Requantization of TDDFT on collective subspace

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Collaboration with
Kai Wen (Univ. of Tsukuba)

- Density functional model
  - Success & Failure
- Requantized TDDFT   cf) Negele, Rev. Mod. Phys. 54 (1982), 913.
  - Why is the requantization necessary?
  - Canonical quantization:
    - Derivation of nuclear reaction model at low energy
  - Torus quantization
    - Microscopic wave function

2022.9.12-16 @RPMBT-XXI, Chapel Hill, NC, USA

Nuclear energy density functional

- Spin & isospin degrees of freedom
- Nuclear superfluidity

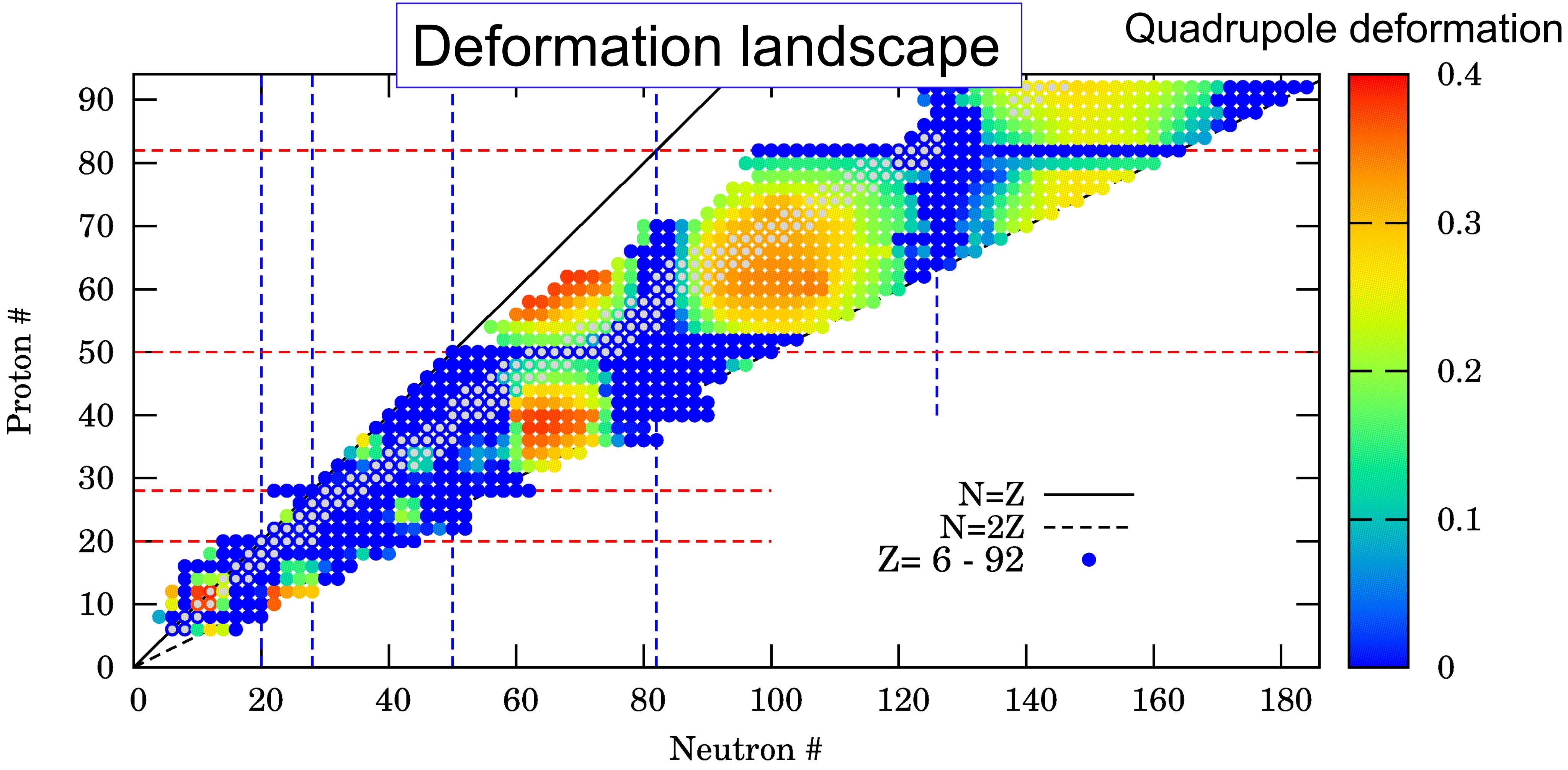
$$E\left[\rho_q(t),\tau_q(t),\overleftrightarrow{J}_q(t),\vec{j}_q(t),\vec{s}_q(t),\vec{T}_q(t);\kappa_q(t)\right]$$

kinetic
spin-current
current
spin
spin-kinetic
pair density

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

Nuclear deformation

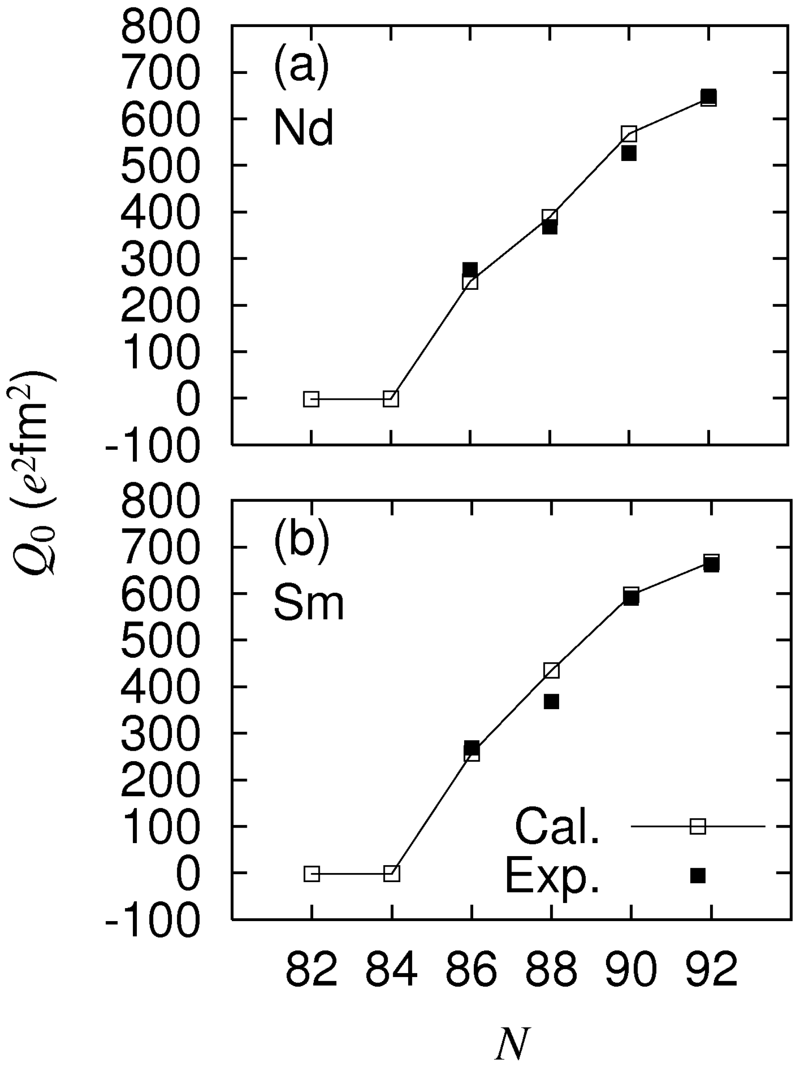
Ebata and T.N., Phys. Scr. 92 (2017) 064005



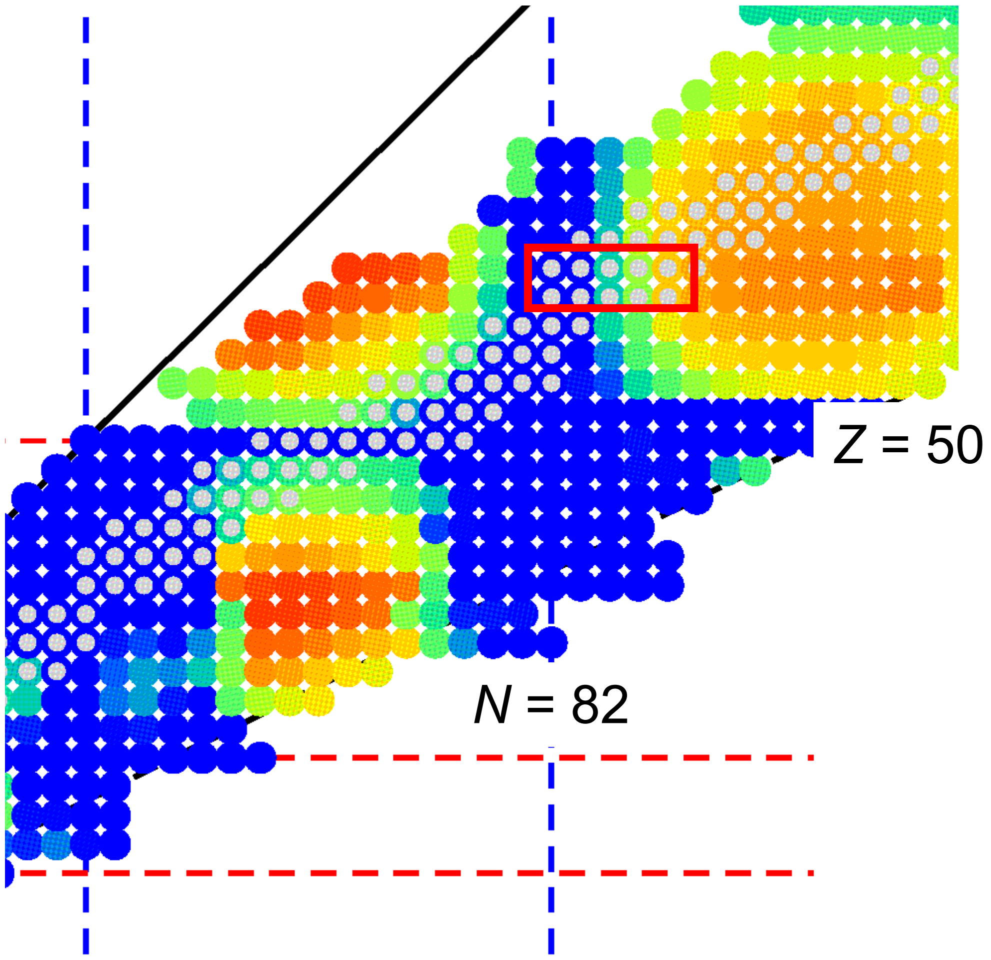
Nuclear deformation predicted by DFT

Intrinsic Q moment

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



Deformation landscape



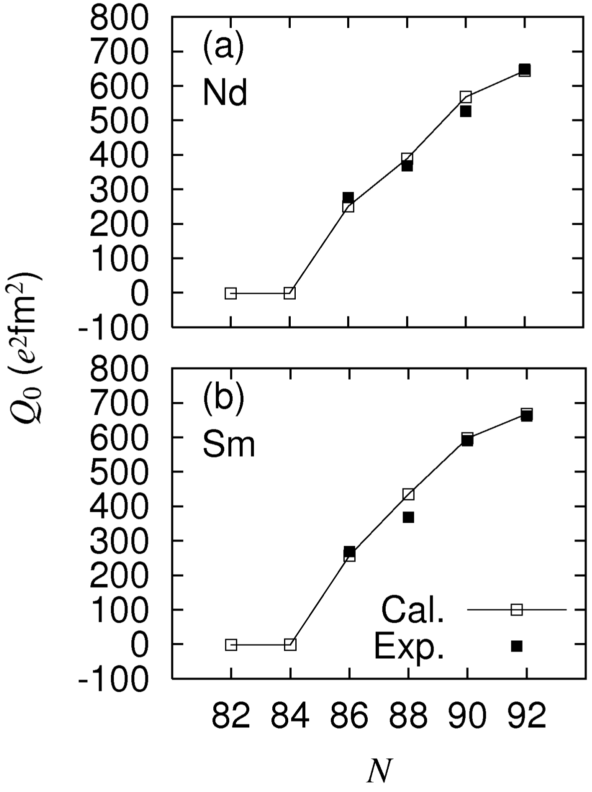
Deformation effects for photoabsorption cross section

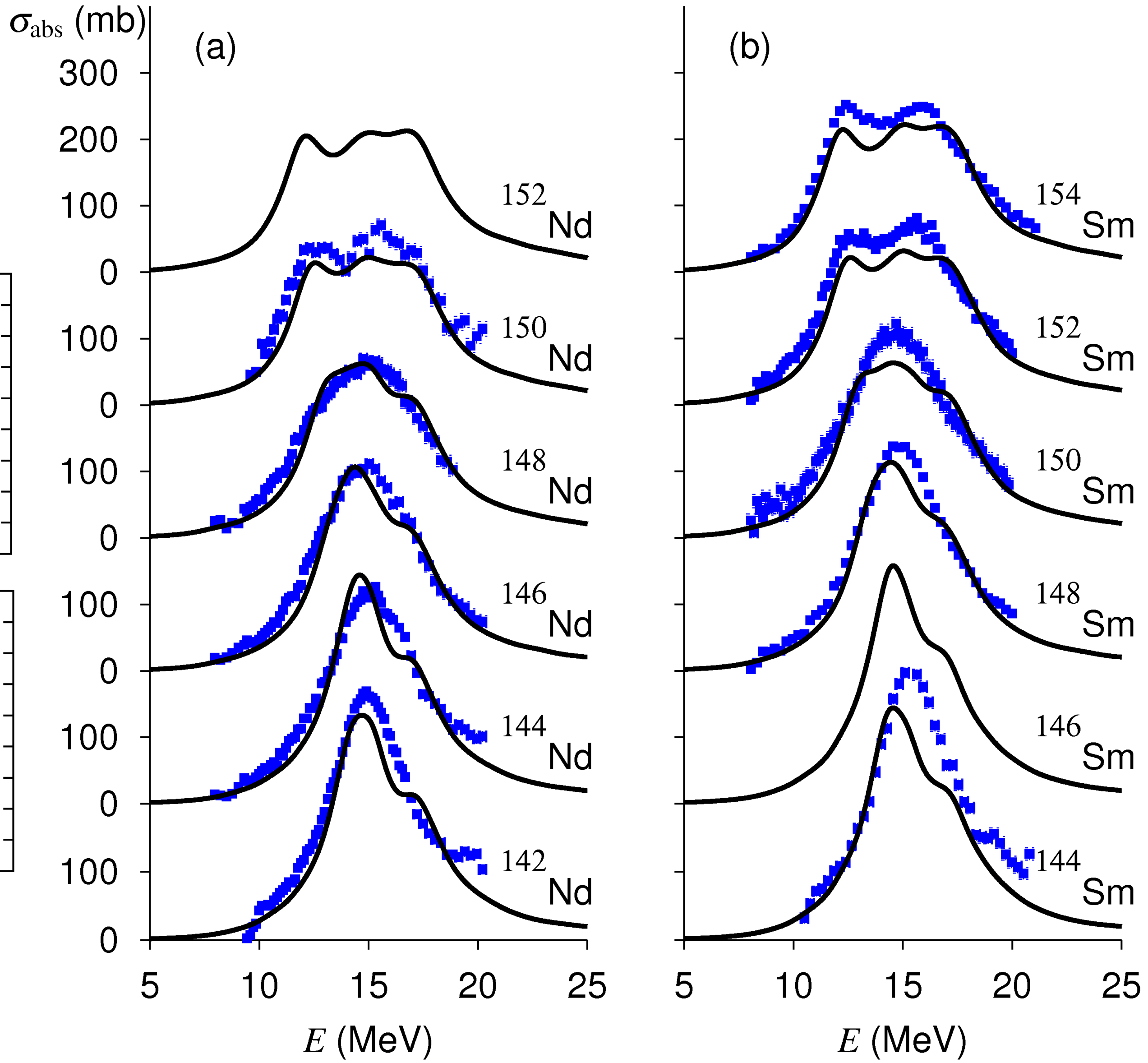
SkM* functional

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

Intrinsic Q moment

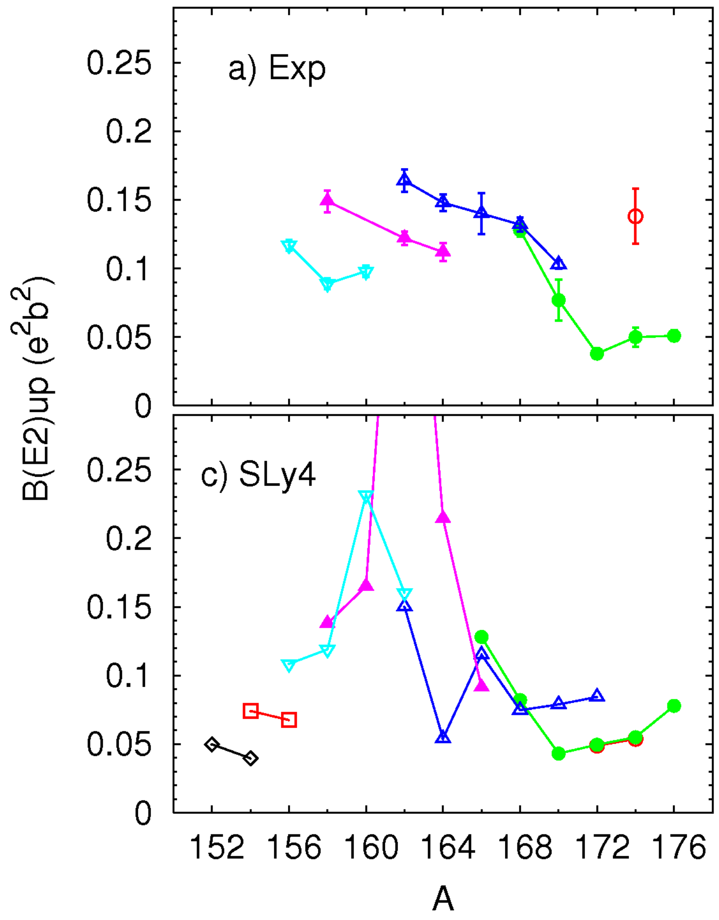
$\langle \hat{Q}_{20} \rangle$

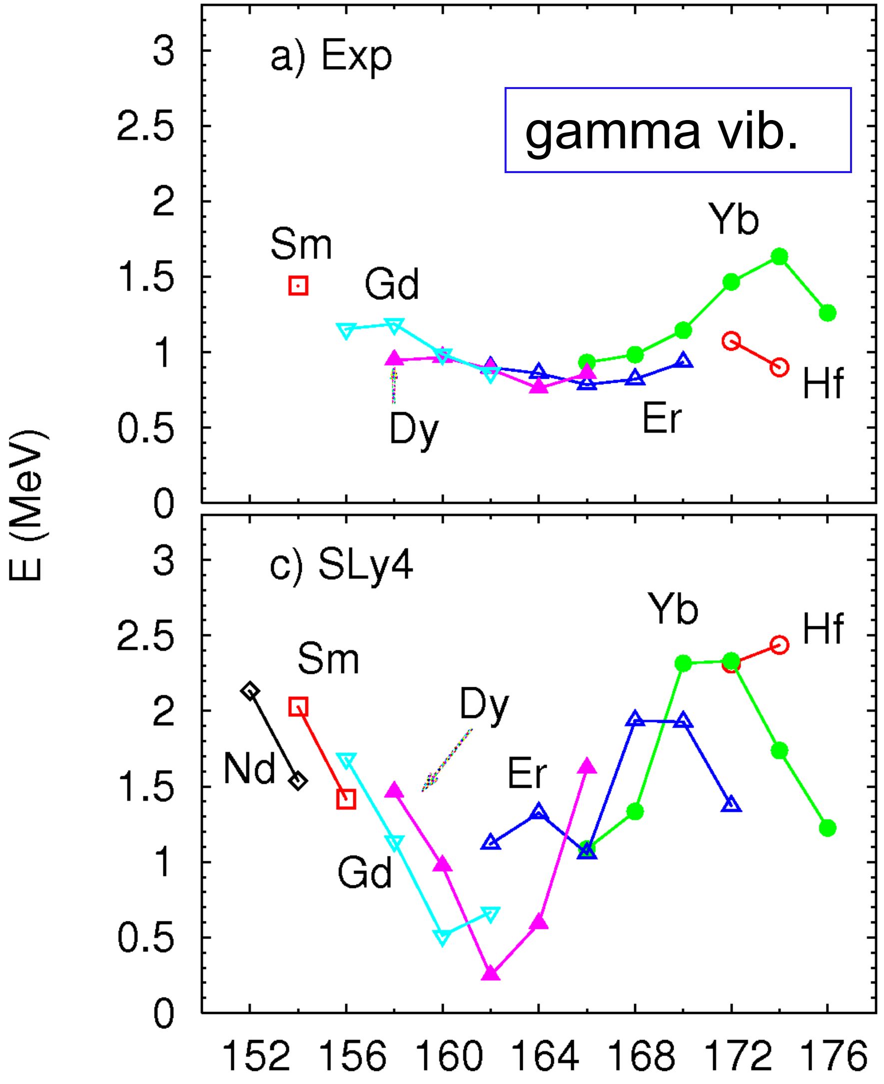




Low-energy states

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

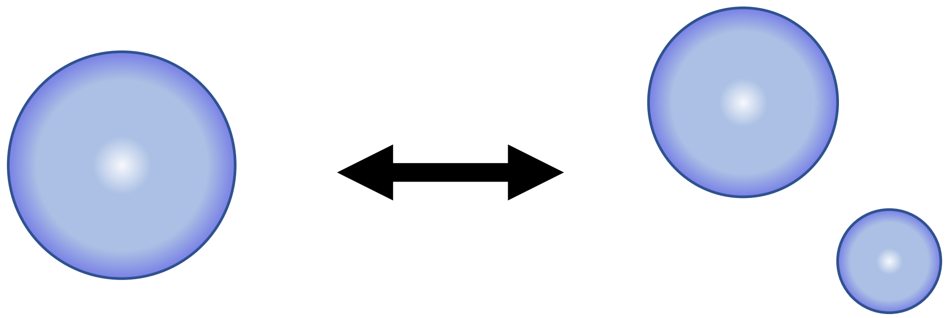




Terasaki, Engel, Phys. Rev. C 84, 014332 (2011)

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)



Problems in nuclear (TD)DFT

- Problems
  - Low-energy collective motion
  - Many-body tunneling (spontaneous fission, sub-barrier fusion, astrophysical reaction)

- Main origin of missing correlations
  - Quantum fluctuation associated with “slow” collective motion

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 $[q, p] = i\hbar$

Adiabatic Self-consistent Collective Coordinate (ASCC) method

TN, et al., RMP 88, 045004 (2016)

- Collective canonical variables (q, p)

$$\{\xi^\alpha, \pi_\alpha\} \to \{q, p;\ q^a, p_a;\quad a = 2, \cdots, N_{ph}\}$$

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

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

- Finding a decoupled subspace

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

Moving mean-field eq.

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

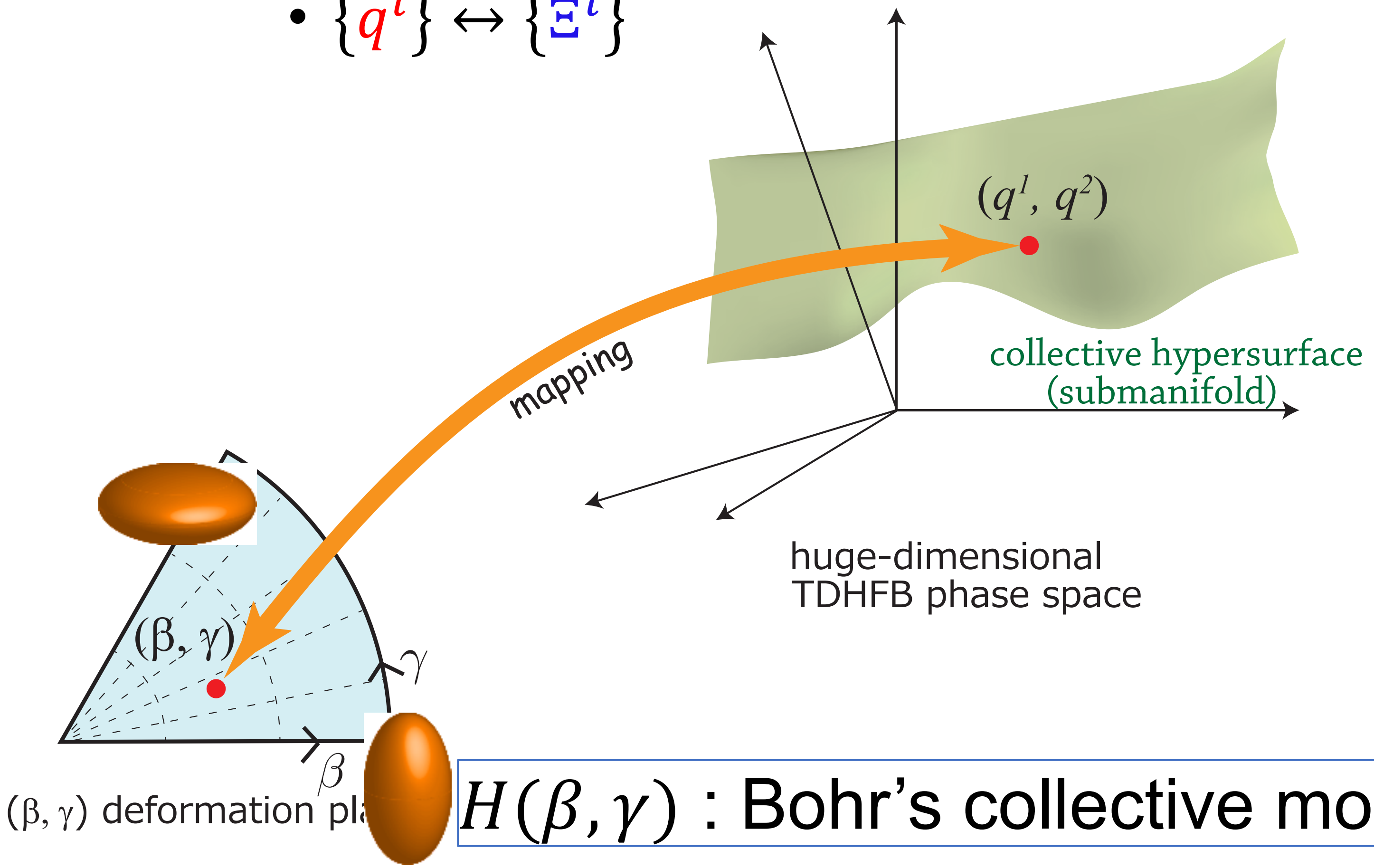
Moving RPA eq.

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

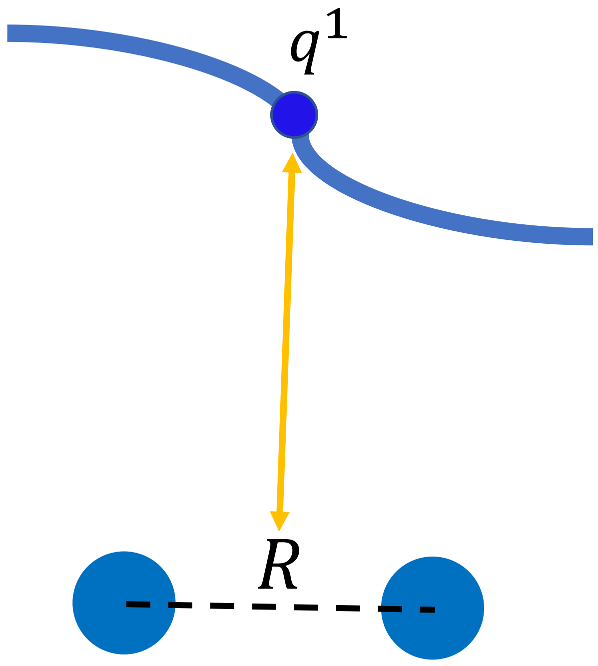
$\Gamma^\beta_{\alpha\gamma}$: Affine connection with metric $g_{\alpha\beta} \equiv \sum_\mu \frac{\partial q^\mu}{\partial \xi^\alpha}\frac{\partial q^\mu}{\partial \xi^\beta}$

One-to-one correspondence

- One-to-one correspondence between the self-consistent collective subspace and a given collective space
  - $\{q^i\} \leftrightarrow \{\Xi^i\}$



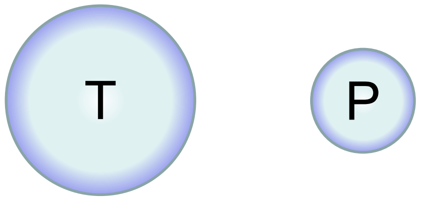
$H(\beta,\gamma)$: Bohr's collective model



$H(R)$: Reaction model

Macroscopic reaction model at low energy

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



$\mu_R = \frac{M_P M_T}{M_P+M_T}$: reduced mass

$V(R)$: Potential

(phenomenological or calculated assuming frozen structure)

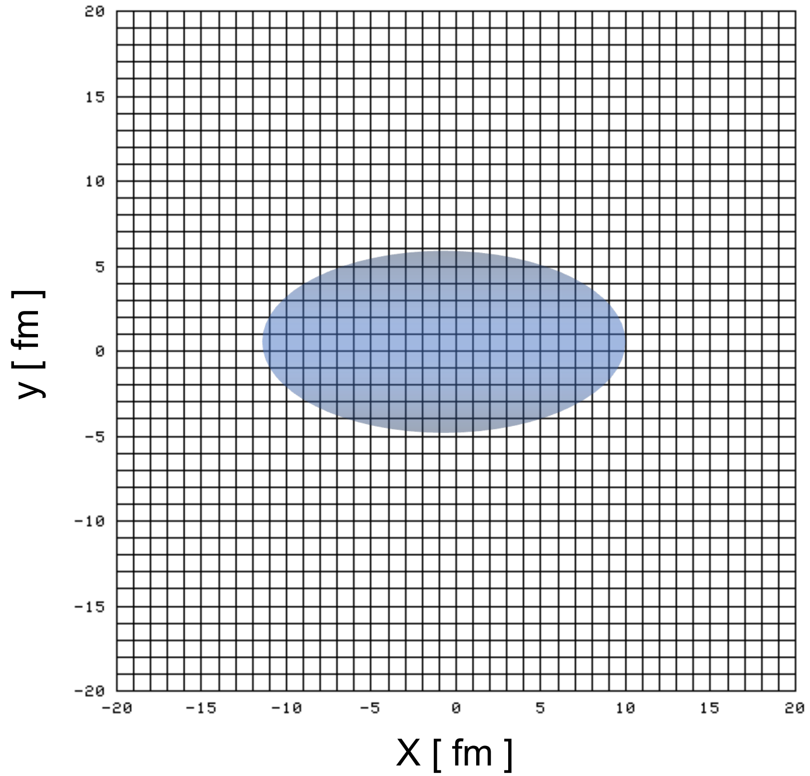
Macroscopic reaction model at low energy

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

- Necessary steps for construction
  - Determination of reaction path
  - Calculation of the potential $V(R)$
  - Calculation of the mass $M(R)$ & M.o.I $I(R)$

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))



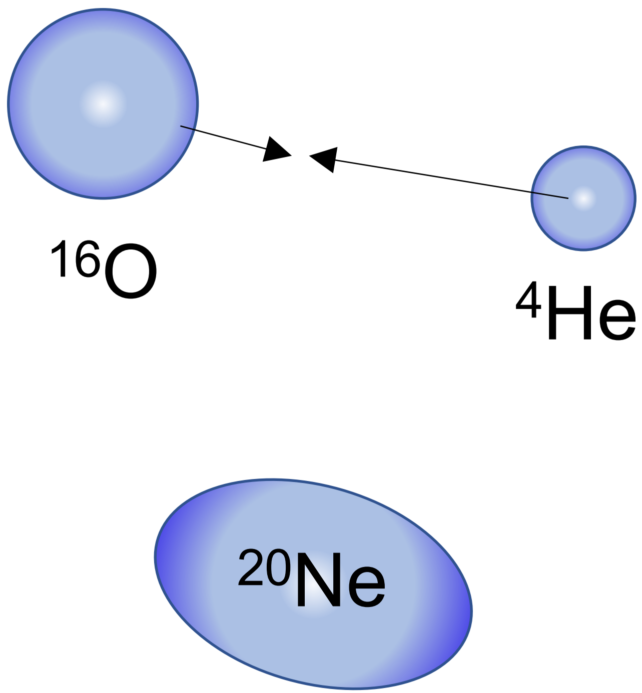
Wen, T.N., PRC 94, 054618 (2016); PRC 96, 014610 (2017); PRC 105, 034603 (2022)

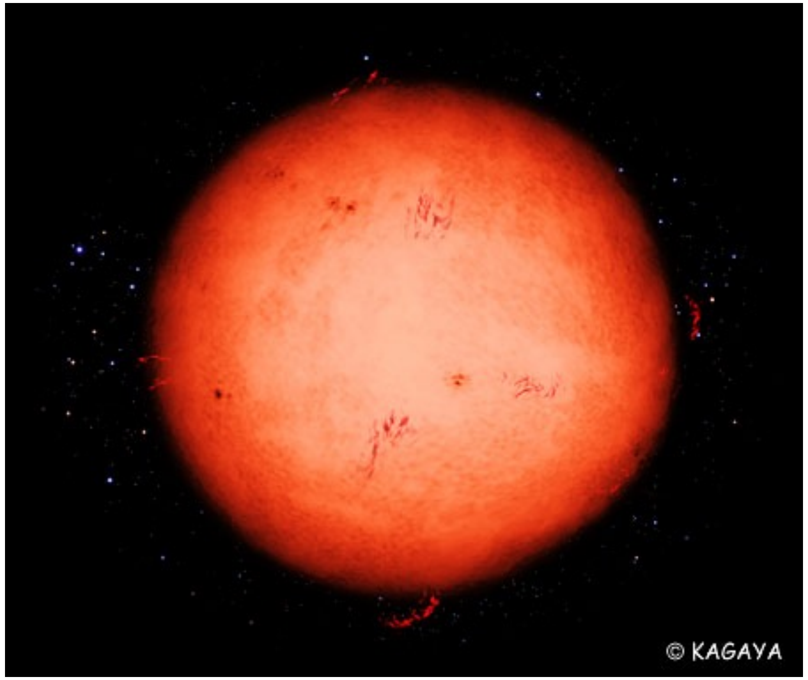
No pairing

1-dimensional reaction path extracted from the space of dimension of 10^4 ~10^5.

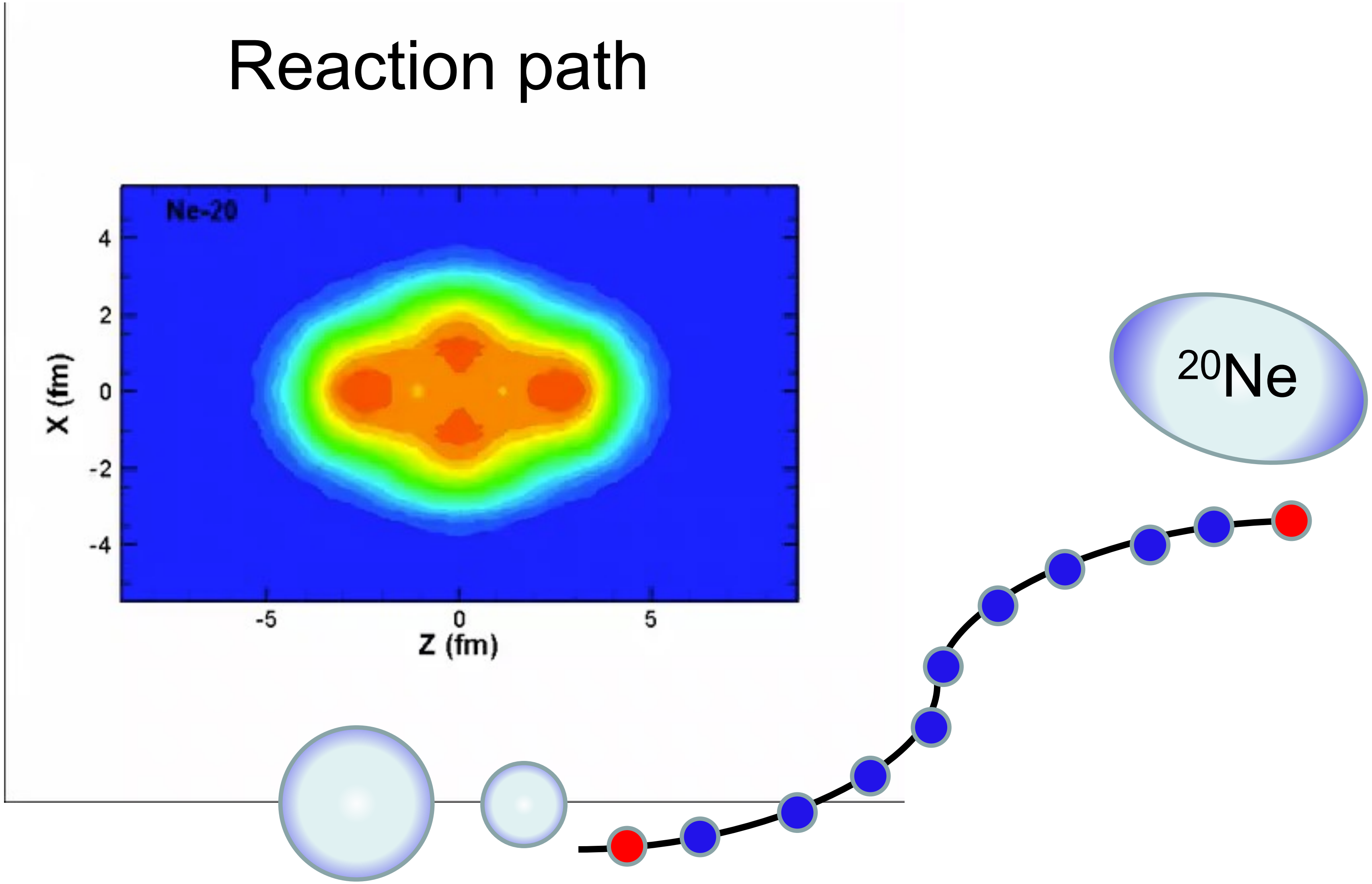
$^{16}O + \alpha$ scattering

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

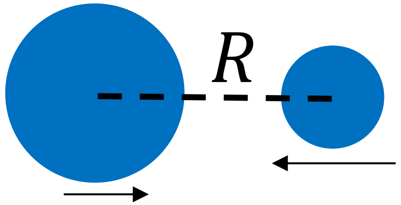


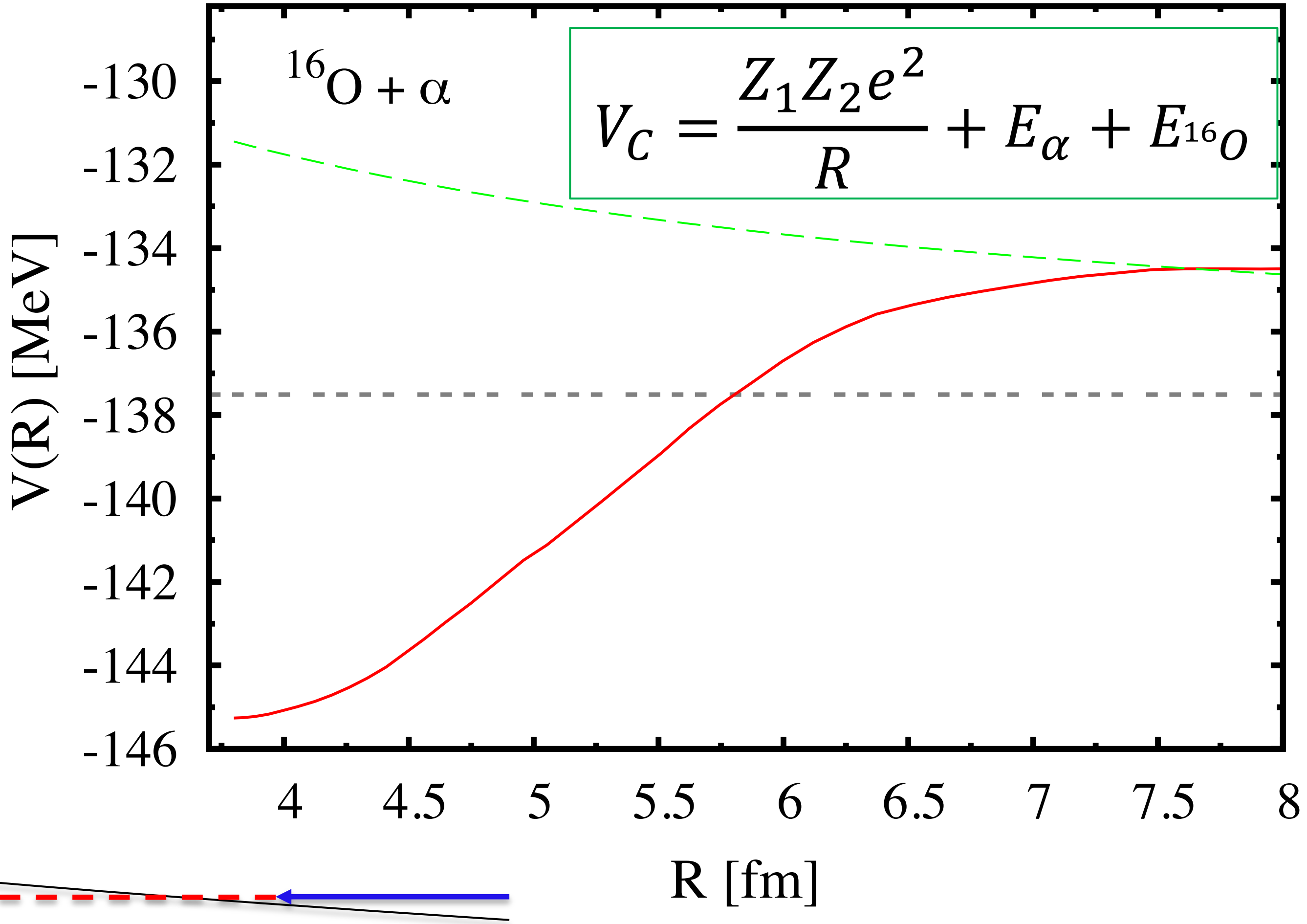


$^{16}O + \alpha$ to/from ^{20}Ne

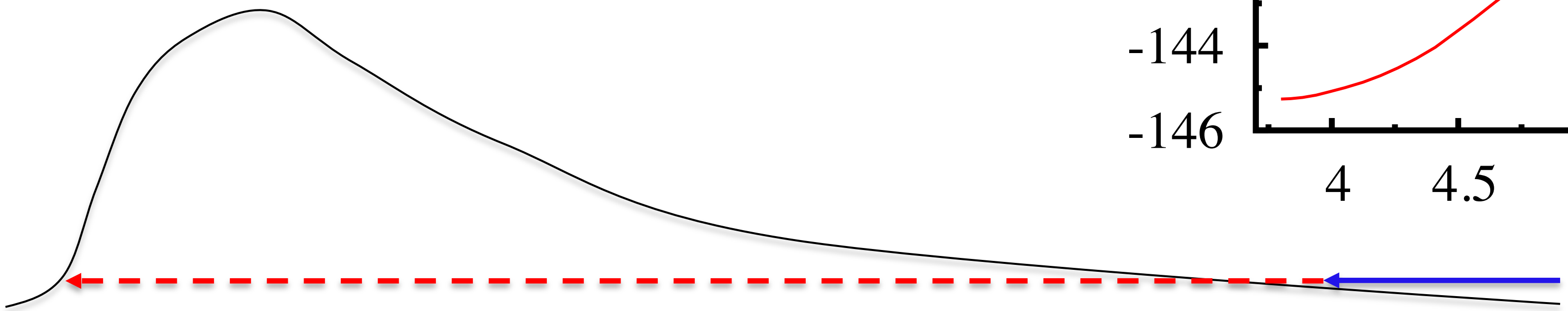


$$V(R) \quad (m^*/m = 1)$$





Quantum tunneling



Energy density functional

$$E[\rho] = \int \frac{1}{2m}\tau(\mathbf{r})d\mathbf{r} + \int d\mathbf{r}\left\{\frac{3}{8}t_0\rho^2(\mathbf{r}) + \frac{1}{16}t_3\rho^3(\mathbf{r})\right\}$$
$$+ \iint d\mathbf{r}d\mathbf{r}'\rho(\mathbf{r})v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}')$$
$$+ B_3\int d\mathbf{r}\{\rho(\mathbf{r})\tau(\mathbf{r}) - \mathbf{j}^2(\mathbf{r})\},$$

BKN functional

Bonche, Koonin, Negele, PRC 13, 1226 (1976)

$$\hat{h}_{\mathrm{HF}}(\mathbf{r}) = -\nabla\frac{1}{2m^*(\mathbf{r})}\nabla + \frac{3}{4}t_0\rho(\mathbf{r}) + \frac{3}{16}t_3\rho^2(\mathbf{r})$$
$$+ \int d\mathbf{r}'v(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}') + B_3[\tau(\mathbf{r}) + i\nabla\cdot\mathbf{j}(\mathbf{r})]$$
$$+ 2iB_3\mathbf{j}(\mathbf{r})\cdot\nabla,$$

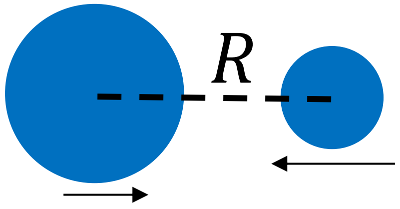
$$B_3 = 0 \quad \rightarrow \quad m^* = m$$

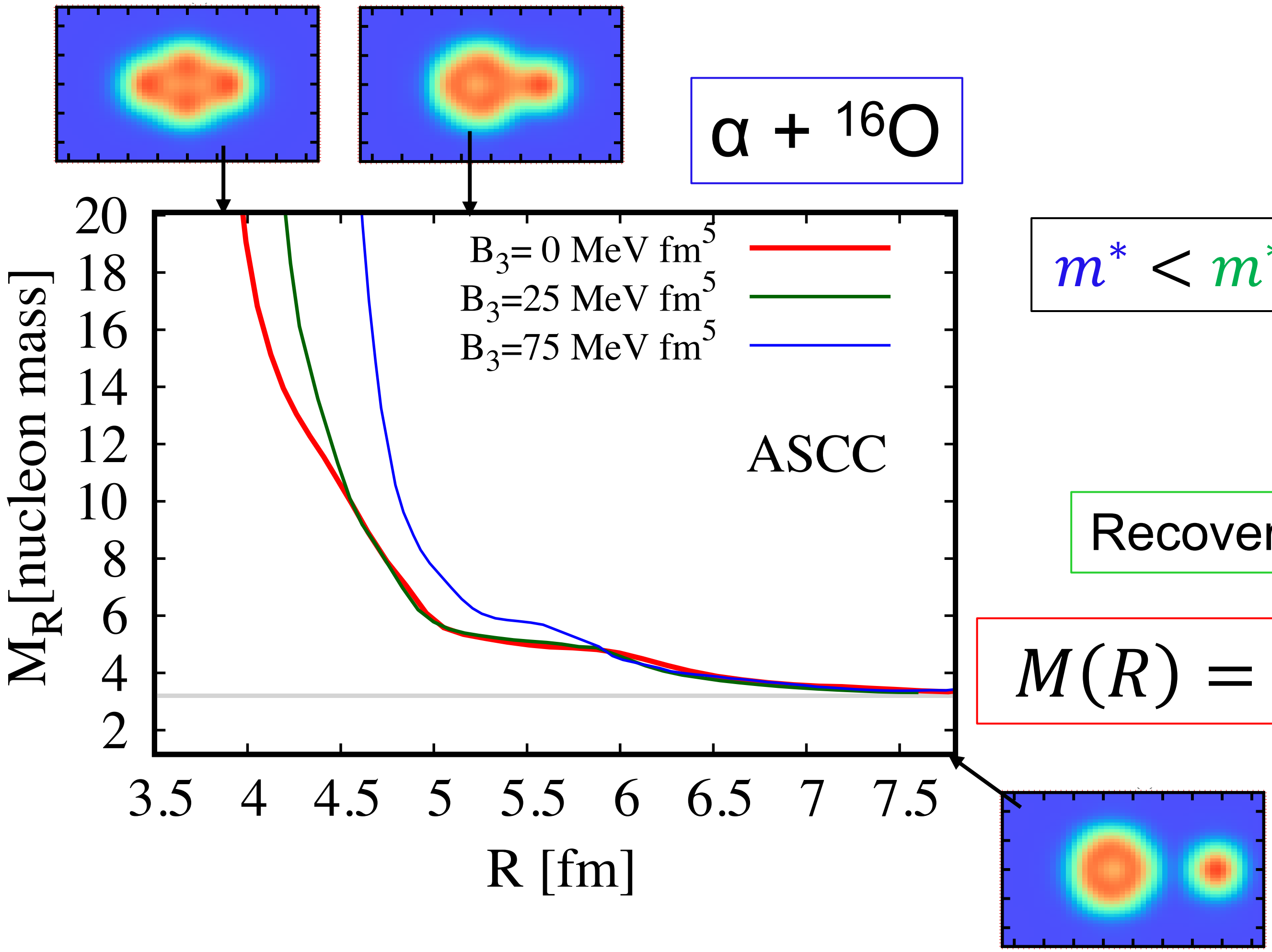
$$B_3 > 0 \quad \rightarrow \quad m^* < m$$

Effect of "effective mass"

- Velocity-dependent potential
- Nucleonic effective mass
  - $\frac{m^*}{m} \sim 0.7 - 0.8$
- Does this affect the inertial mass of nuclear reaction?
  - $\big(M(R), I(R)\big) \to (\mu_R, \mu_R R^2) \times \frac{m^*}{m}?,\ \text{at}\ R \to \infty$

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



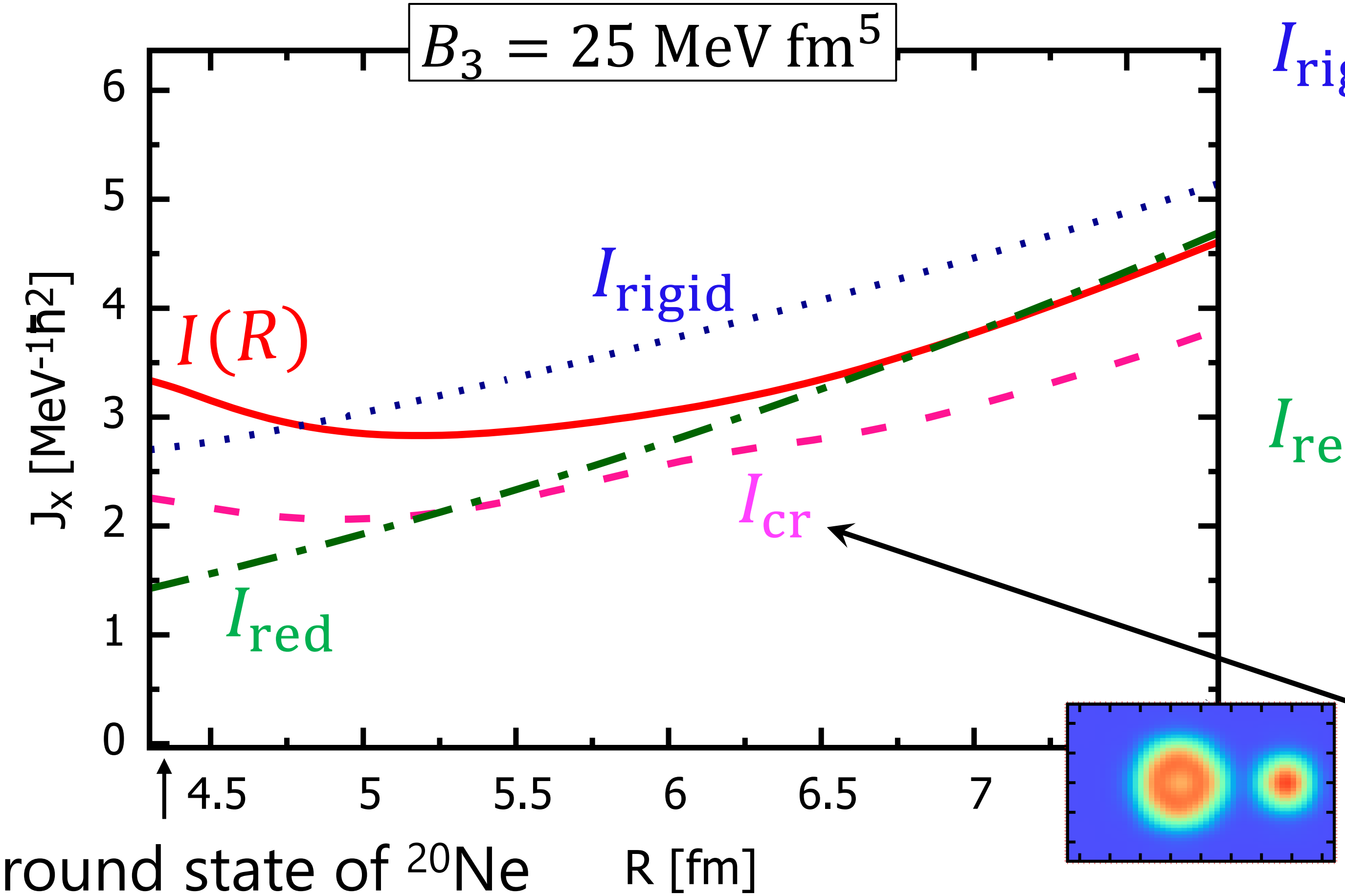


$m^* < m^* < m^* = m$

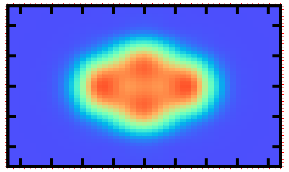
Recovery of the Galilean invariance !!

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

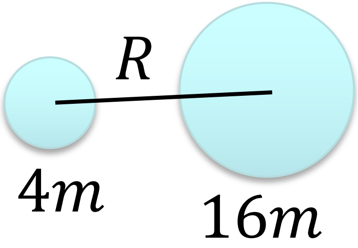
$I(R) \quad (m^*/m < 1)$



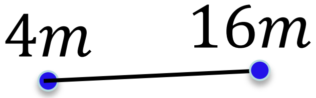
Ground state of ^{20}Ne



$$I_{\mathrm{rigid}} = \int \rho(\boldsymbol{r}) r_\perp^2 d\boldsymbol{r}$$



$I_{\mathrm{red}} = \mu_R R^2$ (Point-particle approx.)



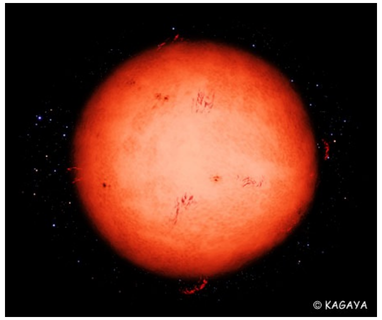
$$I_{\mathrm{cr}} = 2 \sum_{n\in p, j \in h} \frac{|\langle n|\hat{j}_x|j\rangle|^2}{e_n - e_j}$$

Smooth transition from I_{rigid} to I_{red}.

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

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

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

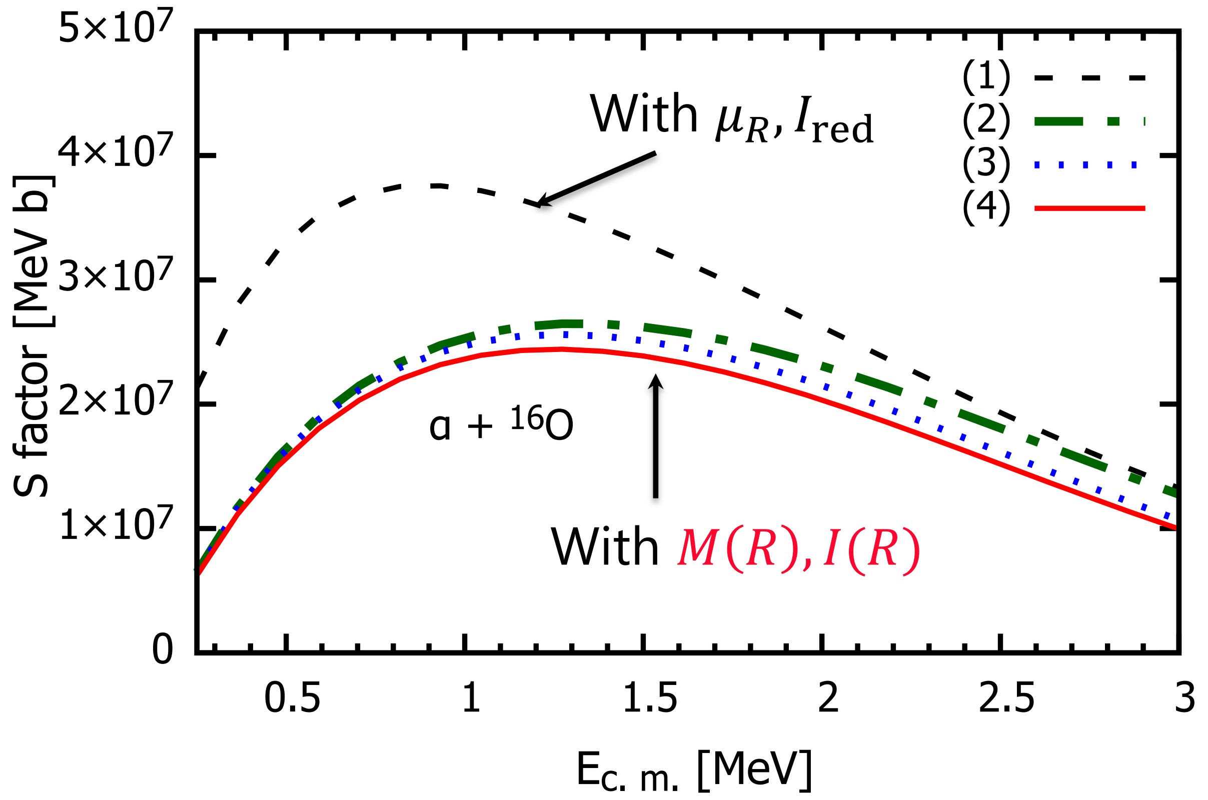


Synthesis of ^{20}Ne

Fusion reaction:
Astrophysical S-factor

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

$$B_3 = 25 \text{ MeV fm}^5$$



Torus quantization

- EBK quantization on invariant torus

$$\oint p_i dq^i = 2\pi\hbar \times k, \qquad k\text{: integer}$$

- Microscopic wave functions for eigenstates

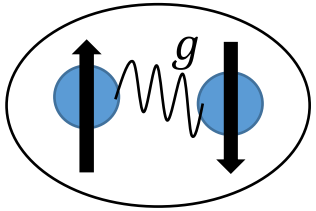
$$|\tilde{\psi}_k\rangle = \oint d\mu(Z_k)|Z_k\rangle e^{iT(Z_k)/\hbar}$$

$|Z_k\rangle$: (Generalized) Slater det. on the torus
$T(Z_k)$: Action
$\mu(Z_k)$: invariant measure

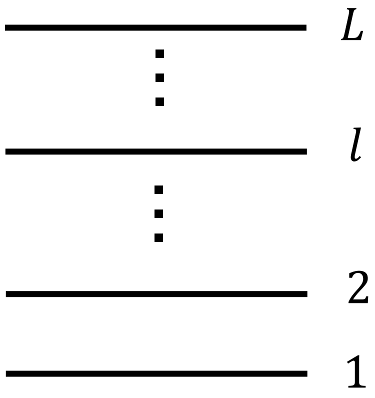
Pairing (Richardson) model

$$H = \sum_l \epsilon_l n_l - g S^+ S^- \qquad S^+ = \sum_l S_l^+ \qquad S^- = (S^+)^\dagger$$

$$\begin{cases} n_l = \sum_m a_{lm}^+ a_{lm} \\ S_l^+ = \sum_{m>0} a_{lm}^+ a_{l\bar{m}}^+ \end{cases}$$



$J = 0$



L s.p. level system

- TDHFB dynamics

$$\begin{cases} \dot{\chi}^\alpha = \dfrac{\partial \mathcal{H}}{\partial j_\alpha} \\ \dot{j}_\alpha = -\dfrac{\partial \mathcal{H}}{\partial \chi^\alpha} \end{cases}$$

$$|Z(t)\rangle = \prod_\alpha \frac{1}{(1 + |Z_\alpha(t)|^2)^{S_\alpha}} e^{Z_\alpha(t) S_\alpha^+} |0\rangle$$

$$Z_\alpha \to (\chi^\alpha, j_\alpha) \qquad \langle Z|H|Z\rangle = \mathcal{H}\big(\chi(t), j(t)\big)$$

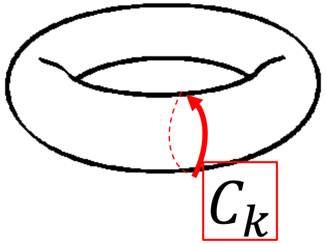
Tow-level pairing model is integrable.
Conserved quantities: *E* and *N*

Stationary phase approximation (SPA) for Integrable systems

Kuratsuji, Suzuki, PLB 92, 19 (1980)
Kuratsuji, PTP 65, 224 (1981)
Suzuki, Mizobuchi PTP 79, 480 (1988)

Ni and TN, PRC **97**, 044310 (2018)

Separable with invariant tori

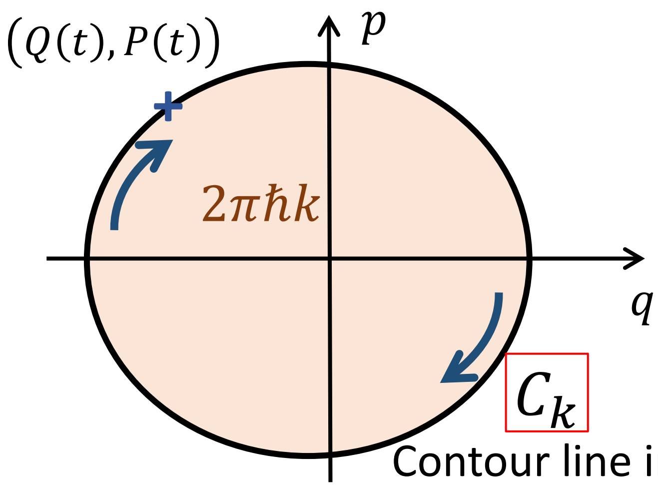


$$|\tilde{\psi}_k\rangle = \oint d\mu(Z_k)|Z_k\rangle e^{iT(Z_k)/\hbar}$$

Integration over a closed trajectory on invariant tori

No diagonalization (variation) involved

2D Phase space



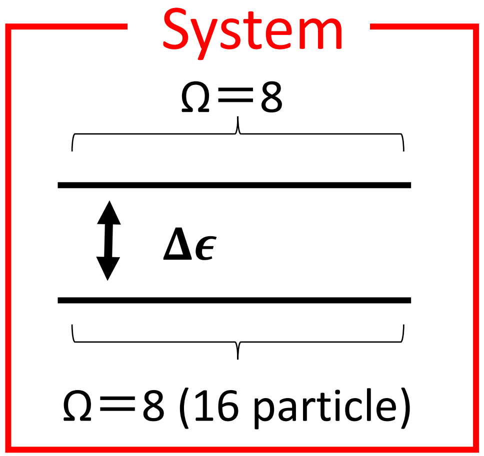
Contour line in k-th excited energy E_k

- EBK quantization condition

$$T_\circ = \oint_{C_k} \langle Z(t')|i\hbar\frac{\partial}{\partial t'}|Z(t')\rangle dt' = \oint_{C_k} \sum_\alpha p_\alpha dq^\alpha = 2\pi\hbar k$$

k: integer

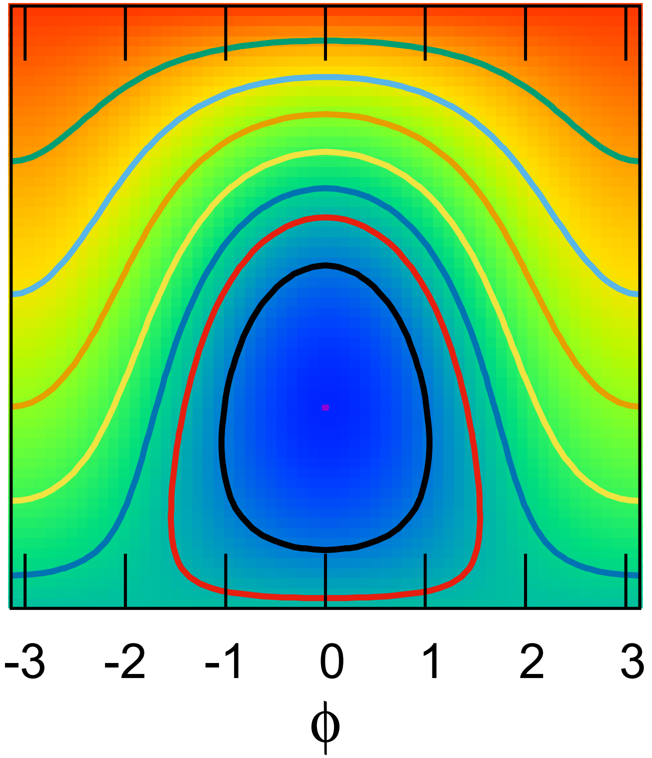
Two-level pairing model



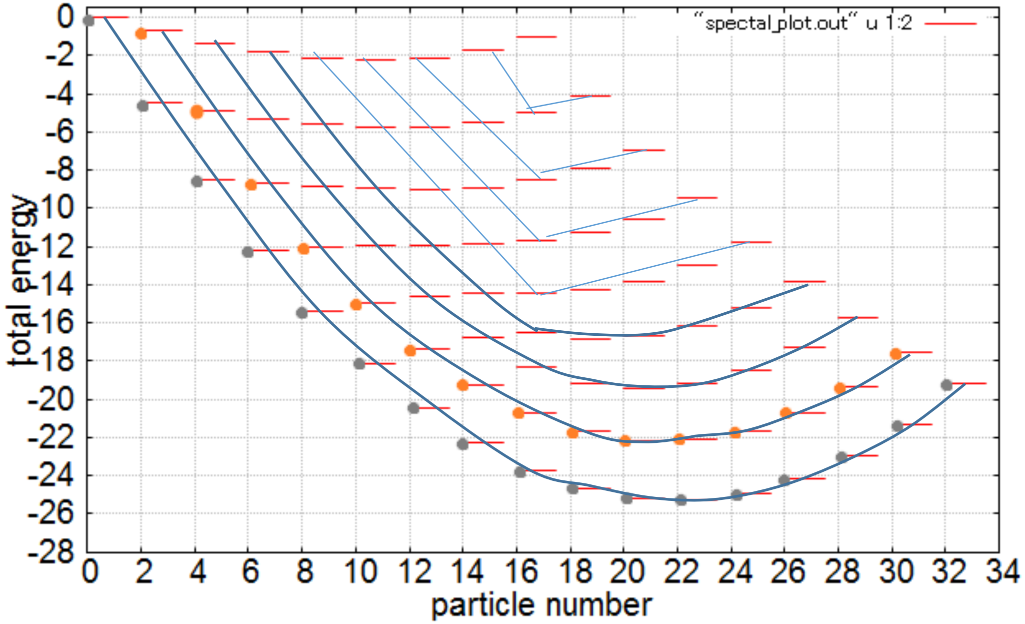
The system is integrable with two sets of *separable* canonical variables: $(N/2, \Phi)$ and (j, ϕ)

$\Phi = \frac{1}{2}(\chi_1 + \chi_2)$: Gauge angle

$\phi = \chi_2 - \chi_1$: Relative angle

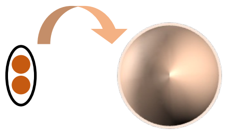


in units of $\Delta\varepsilon$



Ni and TN, PRC **97**, 044310 (2018)

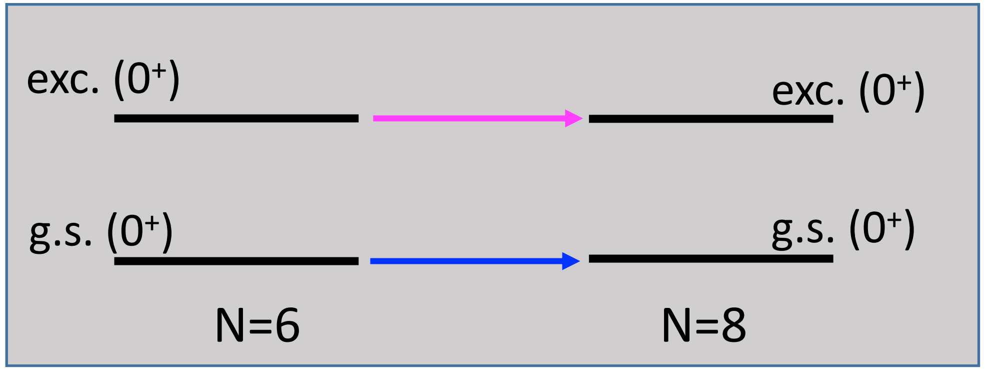
Two-level pairing model

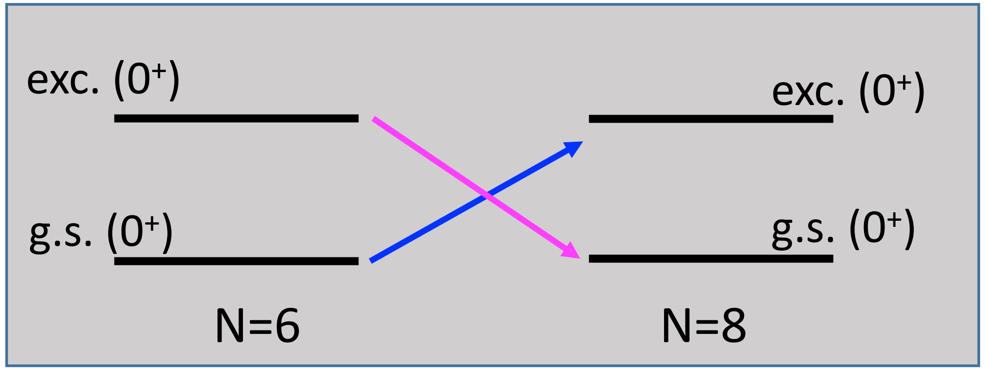


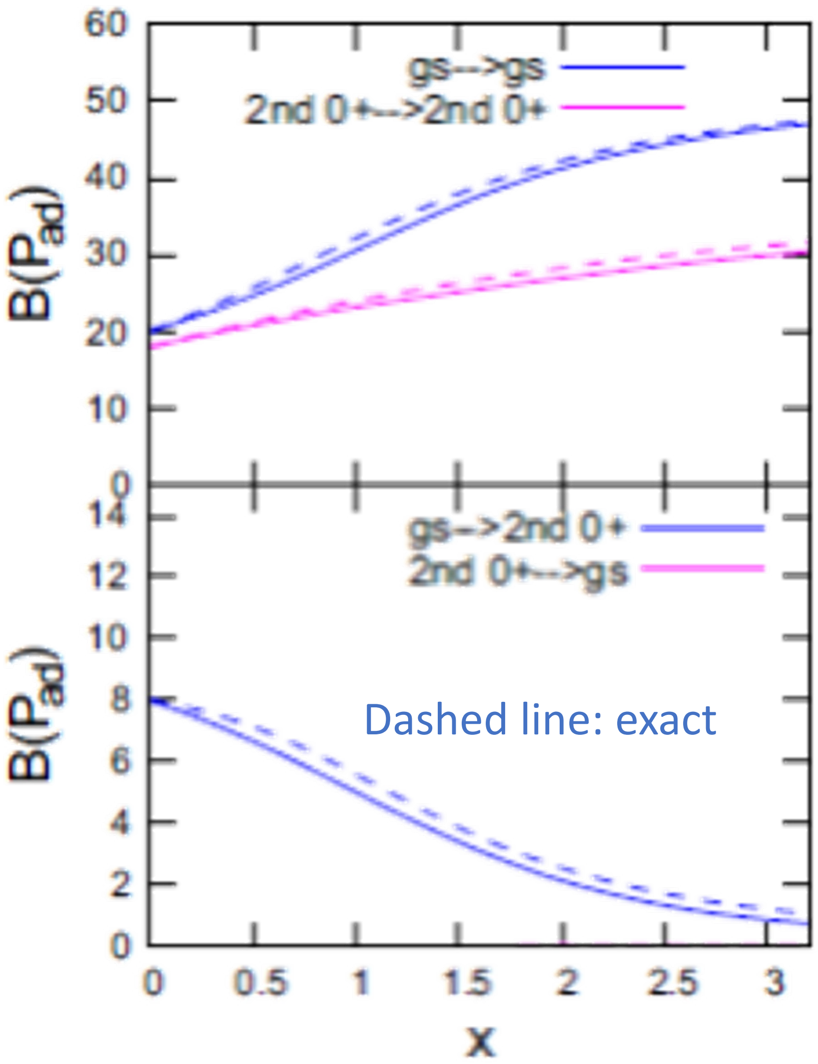
$x = 2g\Omega/\Delta\varepsilon$

- Pair-additional transition

  $B(P_{ad}) = |\langle N = 8, \alpha|S_+|N = 6, \beta\rangle|^2$







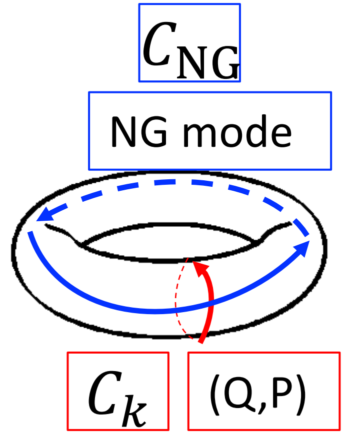
Excellent agreement with exact cal.

ASCC + SPA for non-integrable systems

Find a 2D collective subspace

Pair rotation d.o.f. $\left(\phi, \frac{N}{2}\right)$ (NG modes)

Pair vibration d.o.f. (Q, P).



<u>EBK quantization and a wave function of a collective state</u>

$$\boxed{\frac{N}{2}\pi\hbar + \oint_{C_k} \langle Z(t')| i\hbar \frac{\partial}{\partial t'} |Z(t')\rangle dt' = 2\pi\hbar k}$$

- A closed trajectory C_{NG} automatically leads to the number projection
- A closed trajectory C_k gives an energy E_k and a wave function, $|\tilde{\psi}_k\rangle$

$$|\tilde{\psi}_k\rangle = \oiint_{C_{NG}+C_k} d\mu(Z_k)|Z_k\rangle e^{iT(Z_k)/\hbar}$$

Neutron pairing vibrations in Pb isotopes

Ni, Hinohara, TN, PRC **98**, 064327 (2018)

Neutron pairing vibrations in N-deficient Pb isotopes

Input:

126

Neutron

s.p. level	Energy (MeV)
p1/2	-7.45
f5/2	-8.16
p3/2	-8.44
i13/2	-8.74
f7/2	-10.69
h9/2	-10.94

82

- $g = 0.138$ (MeV) is adopted so as to reproduce experimental pairing gap of $^{192}\mathrm{Pb}$ in three-point formula

$$H = \sum_{l} \epsilon_l n_l - g S^+ S^-$$

- Results: Excitation energy of $|0_2^+\rangle$

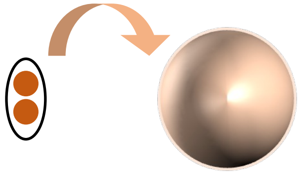
	Exact	**ASCC+SPA**
$^{188}\mathbf{Pb}$	2.44	2.31
$^{190}\mathbf{Pb}$	2.34	2.21
$^{192}\mathbf{Pb}$	2.25	2.12
$^{194}\mathbf{Pb}$	2.2	2.04

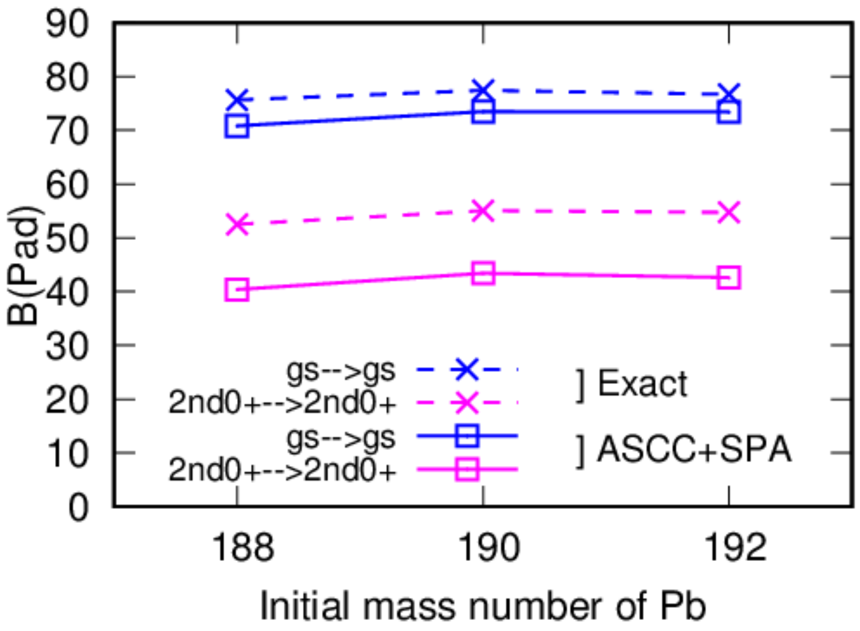
Pair transfer transition strengths

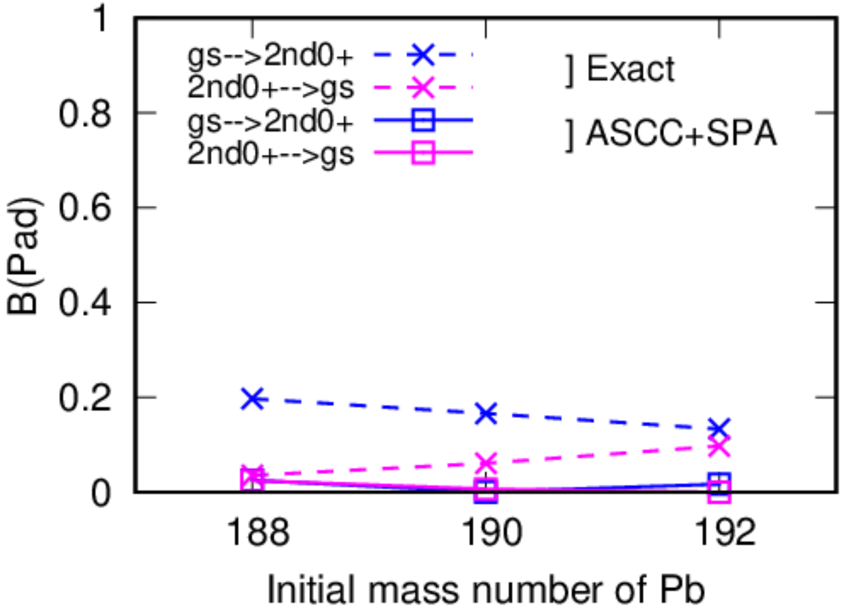
Ni, Hinohara, TN, PRC **98**, 064327 (2018)

- Two-neutron additional transition

$$B(Pad) = \left|\langle {}^{A+2}\mathrm{Pb}, \alpha \middle| S_+ \middle| {}^{A}\mathrm{Pb}, \beta \rangle\right|^2$$







For $|0_2^+\rangle \rightarrow |0_2^+\rangle$, 20% smaller than exact solution.

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
- Application to nuclear reaction
  - Finding a reaction path & construct a collective Hamiltonian
  - Quantum tunneling in many-body systems
- Application to nuclear pairing problems
  - Torus quantization to produce wave functions of energy eigenstates
  - An alternative to GCM, without Hamiltonian matrix diagonalization