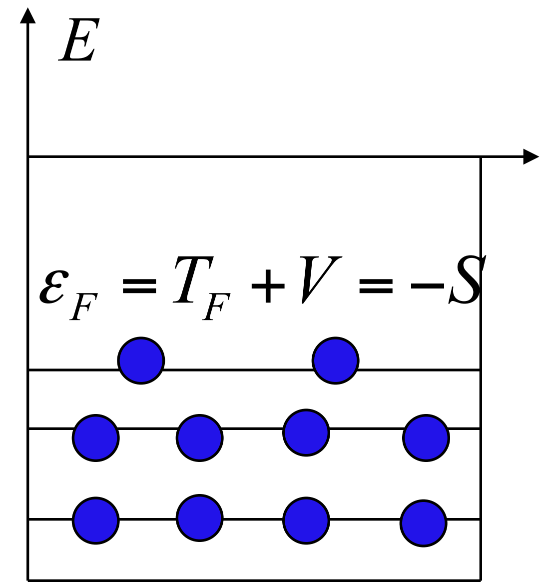
$$B_{mi,nj} = \left\langle \phi_m \left| \frac{\partial V}{\partial \rho_{jn}} \right|_{\rho_0} \left| \phi_i \right\rangle \right.$$

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

Saturation properties of nuclear matter

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

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

- Saturation density

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

  - Fermi energy

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

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

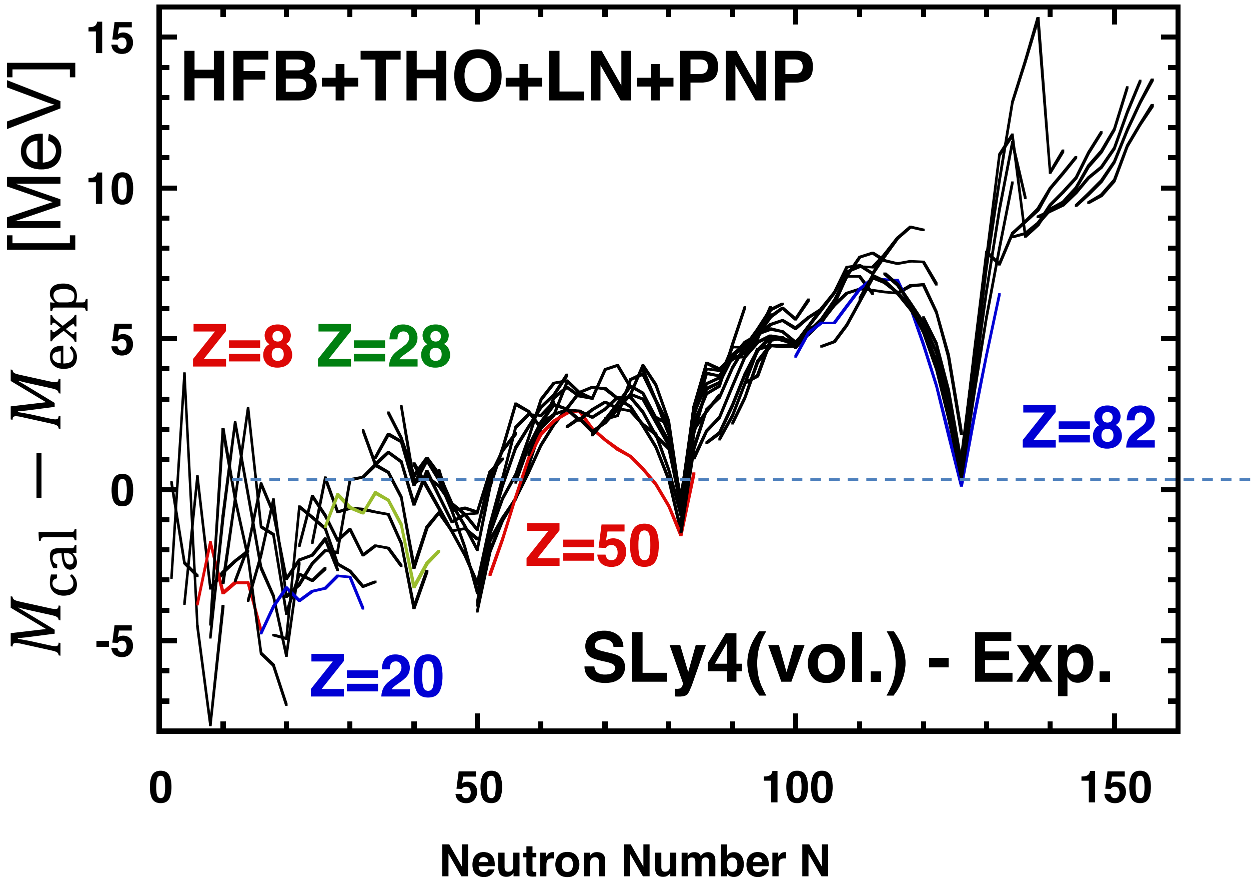
- Energy density functional

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

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

- State-dependent effective interaction
  – Rearrangement terms

Predicted nuclear mass



Dobaczewski et al., 2004

Missing correlations for open-shell nuclei

Inertial mass

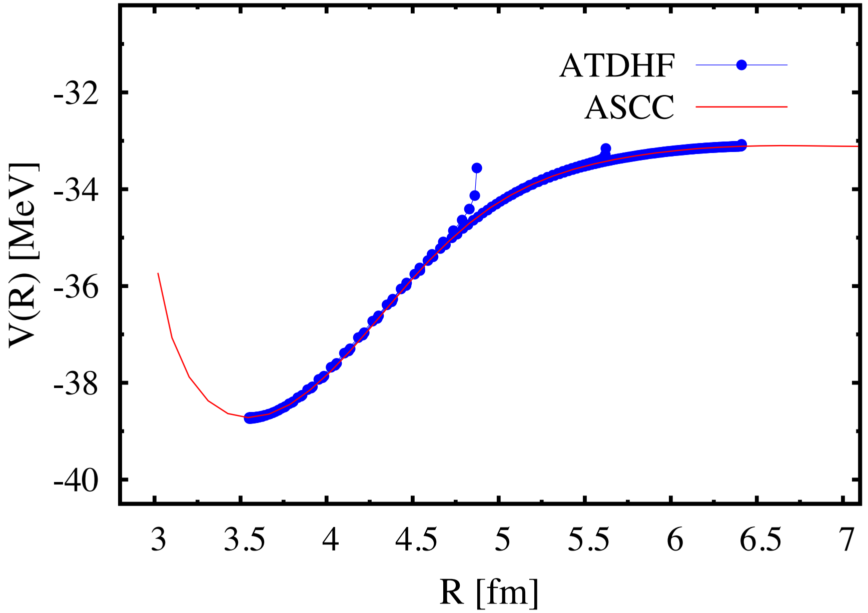
- Cranking (Inglis-Belyaev) inertial mass
  - Neglect time-odd mean-field effects
- GCM-GOA
  - Realistic applications: real coordinates only
- Wrong total mass for translation

- ASCC inertial mass (extension of RPA mass)
  - Time-odd effects
  - Correctly reproduce the total mass

ATDHF: ^{8}Be:

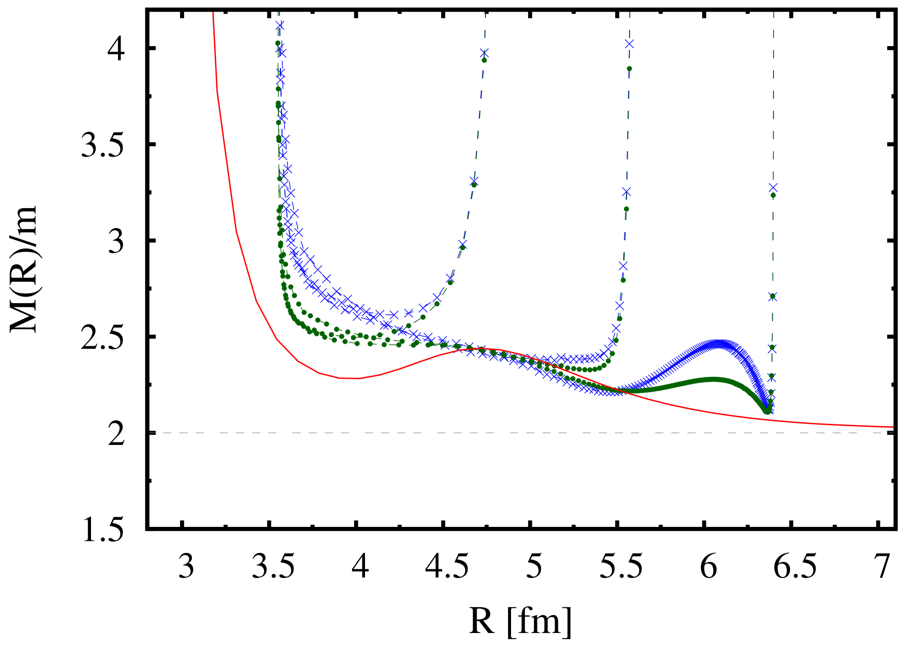
ATDHF method (Goeke, Gruemmer, Reinhard 1983)

$$\frac{\partial}{\partial q}|\psi(q)\rangle = \frac{M_{\mathrm{atdhf}}(q)}{dV/dq}[\hat{H}, \hat{H}_{\mathrm{ph}}]_{\mathrm{ph}}|\psi(q)\rangle,$$



Calculate many trajectories to construct an "envelope"

$$M_{\mathrm{atdhf}}(q) = \langle\psi(q)|[\hat{Q}(q), [\hat{H}, \hat{Q}(q)]]|\psi(q)\rangle^{-1}$$



Difficulties:

- Around the saddle point
- Convergence