

Nuclear reaction path and inertial mass in the self-consistent collective coordinate method

Kai Wen

Takashi Nakatsukasa



*Center for Computational Sciences,
University of Tsukuba*



INPC2016, Adelaide, Australia, September 11-16, 2016

This work was supported in part by ImPACT Program of Council for Science, Technology and Innovation (Cabinet Office, Government of Japan).

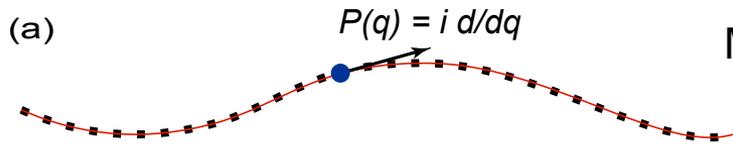
Contents

- Large amplitude collective motion
 - Determination of optimal reaction path
 - “Macroscopic” quantities (potential, mass)
 - ASCC method
- Reaction path, potential, and inertial mass
 - Symmetric reaction: ${}^8\text{Be} \leftrightarrow \alpha + \alpha$
 - Symmetric reaction: ${}^{32}\text{S} \leftrightarrow {}^{16}\text{O} + {}^{16}\text{O}$
 - Asymmetric reaction: ${}^{20}\text{Ne} \leftrightarrow {}^{16}\text{O} + \alpha$

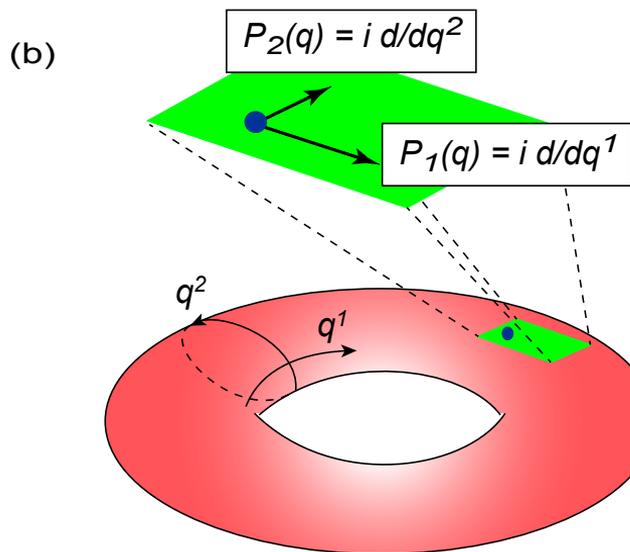
Microscopic determination of reaction path

- RGM
 - Assuming the “cluster configurations”
- GCM
 - Assuming the “generator coordinates”
- TDHF
 - An initial state produces a reaction path.
 - Not applicable to sub-barrier reaction.

Adiabatic Self-consistent Collective Coordinate (ASCC) method



Matsuo, Nakatsukasa, Matsuyanagi, PTP 103, 959 (2000)



Generators for canonical variables (q,p) are self-consistently constructed.

Collective submanifold spanned by (q,p) are determined.

ASCC method

Matsuo, Nakatsukasa, Matsuyanagi, PTP 103, 959 (2000) “Moving mean-field equation”

$$(0\text{th}) \quad \delta \langle \Psi(q) | \hat{H}_M(q) | \Psi(q) \rangle = 0, \quad \hat{H}_M(q) \equiv \hat{H} - (\partial V / \partial q) \hat{Q}(q)$$

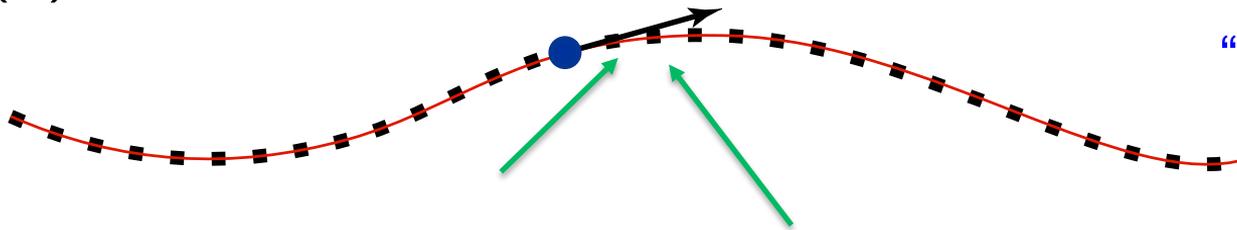
$$(1\text{st}) \quad \delta \langle \Psi(q) | [\hat{H}_M(q), i\hat{Q}(q)] - B(q)\hat{P}(q) | \Psi(q) \rangle = 0$$

$$(2\text{nd}) \quad \delta \langle \Psi(q) | [\hat{H}_M(q), \hat{P}(q)/i] - C(q)\hat{Q}(q)$$

$$- \frac{1}{2B(q)} \left[[\hat{H}_M(q), (\partial V / \partial q) \hat{Q}(q)], \hat{Q}(q) \right] | \Psi(q) \rangle = 0$$

(a)

$$P(q) = i d/dq$$



“Moving RPA equation”

Collective Hamiltonian

Identification of collective canonical variables; (q,p)

Determination of the optimal reaction path

Determination of collective mass

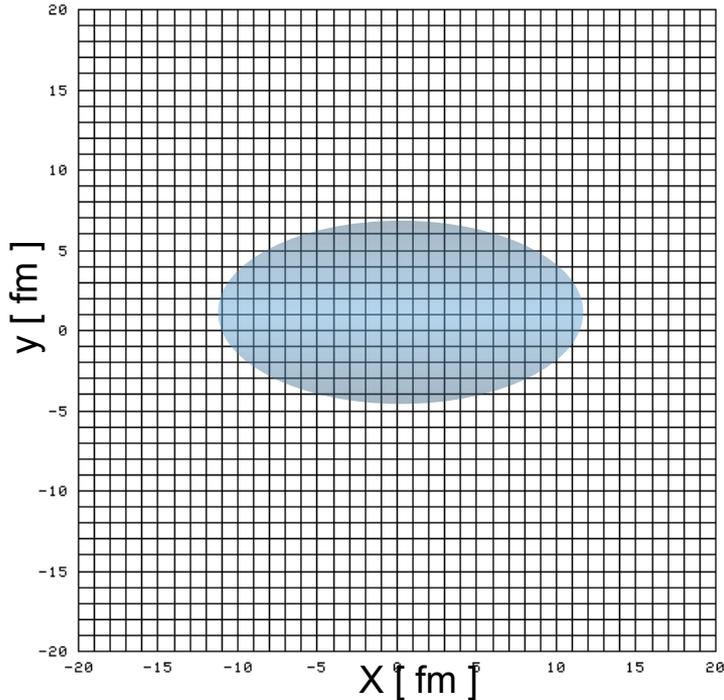
Construction of a collective Hamiltonian

$$H(q,p) = \langle \Psi(q,p) | \hat{H} | \Psi(q,p) \rangle \approx \frac{1}{2} B(q) p^2 + V(q)$$

$$V(q) = \langle \Psi(q) | \hat{H} | \Psi(q) \rangle, \quad B(q) = \langle \Psi(q) | \left[[\hat{H}, \hat{Q}(q)], \hat{Q}(q) \right] | \Psi(q) \rangle$$

Coordinate transformation; $(q,p) \rightarrow (R,P)$

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, Nakatsukasa, arXiv: 1608.02294

Wen, Washiyama, Ni, Nakatsukasa,
Acta Phys. Pol. B Proc. Suppl. 8, 637 (2015)

^8Be : Canonical generators

of the axial symmetry of the ground state
tion about the symmetry axis (z axis)
pear. In Fig. 2 the calculation produces
modes of excitation around 2.8 MeV with
tion matrix element of the $K = 1$ quadr
 $\hat{Q}_{2\pm 1} \equiv \int r^2 Y_{2\pm 1}(\hat{r}) \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) d\vec{r}$. The
these rotational modes comes from the
discretizing the space. Besides these fi
the lowest mode of excitation turns out t

$$\rho(r)$$

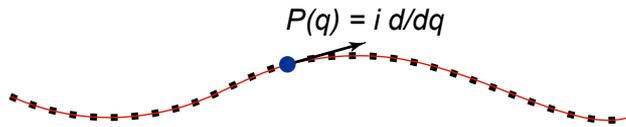


$$\delta\rho(r)$$



^8Be : Collective potential

- $V(q) = \Psi(q) H \Psi(q)$



▪
▪
▪

distance $R \equiv \langle \psi(q) | R | \psi(q) \rangle$ with Eq. shows the obtained potential energy along a collective path. As a reference, we also show the Coulomb potential between two α particles, $4e^2/R + 2E_\alpha$, where E_α is the calculated energy of the isolated α particle. As the two α 's get closer, the potential starts to deviate from the pure Coulomb potential at $R < 6$ fm and finally

^8Be : Collective inertial mass

$$k^2(R) = 2M(R) \left\{ E \right.$$

$$k_c^2(R) = 4m \left\{ E - \frac{4}{R} \right.$$

where $k(R)$ and $k_c(R)$ a radial motion with and v

distance $R \equiv \langle \psi(q) | R | \psi(q) \rangle$ with Eq. shows the obtained potential energy a collective path. As a reference, we also Coulomb potential between two α parti R , $4e^2/R + 2E_\alpha$, where E_α is the calculat energy of the isolated α particle. Appar totically approaches the pure Coulomb p α 's get closer, the potential starts to d Coulomb potential at $R < 6$ fm and fin

Reduced
mass

$\alpha + \alpha$ scattering (phase shift)

$$k^2(R) = 2M(R) \left\{ E - V(R) - \frac{(L+1/2)^2}{4R^2} \right\}$$

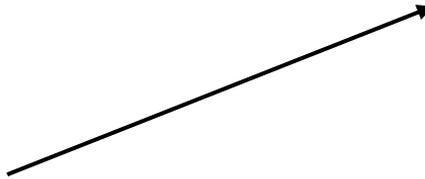
Nuclear phase shift

$$k_c^2(R) = 4m \left\{ E - \frac{4e^2}{R} - \frac{(L+1/2)^2}{4mR^2} \right\}$$

where $k(R)$ and $k_c(R)$ are the wave radial motion with and without the n

Dashed: Constant reduced mass

($M(R) \rightarrow 2m$)



^8Be : CHF+Cranking

larger than the BSCU inertia. The s
perturbative and perturbative cranking
are significantly different. For instance,
with \hat{Q}_{20} constraint suggest prominent
in $M_{\text{cr}}^{\text{NP(P)}}(R)$. However, the peak po
different. It should be noted that the
should not be generalized to other energ
tionals, because the BKN interaction h
mean fields.

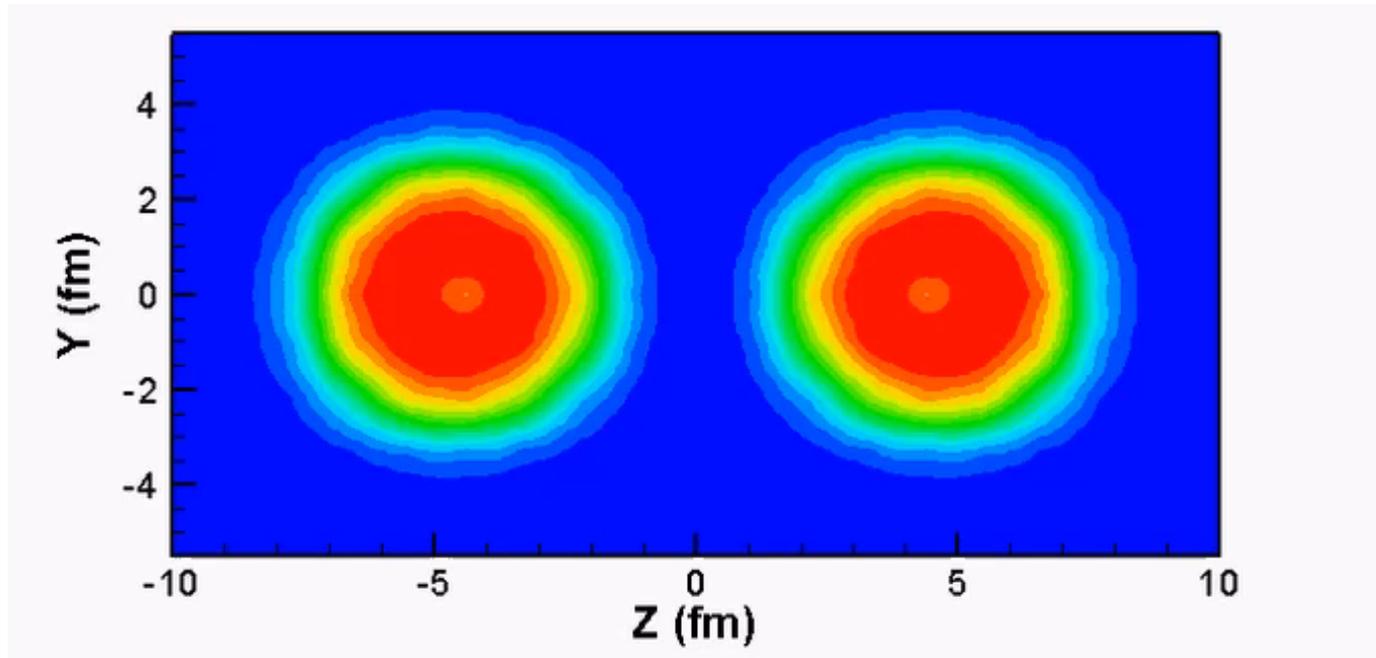
Perturbative cranking formula

Cranking formula for translational mass

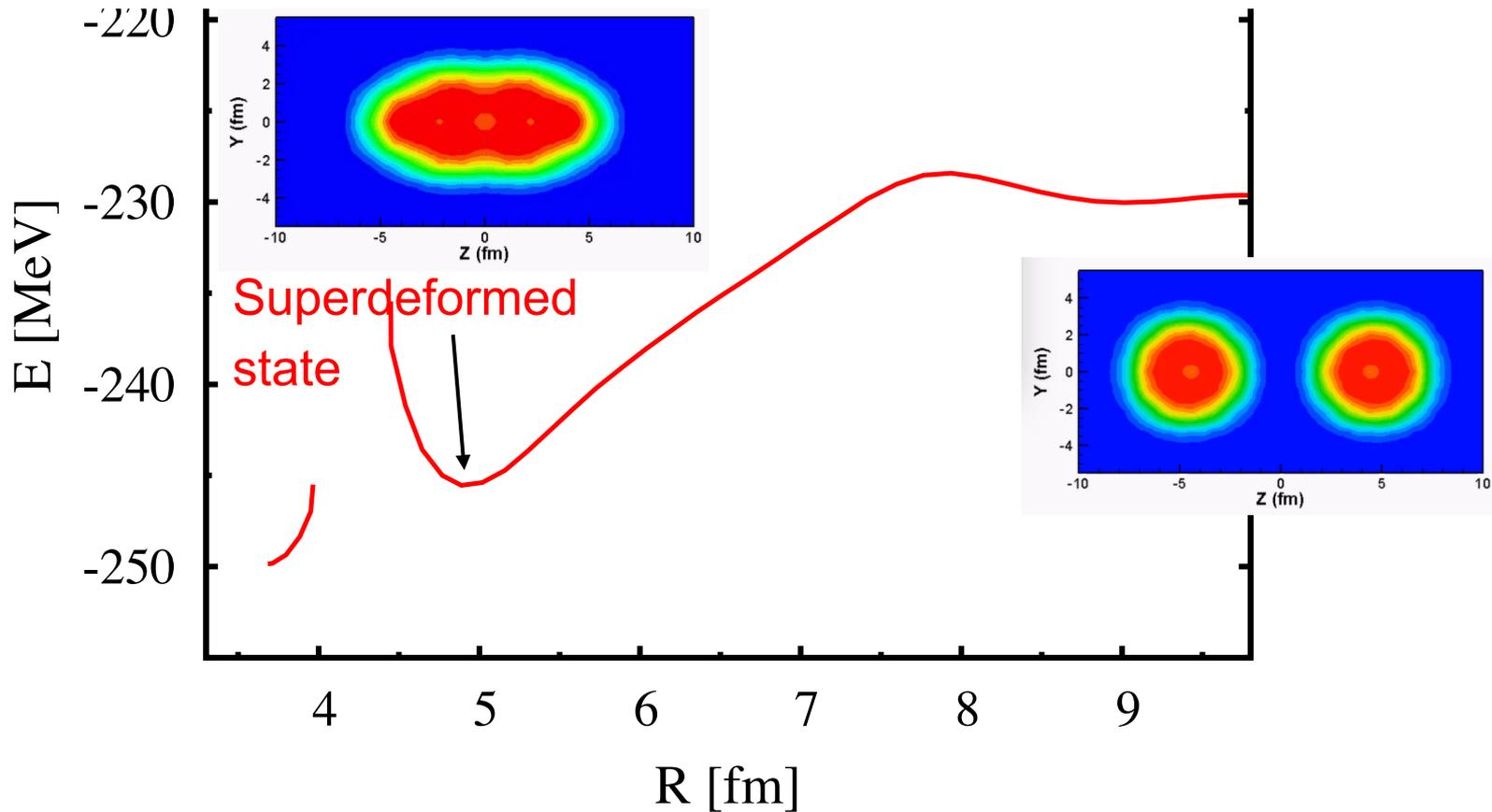
e.g.) $M \downarrow \alpha = 3.1 m$ for $E \downarrow \text{BKN} [\rho] + B(\rho\tau - j \uparrow 2)$ with $B = 50 \text{ MeV fm}^5$

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

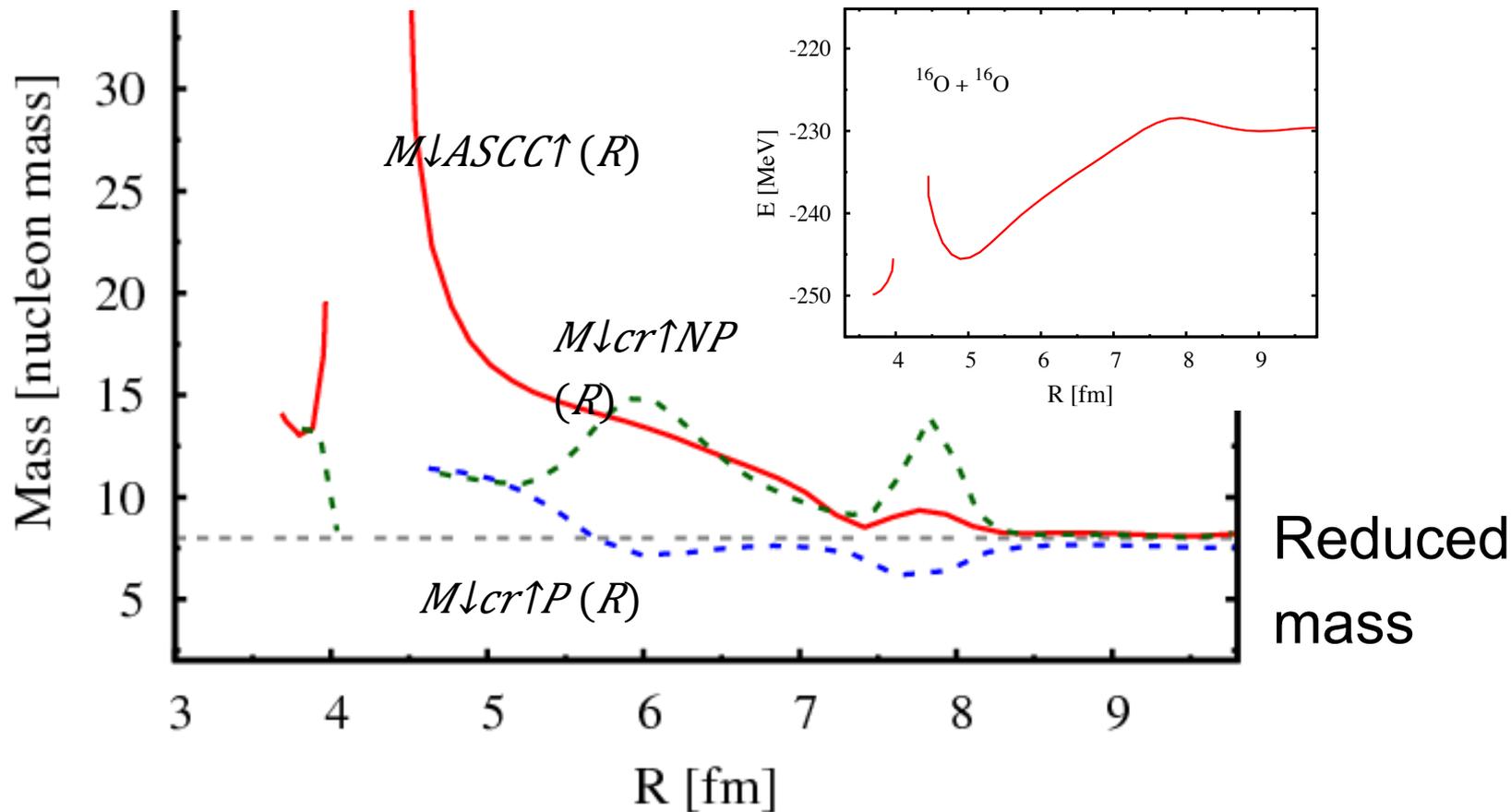
Starting from two ^{16}O configuration



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

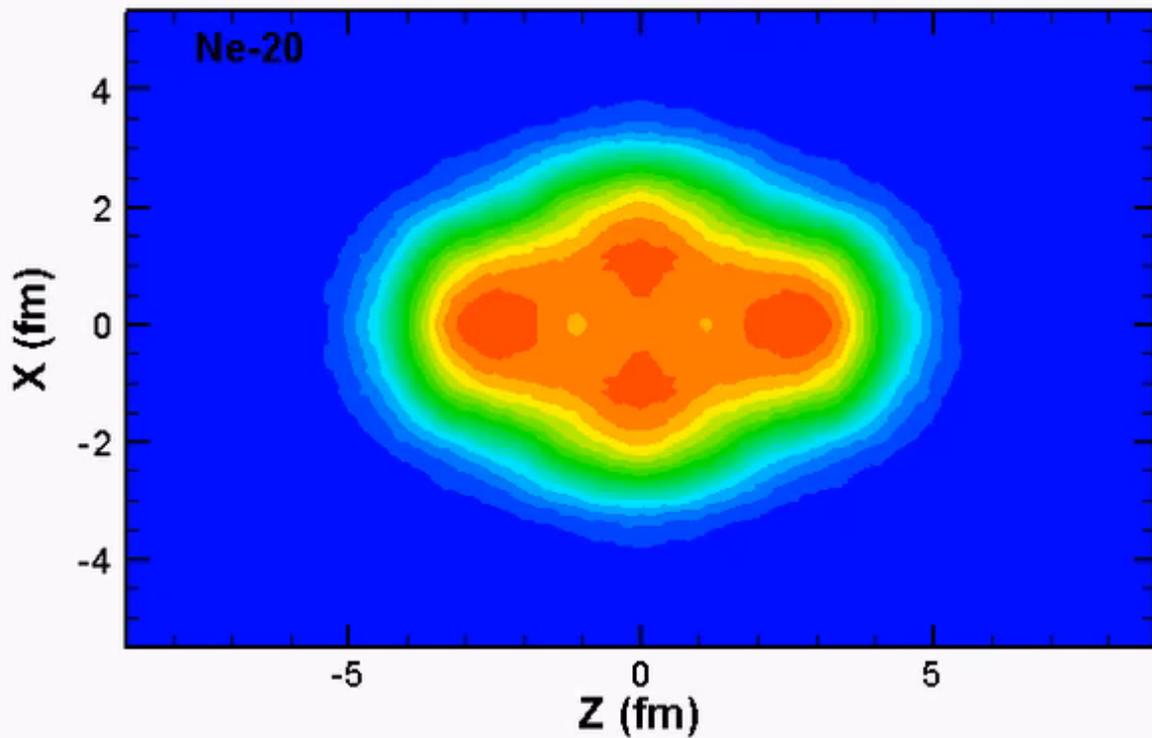


$^{16}\text{O} + ^{16}\text{O} \rightarrow ^{32}\text{S}$: Collective mass



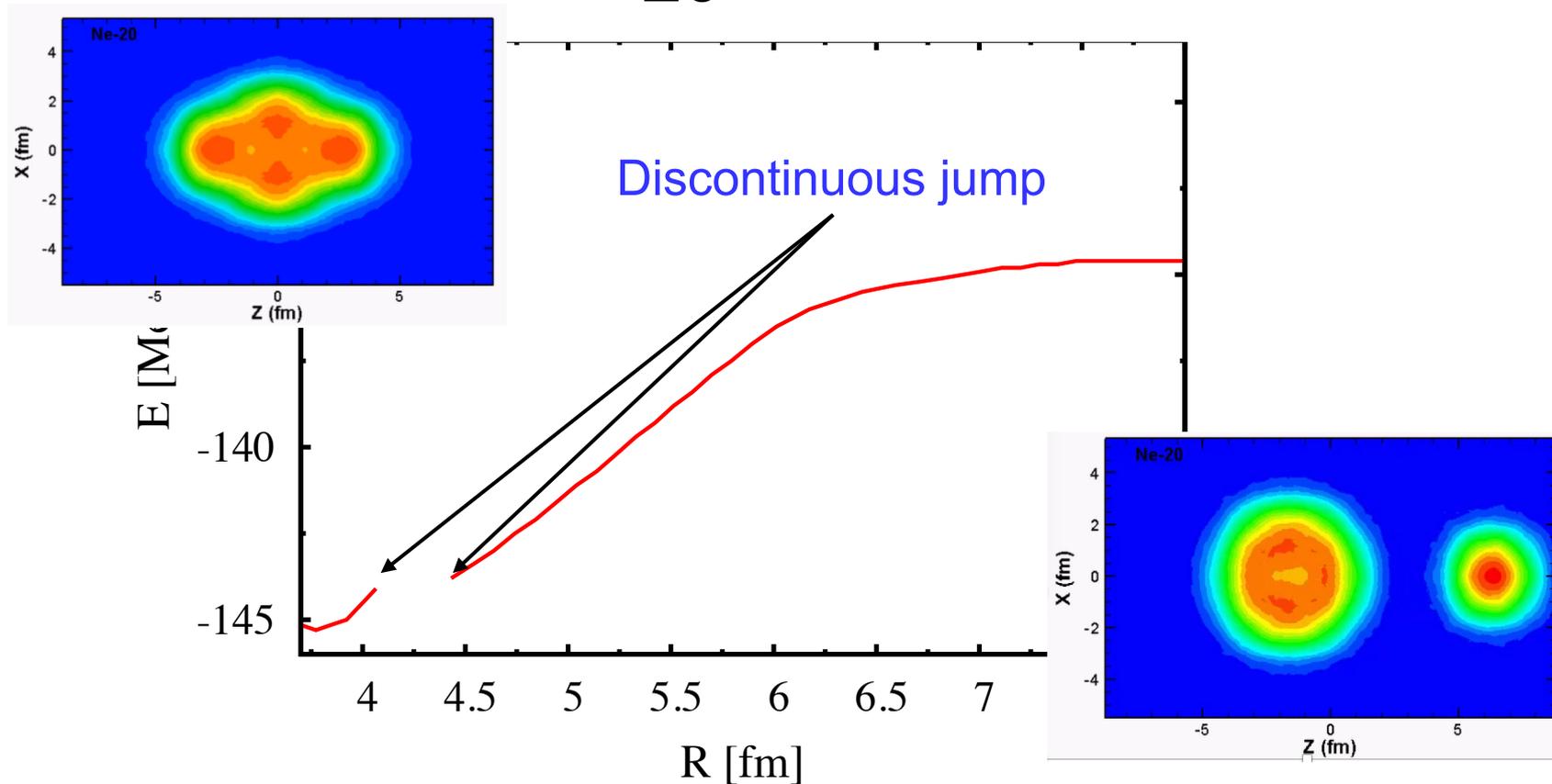
^{20}Ne : Reaction path

Starting from the ground state of ^{20}Ne

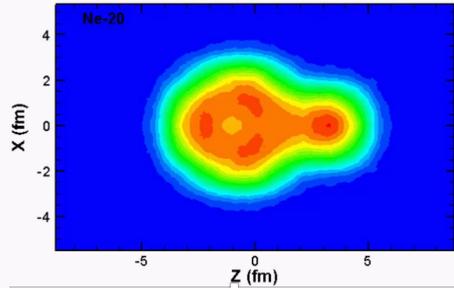
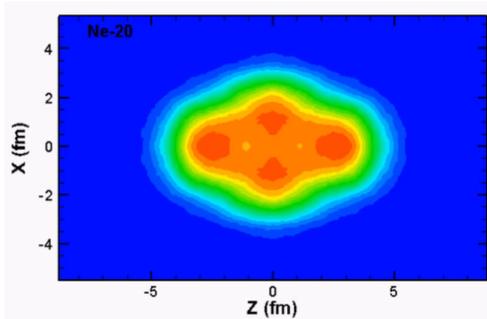


The final state automatically becomes $^{16}\text{O} + \alpha$

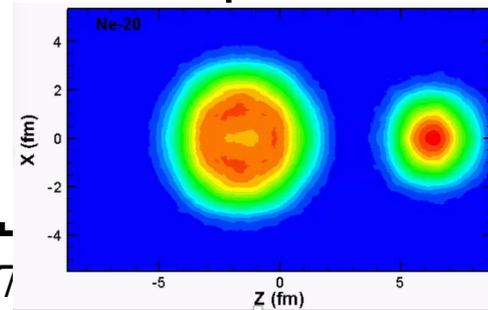
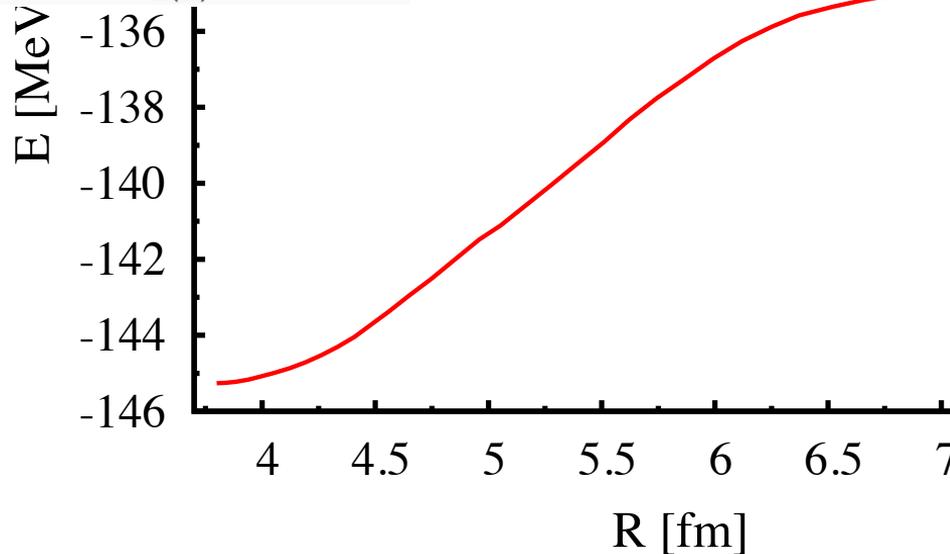
^{20}Ne : r^2Y_{20} -constrained cal.



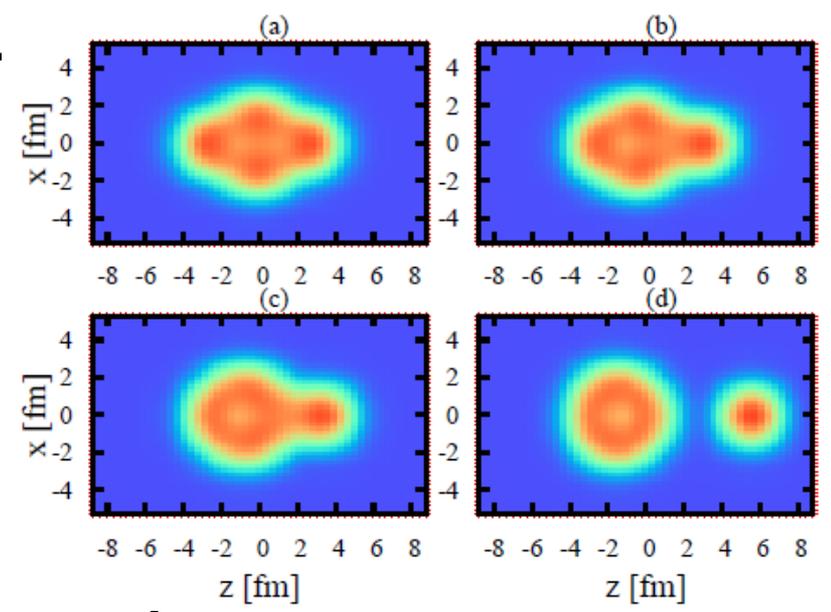
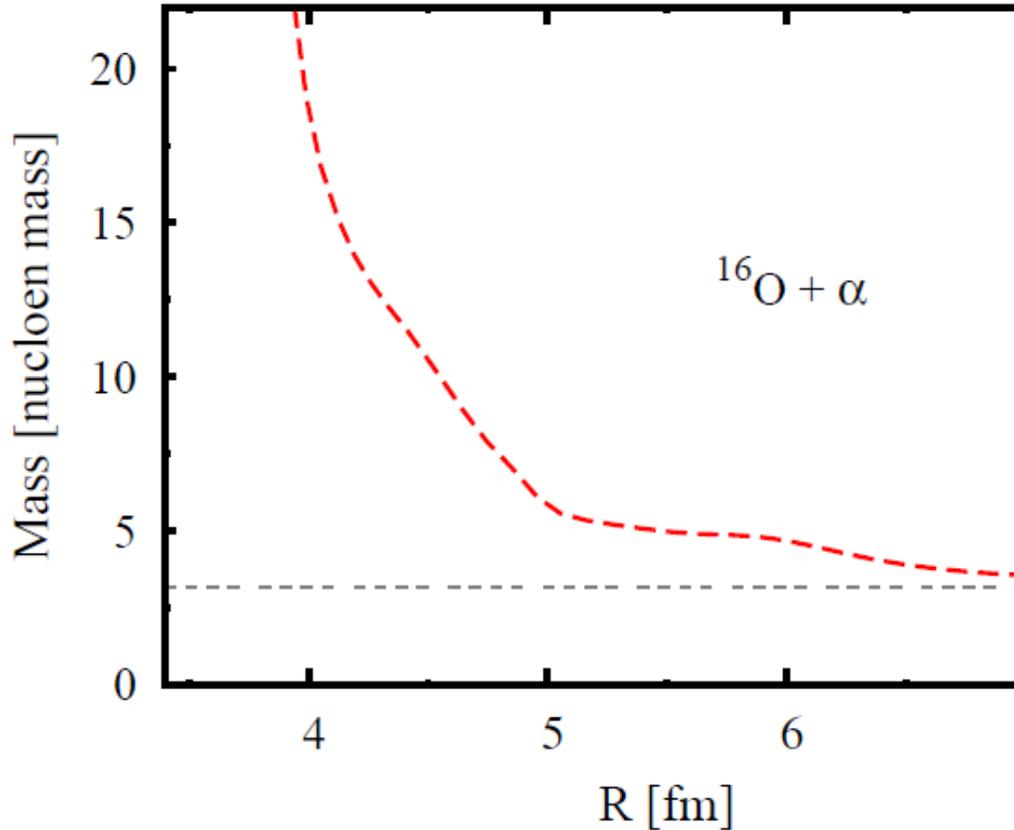
^{20}Ne : Collective potential



Continuous curve
without a jump



^{20}Ne : Collective inertial mass

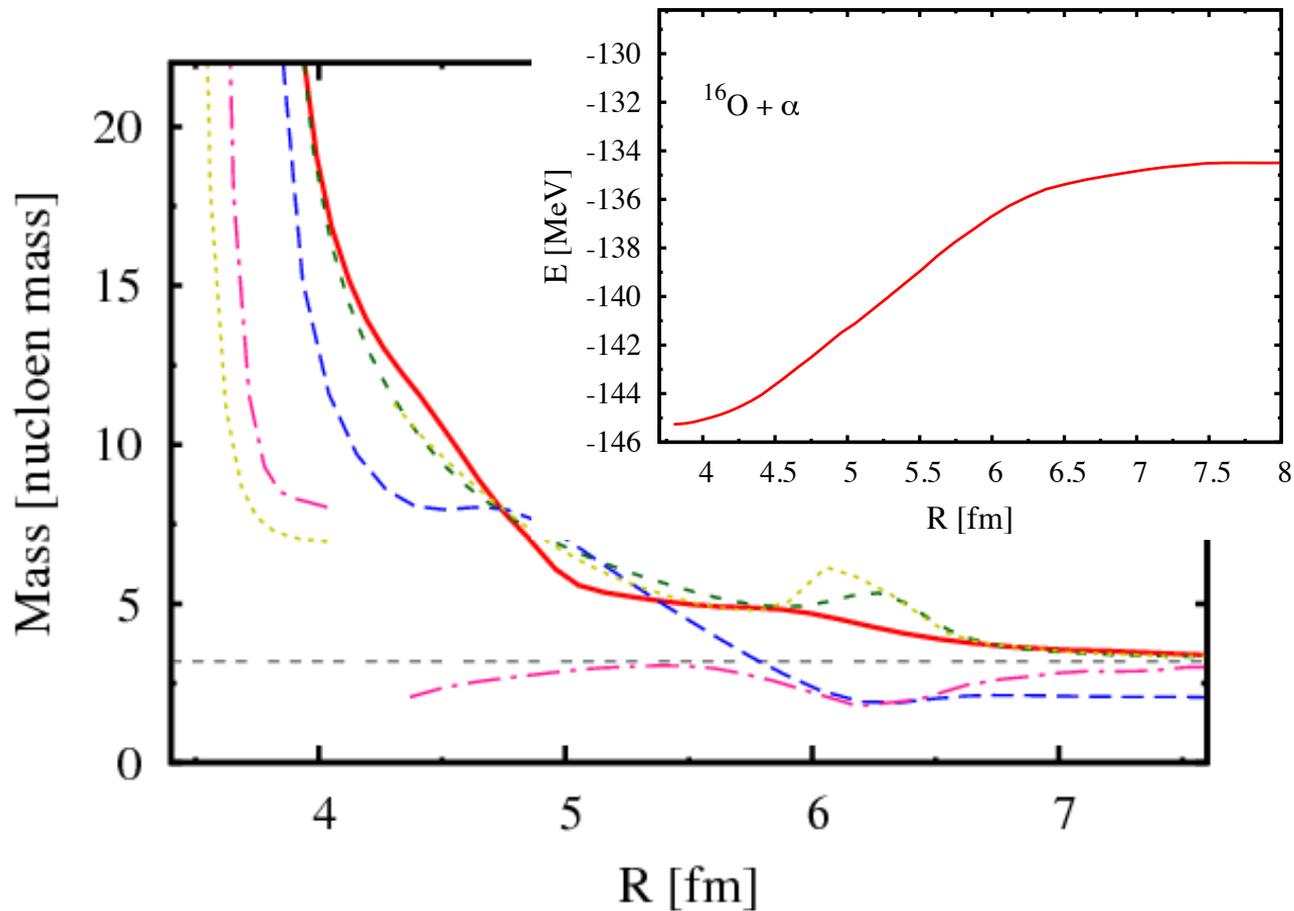


Reduced mass
for $^{16}\text{O} + \alpha$

Summary

- Reaction path and inertial mass
 - Scattering/fusion/fission reaction
 - Determination of the reaction path
 - Inertial mass with proper account of time-odd effects (different from the cranking/GOA inertia)
- Applications
 - Symmetric mode: $\alpha + \alpha \leftrightarrow {}^8\text{Be}$
 - Reaction path: Quadrupole vib. into rel. motion between two α 's
 - Symmetric mode: ${}^{16}\text{O} + {}^{16}\text{O} \leftrightarrow {}^{32}\text{S}(\text{SD})$
 - Reaction path: Two ${}^{16}\text{O}$'s into the superdeformed ${}^{32}\text{S}$
 - Asymmetric mode: ${}^{20}\text{Ne} \leftrightarrow {}^{16}\text{O} + \alpha$
 - Reaction path: Octupole vib. into ${}^{16}\text{O} + \alpha$

^{20}Ne : Collective inertial mass



Constrained Hartree-Fock + cranking inertial mass

larger than the ASOC inertia. The self-consistent and perturbative cranking results are significantly different. For instance, the results with \hat{Q}_{20} constraint suggest prominent peaks in $M_{cr}^{NP(P)}(R)$. However, the peak positions are quite different. It should be noted that the results should not be generalized to other energy functionals, because the BKN interaction has different mean fields.

ATDHF method

(Goeke, Gruemmer, Reinhard

1983) Inertial mass increases drastically. This is due to the result of the former calculation. The reason of which is currently under investigation. We encounter a difficulty to obtain the collective inertia in the asymptotic region at large R . A larger and finer mesh size seems to be needed to obtain the inertia in the asymptotic region and to reproduce the mass $2m$. We should also mention that the calculation with $dV/dR = 0$ is extremely difficult to

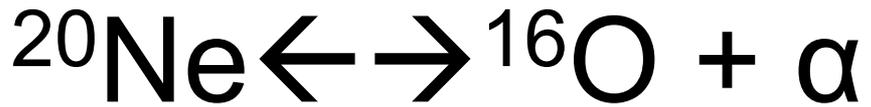
Translational motion of α particle

Dipole
Quadrupole
Monopole

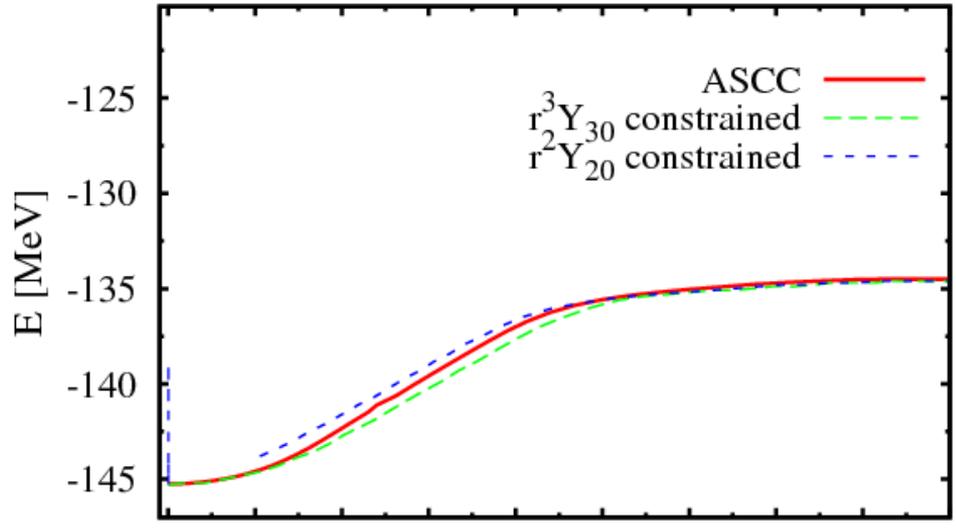
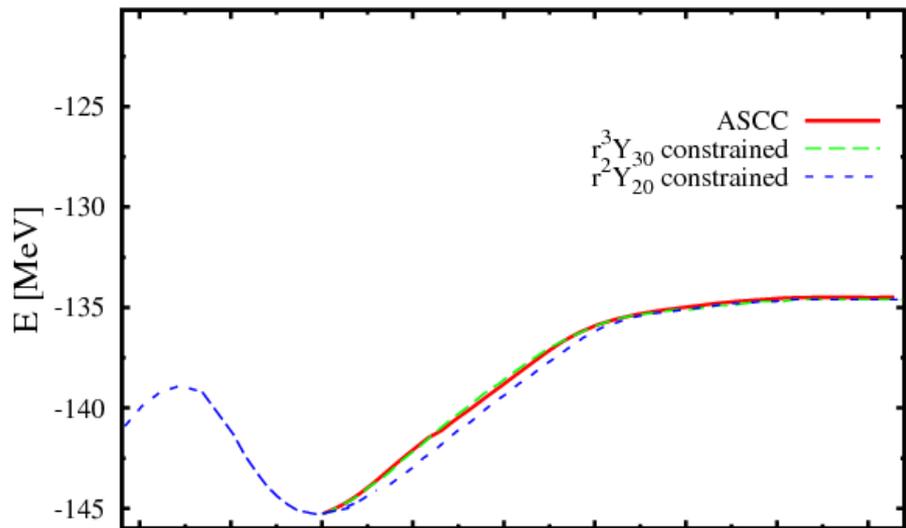
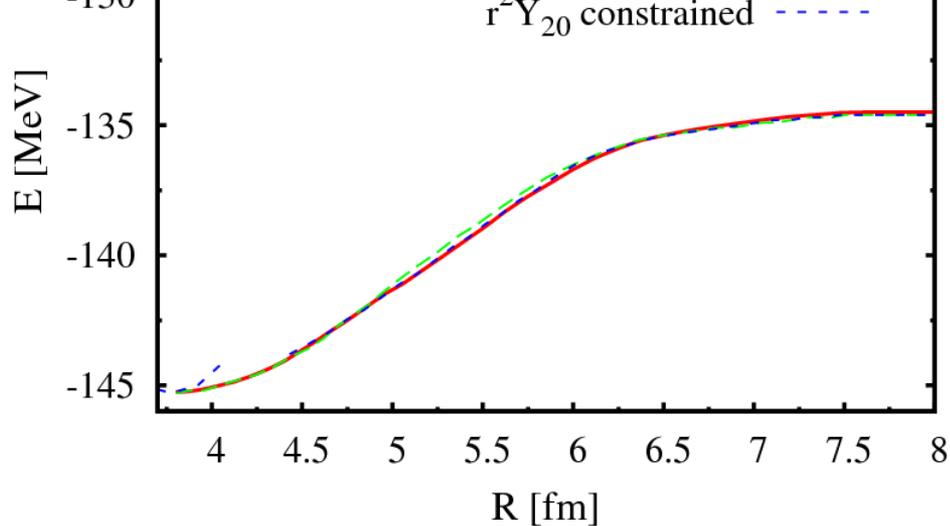
which is degenerated with the other modes along the x and y axis at about the calculation of Fig. (1) the space is discretized equal to 0.8 fm. With finer mesh size translational motion approaches to the compact nature of alpha particle, the energy is 20 MeV higher than these translational

can be picked out with non-zero values which is degenerated with the other modes along the x and y axis at about the calculation of Fig. (1) the space is discretized equal to 0.8 fm. With finer mesh size translational motion approaches to the compact nature of alpha particle, the energy is 20 MeV higher than these translational

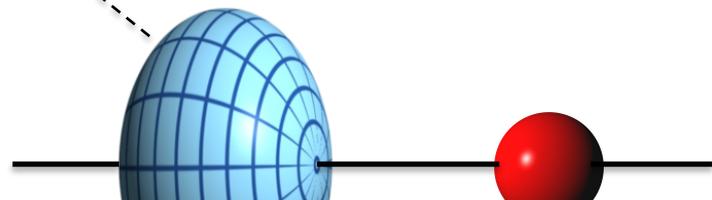
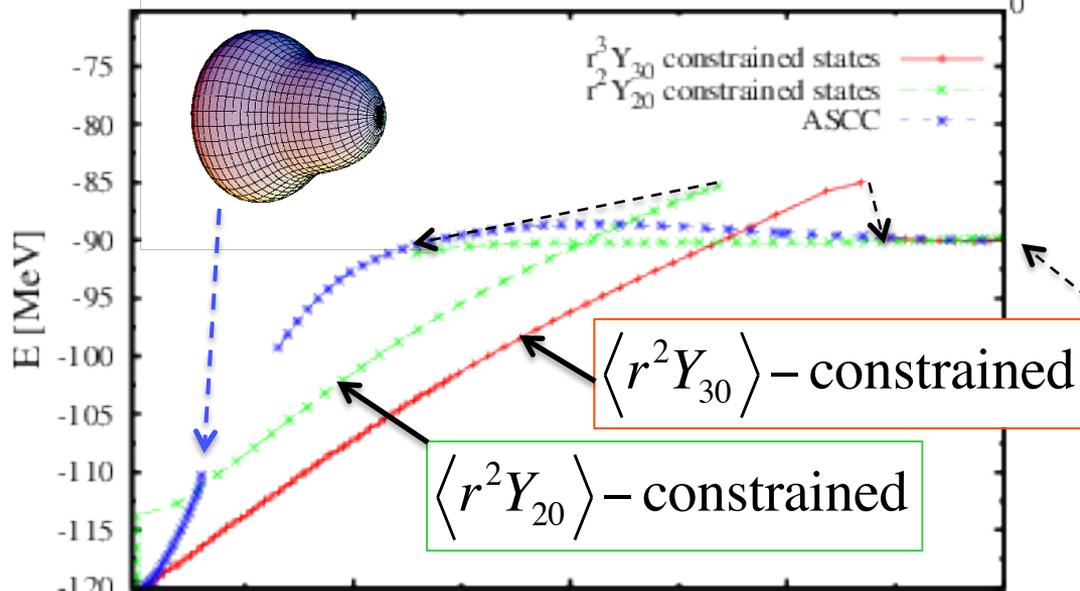
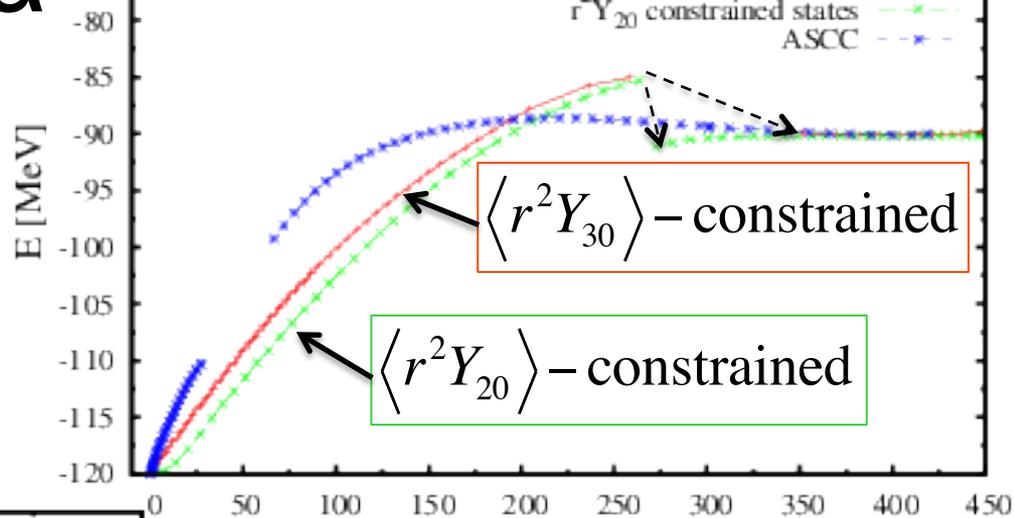
CoM



Preliminary result

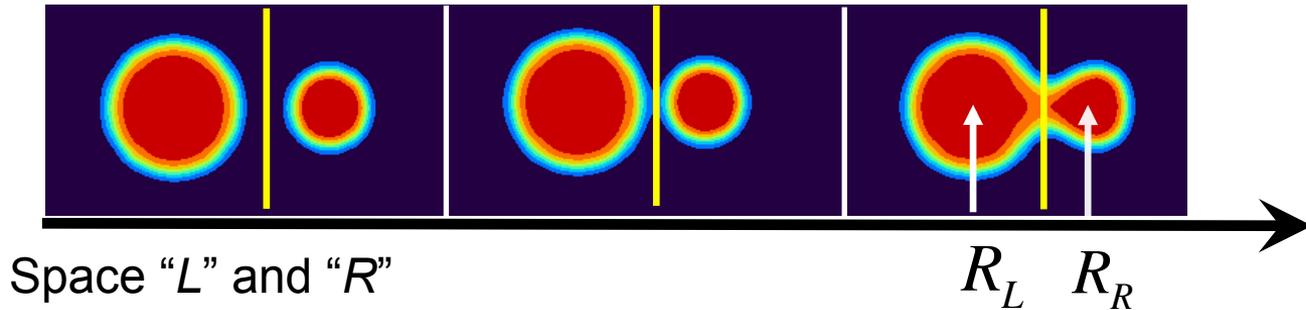


- Constraint operator
 - LHE generator
 - IS Quadrupole op.
 - IS Octupole op.
- Different path



Choice of variables (R, P)

- R is defined by $R = |R_R - R_L|$



- P is calculated from current in L & R
- This definition is questionable after two nuclei touch each other.
- *Need reliable definition of canonical*

Inertial mass & coordinate transf.

Finding decoupled canonical variables

$$(\xi^\alpha, \pi_\alpha) \rightarrow (q, p; \bar{q}^i, \bar{p}_i)$$

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

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

(map from q to R)

$$\Rightarrow \frac{1}{2} B(R) P_R^2 + V(q(R))$$

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

Assuming the collective variables

$$R = R(\xi) \quad R \text{ is chosen by hand}$$

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

$$\Rightarrow \frac{1}{2} \tilde{B}(R) P_R^2 + V(R)$$

$$\tilde{B}(R) = \frac{\partial R}{\partial \xi^\alpha} \frac{\partial R}{\partial \xi^\beta} B^{\alpha\beta}(\xi)$$

$$= B(R) + \frac{\partial R}{\partial \bar{q}^i} \frac{\partial R}{\partial \bar{q}^j} B^{ij}(\bar{q})$$

$$B(R) \neq \tilde{B}(R)$$

Reaction path

