Self-consistent collective path and inertial mass in nuclear fusion/fission reactions

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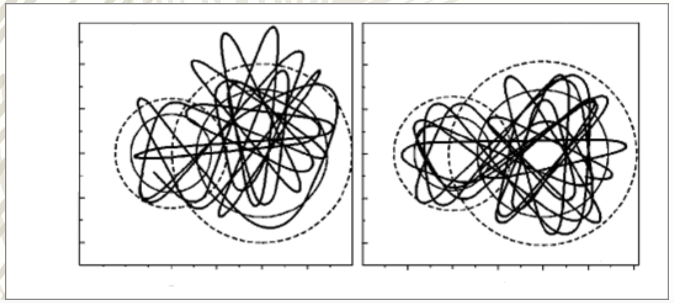
NTSE-2016 Sep. 20th

To study the **nuclear large amplitude collective motion**

Microscopic description

- Time dependent density functional theory(TDHF);
- Quantum molecular dynamics (QMD);
- … …



$$\Psi(t) = \frac{1}{\sqrt{A!}} \det\{\psi_1(t)\psi_2(t)\cdots\psi_A(t)\},$$
$$i\hbar\frac{\partial}{\partial t}\psi_j(r) = h(\rho)\psi_j(t).$$

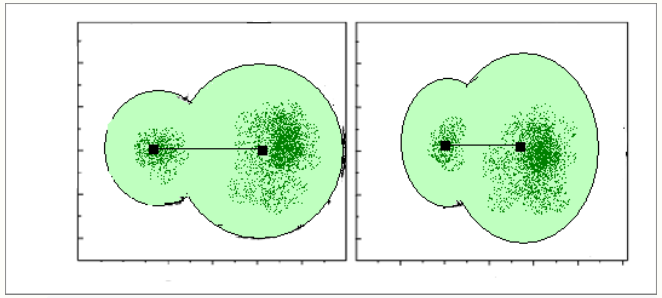
P. Bonche et al., Phys. Rev. C 13, 1226 (1976).

J. Aichelin, Phys. Rep. 202, 233 (1991).

… …

Collective dynamics

- Adiabatic Self-consistent Collective Coordinate (ASCC) method
  - Define the collective coordinates;
  - Construct the collective Hamiltonian



$$H(p,q) = \frac{p^2}{2M} + V(q),$$

- M. Matsuo, T. Nakatsukasa, and K. Matsuyanagi, Prog. Theor. Phys. **103**, 959 (2000)
- N. Hinohara, T. Nakatsukasa, M. Matsuo, and K. Matsuyanagi, Prog. Theor. Phys. **117**, 451 (2007).

Content:

- **The Adiabatic Self-consistent Collective Coordinate (ASCC) Method**
- The inertial mass for ^{8}Be $\leftrightarrow$ $\alpha + \alpha$.
  - CHF+LRPA mass
  - ASCC mass
  - Cranking mass and ATDHF
- The collective motion paths.
- Summary

The ASCC Method

Purpose:

Determine a collective motion path parameterized by ψ(p, q). The evolution of p and q obey the classical Hamilton's equation with Hamiltonian

$$H(p,q) = \frac{p^2}{2M} + V(q),$$

Assumption:

The adiabatic limit: collective momentum p is assumed to be small:

$$|\psi(p,q)\rangle = (1 + i\hat{Q}p - \frac{1}{2}\hat{Q}^2 p^2)|\psi(q)\rangle,$$

Starting point:

The Time dependent variational principle:

$$\delta\langle\psi(q,p)|i\frac{\partial}{\partial t} - \hat{H}|\psi(q,p)\rangle = 0,$$

The ASCC equations

$$\delta\langle\psi(q)|\hat{H}_{\rm mv}(q)|\psi(q)\rangle = 0$$

(1): moving mean field equation

$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), \frac{1}{i}\hat{P}(q)] - \frac{\partial^2 V}{\partial q^2}\hat{Q}(q)|\psi(q)\rangle = 0,$$
$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), i\hat{Q}(q)] - \frac{1}{M(q)}\hat{P}(q)|\psi(q)\rangle = 0,$$

(2): moving RPA equation

with moving mean field Hamiltonian:

$$\hat{H}_{\rm mv}(q) \equiv \hat{H} - (\partial V/\partial q)\hat{Q}(q)$$

Eqs. (2) can be transformed to a eigenvalue problem:

$$(A+B)(A-B)Q = \omega^2 Q,$$
$$\frac{\partial^2 V}{\partial q^2}\frac{1}{M} = \omega^2,$$

To calculate the inertial mass

1. Pick out the one desired RPA solution (e.g. quadrupole motion):

$$\langle n | \hat{Y}_{20} | 0 \rangle \neq 0$$

From many RPA solutions:

$\{ Q_1, Q_2, Q_3, \ldots Q_x \ldots Q_n, Q_{n+1} \ldots \ldots \}$

2. Transformation between collective coordinates

Collective Hamiltonian in q
(the solution of ASCC equations)

$$\hat{H}^q_{\rm coll} = \hat{T} + V(q), \quad \hat{T} = \frac{1}{2M_q}\frac{\partial^2}{\partial q^2}.$$

Collective Hamiltonian in R
(Defined at our convenience)

$$\hat{H}^R_{\rm coll} = \hat{T} + V(R), \quad \hat{T} = -\frac{1}{2}\frac{1}{\sqrt{M(R)}}\frac{d}{dR}\frac{1}{\sqrt{M(R)}}\frac{d}{dR}.$$

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

Numerical Details

- Coordinate-space and mixed representation

$$\hat{Q} = \sum_n \sum_j Q_{nj} a_n^\dagger a_j + \text{h.c.}$$

$$\hat{Q} = \int d\vec{r} \sum_j Q_j(\vec{r}) a^\dagger(\vec{r}) a_j + \text{h.c.}$$

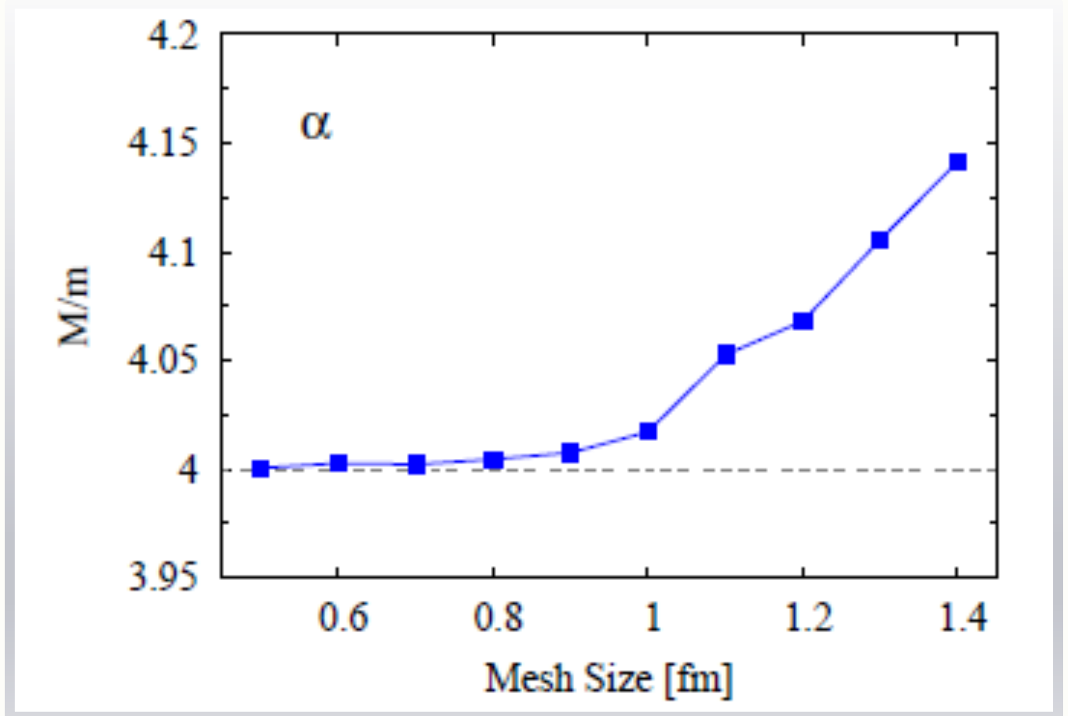
- Finite amplitude method for the moving RPA solution

P. Avogadro, T. Nakatsukasa, PRC **87**, 014331(2013)

- the BKN interaction applied

P. Bonche, S. Koonin, and J. W. Negele, Phys. Rev. C **13**, 1226 (1976).

Test calculation for the mass of one alpha particle:



Content:

- The Adiabatic Self-consistent Collective Coordinate (ASCC) Method
- **The inertial mass for ^{8}Be ↔ α + α .**
  - CHF+LRPA mass
  - ASCC mass
  - Cranking mass and ATDHF
- The ASCC collective motion paths.
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CHF+RPA Mass for ^{8}Be ↔ α + α

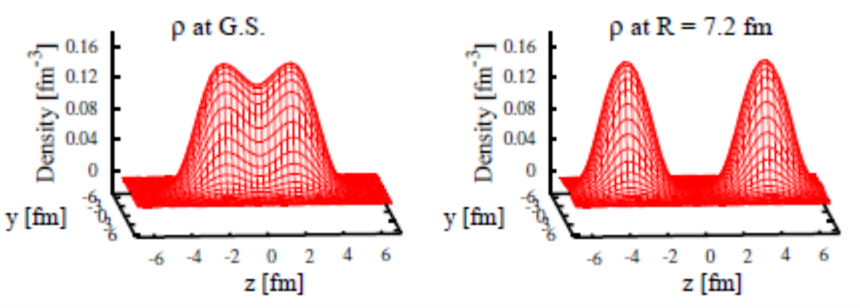
$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), \frac{1}{i}\hat{P}(q)] - \frac{\partial^2 V}{\partial q^2}\hat{Q}(q)|\psi(q)\rangle = 0,$$

$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), i\hat{Q}(q)] - \frac{1}{M(q)}\hat{P}(q)|\psi(q)\rangle = 0,$$

$\psi(q)$ is set to be the Constrained Hartree Fock states. We adopt the two constraints respectively:

1. *quadrupole deformation Q_{20}*
2. *Relative distance R defined as:*

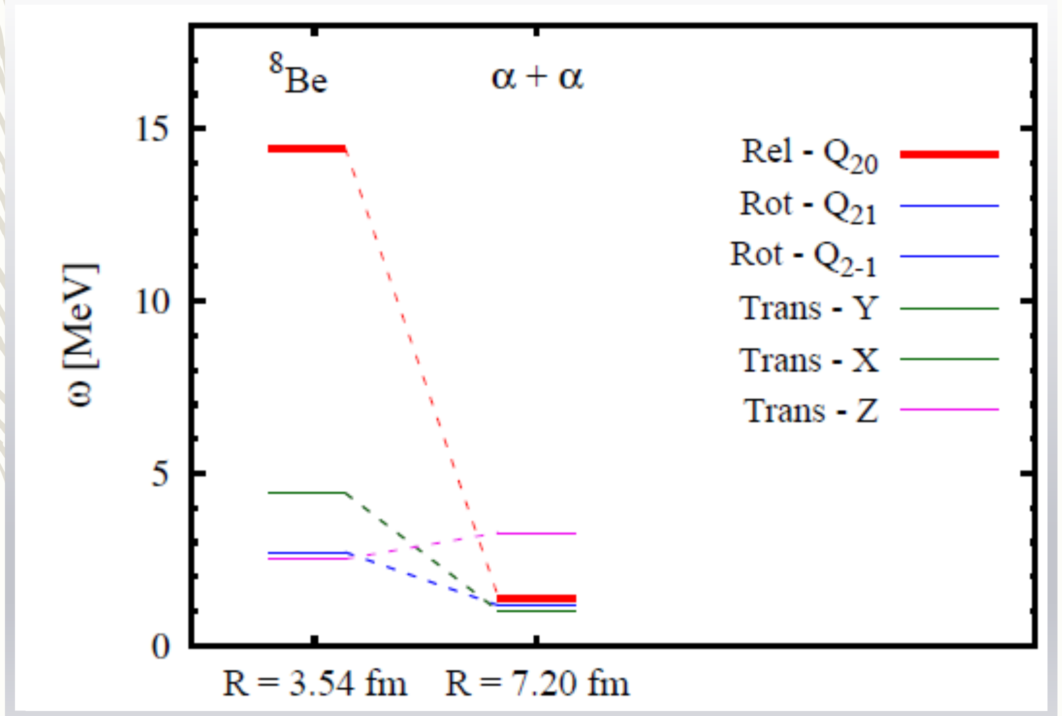
$$\hat{R} \equiv \frac{1}{A/2}\int d\vec{r}\hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r})\left\{z\theta(z) - z\theta(-z)\right\}$$



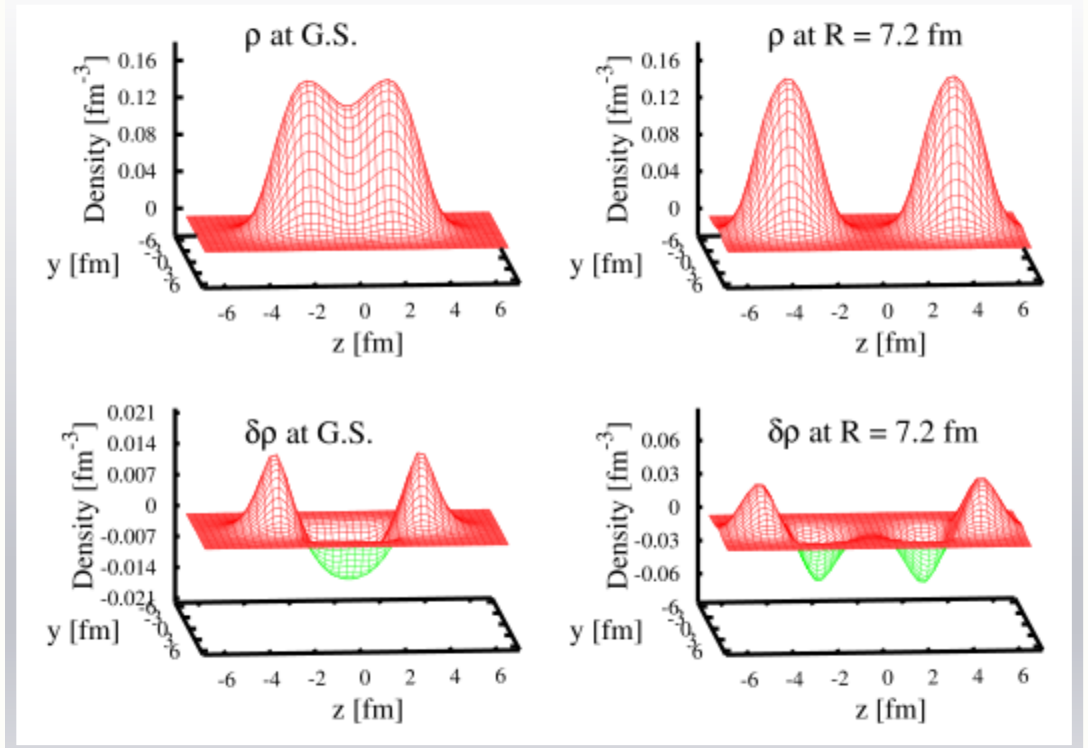
CHF+LRPA mass for ^{8}Be ↔ $\alpha + \alpha$

- Calculation in 3D coordinate space. In the rectangular box of volume 10×10×16 fm^3 with grid size 0.8 fm.

RPA eigenvalues

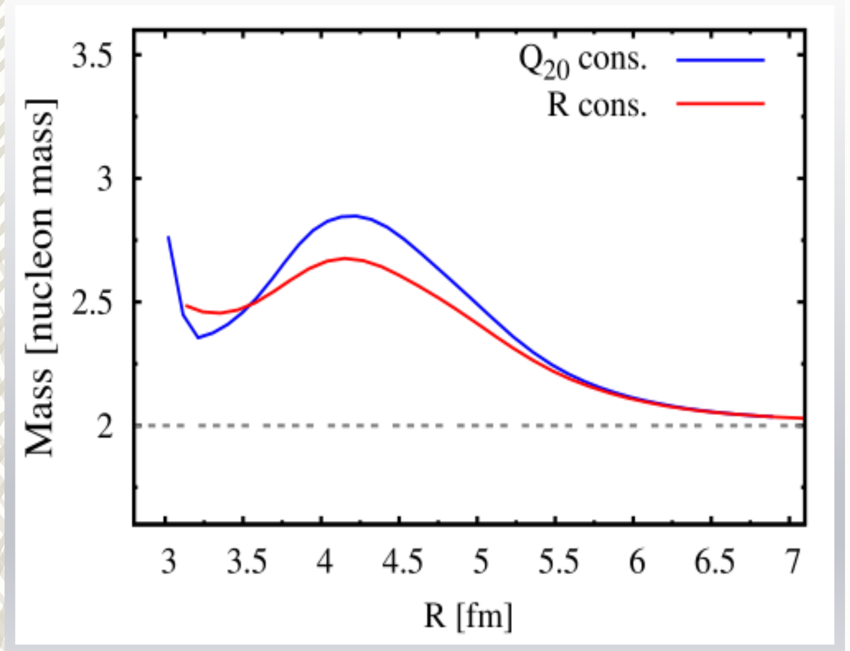


Density and transition density

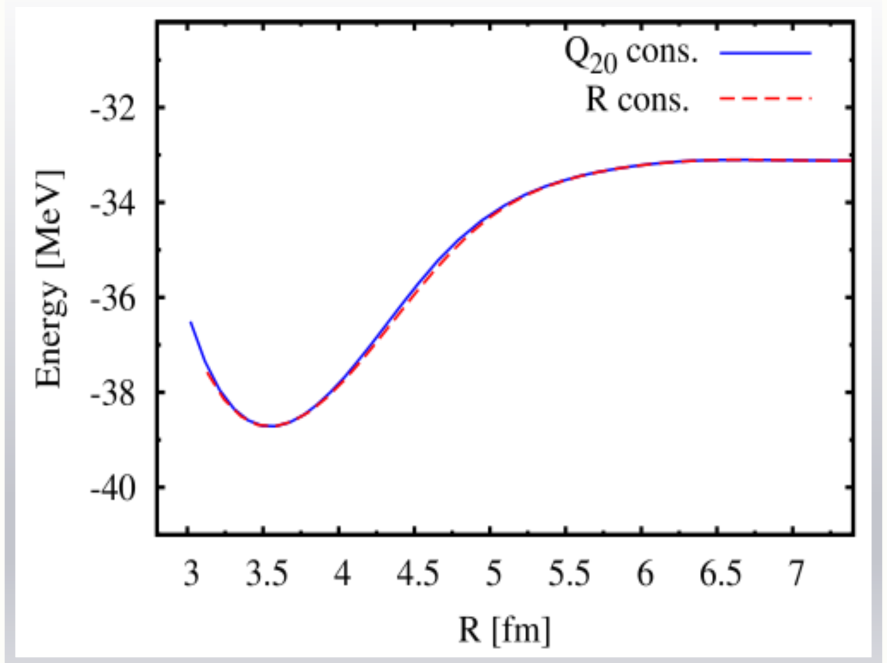


CHF+RPA mass and potential of CHF states

Inertial Mass with coordinate R



Potential energy of CHF states



Results depend on the choice of the constraint.

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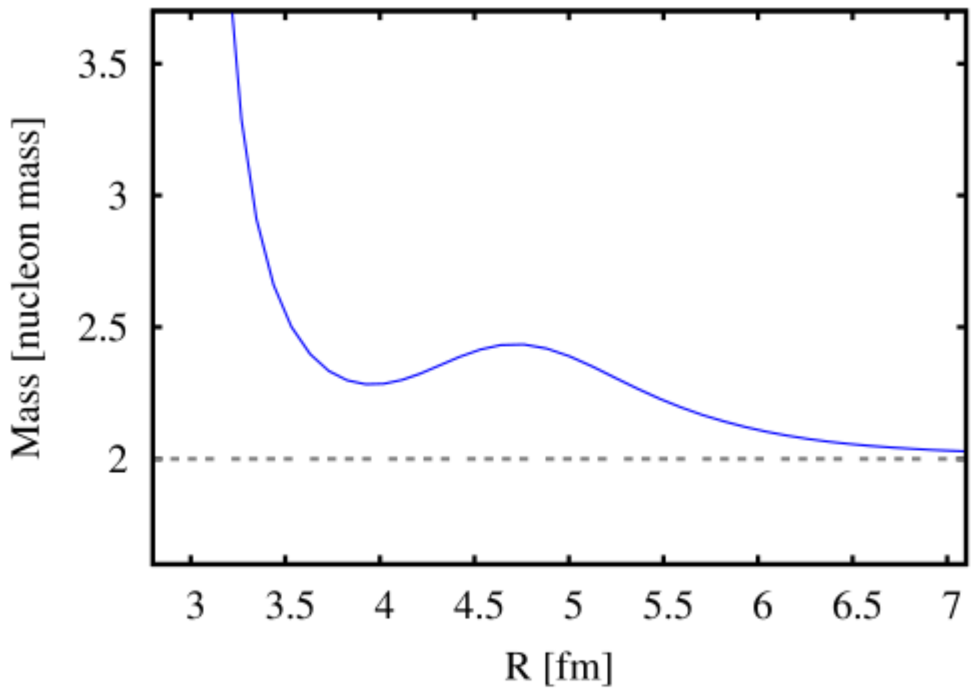
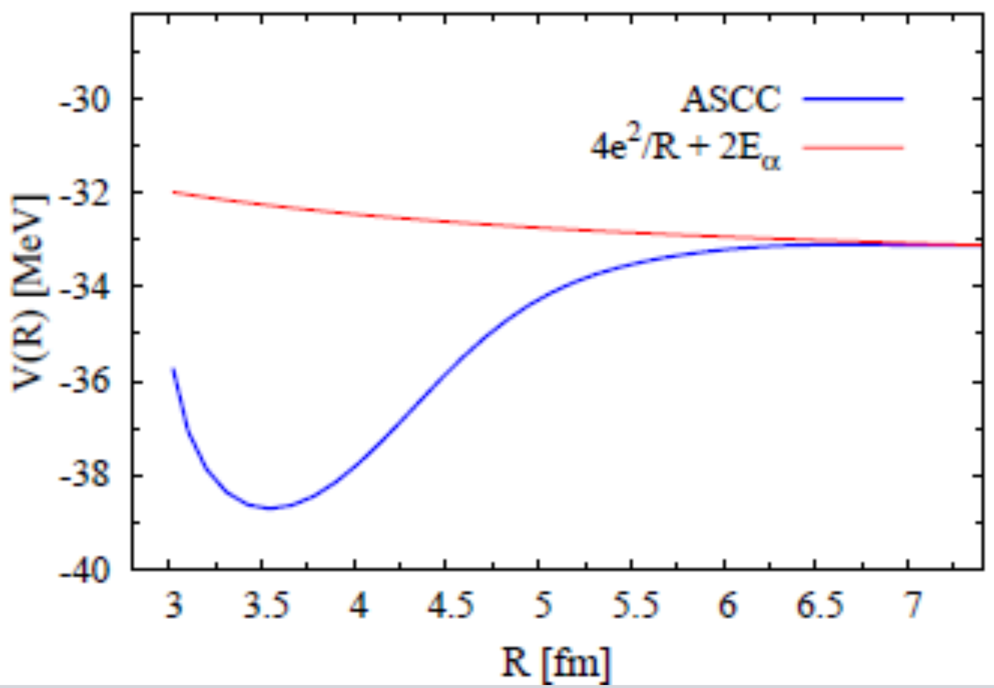
ASCC mass: fission path ^{8}Be

$$\delta\langle\psi(q)|\hat{H}_{\rm mv}(q)|\psi(q)\rangle = 0$$

$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), \frac{1}{i}\hat{P}(q)] - \frac{\partial^2 V}{\partial q^2}\hat{Q}(q)|\psi(q)\rangle = 0,$$
$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), i\hat{Q}(q)] - \frac{1}{M(q)}\hat{P}(q)|\psi(q)\rangle = 0,$$

Iteration starts from the Q_{20} and R constrained state respectively, M converges



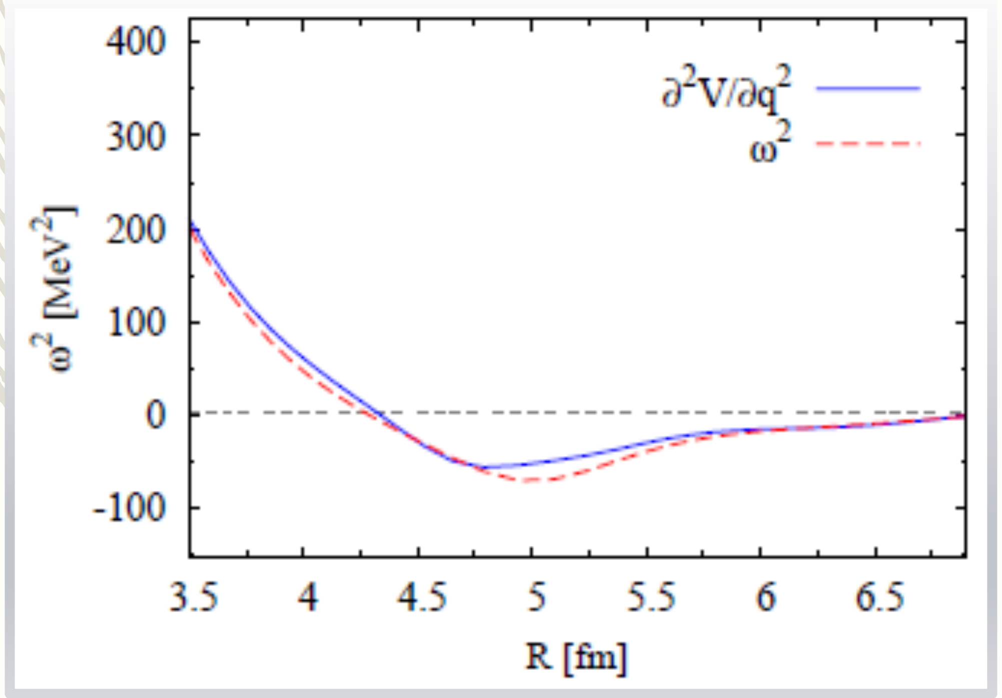


Self-consistency of CHF+LRPA and ASCC mass

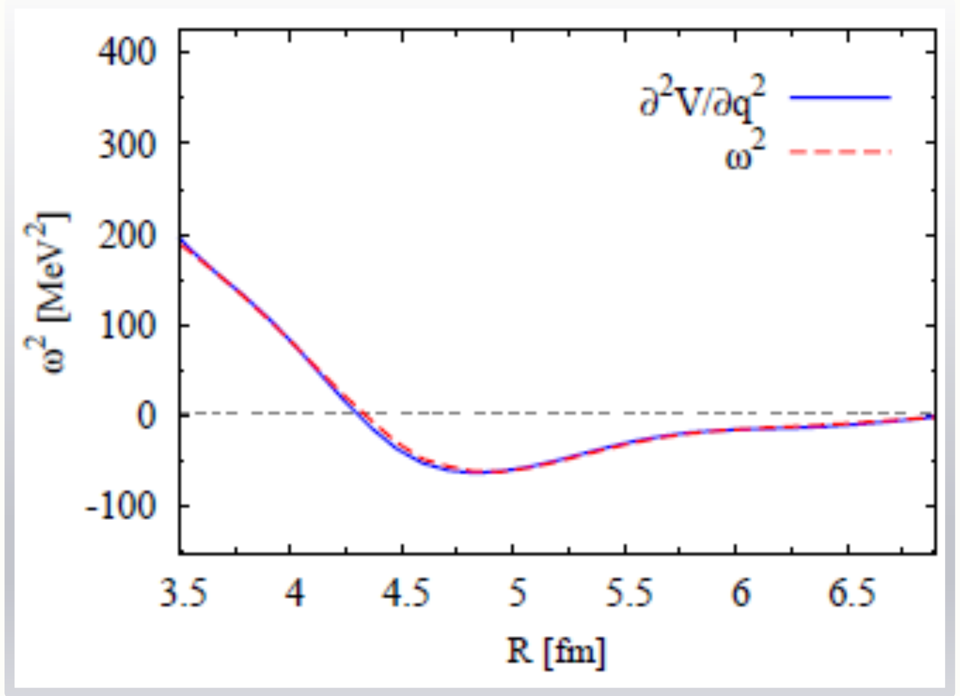
Whether the collective path follows the direction defined by the local generators?

- Interpretation of RPA eigenvalue ω^2 : $$\omega^2 = \frac{d^2 V_{\text{local}}}{dq^2}$$
- The second order derivative of CHF potential: $$\frac{d^2V}{dq^2} = \frac{d^2V}{dR^2}\left(\frac{dR}{dq}\right)^2 = \frac{d^2V}{dR^2}\frac{1}{M}$$

CHF+LRPA



ASCC



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Cranking Mass

Inglis cranking mass
(non-perturbative cranking mass):

$$M_{\rm cr}^{\rm NP}(R) = 2\sum_{m,i} \frac{|\langle\varphi_m(R)|\partial/\partial R|\varphi_i(R)\rangle|^2}{e_m(R) - e_i(R)},$$

$$h_{\rm CHF}(R)|\varphi_\mu(R)\rangle = e_\mu(R))|\varphi_\mu(R)\rangle, \quad \mu = i, m.$$

D. R. Inglis, Phys.Rev. 96, 1059(1954);
D. R. Inglis, Phys.Rev. 103, 1786(1956);
… …

Perturbative cranking mass:

$$M_{\rm cr}^{\rm P}(R) = \frac{1}{2}\left\{S^{(1)}(R)\right\}^{-1} S^{(3)}(R)\left\{S^{(1)}(R)\right\}^{-1},$$

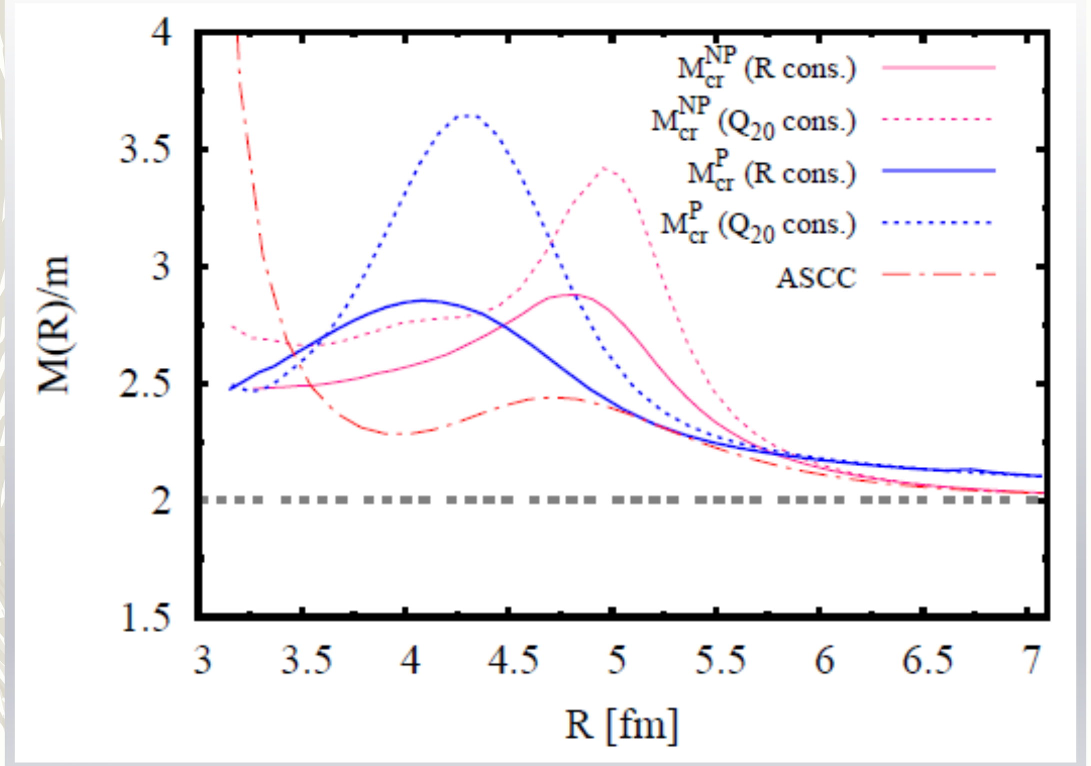
with

$$S^{(k)}(R) = \sum_{m,i} \frac{|\langle\varphi_m(R)|\hat{R}|\varphi_i(R)\rangle|^2}{\{e_m(R) - e_i(R)\}^k}.$$

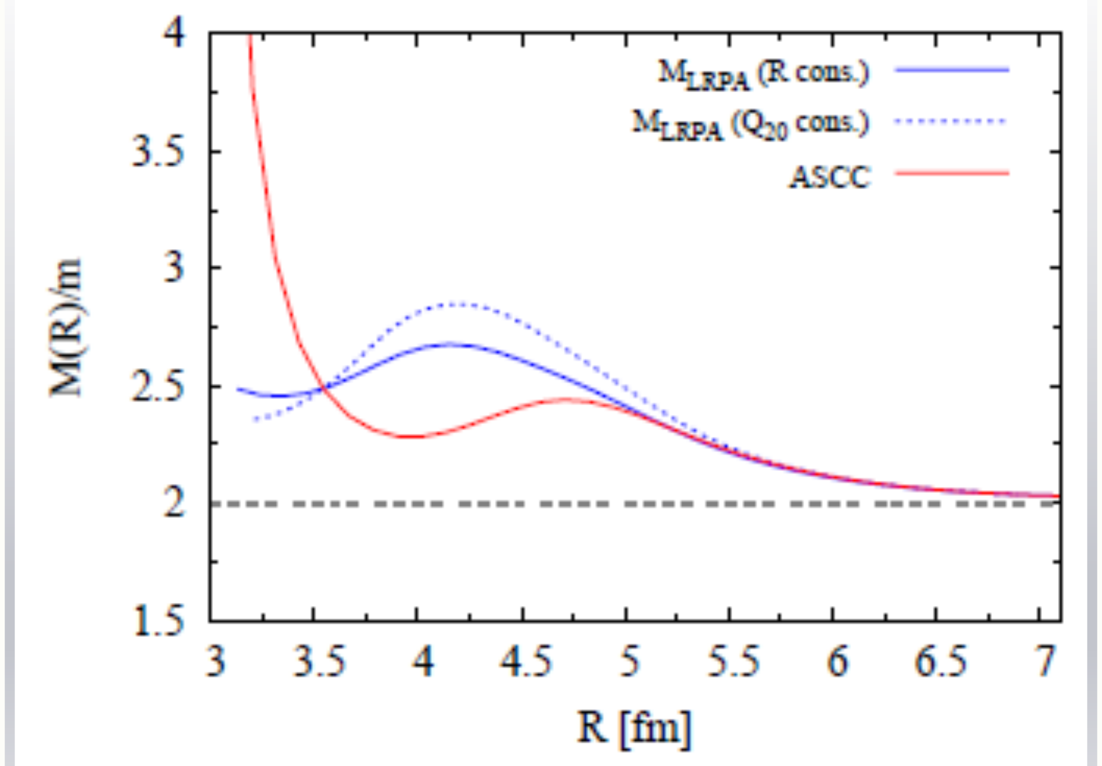
A. Baran et. al. Phys. Rev. C **84**, 054321(2011);
D. Vautherin Phys. Lett.69B, 4(1977);
… …

Comparison between different masses

Cranking and ASCC



CHF+LRPA and ASCC

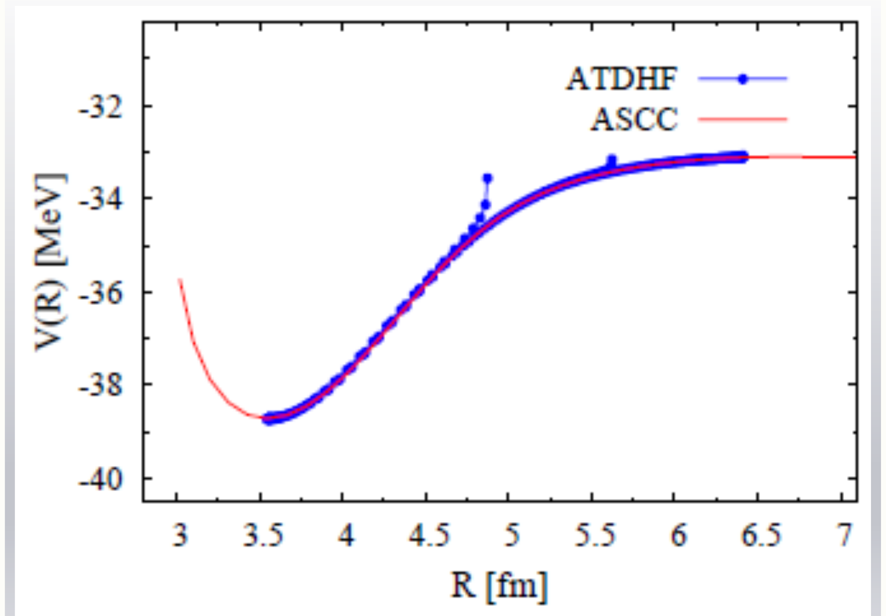


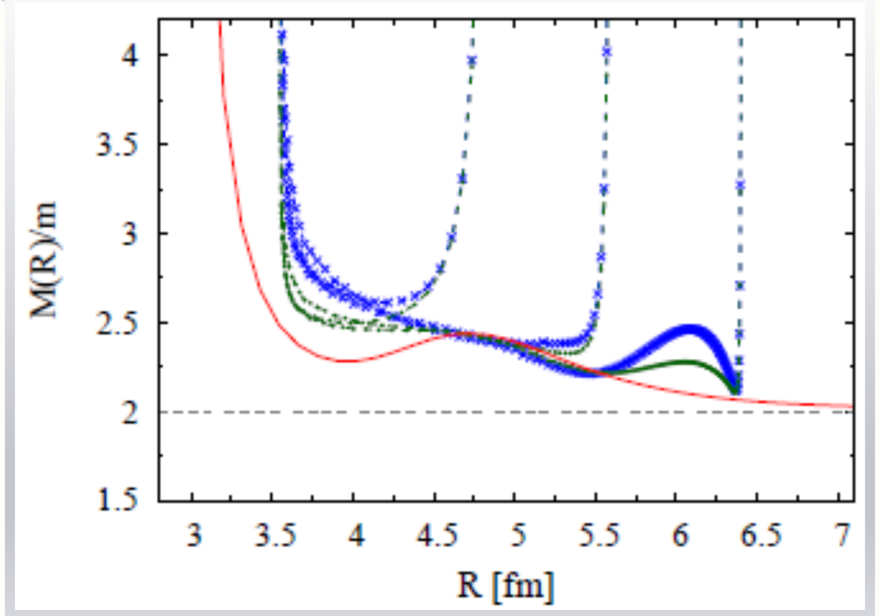
Adiabatic Time-Dependent Hartree-Fock(ATDHF)

- Equation for the collective path ψ(q):

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

- Mass parameter can be calculated in two way:
  - (1) $$M_{\mathrm{atdhf}}(R) = \left(\frac{dV}{dR}\right)^2 \langle\psi(q)|[\hat{H}_{\mathrm{ph}}(q),[\hat{H},\hat{H}_{\mathrm{ph}}(q)]]|\psi(q)\rangle^{-1}.$$
  - (2) $$M_{\mathrm{atdhf}}(R) = \left(\frac{dq}{dR}\right)^2 \frac{\varepsilon}{\delta q}\frac{dV}{dq} = \frac{\varepsilon}{\delta R}\frac{dV}{dR}.$$
- Drawbacks:
  - Non-uniqueness(initial value problem)
  - Trajectory can only go from high energy to low energy
  - Difficult to find find the saddle point





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- The Adiabatic Self-consistent Collective Coordinate (ASCC) Method
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- **The ASCC collective motion paths.**
  - $^{20}Ne \leftrightarrow {}^{16}O + \alpha$
  - $^{16}O \leftrightarrow {}^{12}C + \alpha$
  - $^{32}S \leftrightarrow {}^{16}O + {}^{16}O$
- Summary

Procedure to develop the collective path

$$\Psi(q)$$

Initial state

$$\delta\langle\Psi(q)|[\hat{H}_{\rm mv}(q), \frac{1}{i}\hat{P}(q)] - \frac{\partial^2 V}{\partial q^2}\hat{Q}(q)|\Psi(q)\rangle = 0,$$

$$\delta\langle\Psi(q)|[\hat{H}_{\rm mv}(q), i\hat{Q}(q)] - \frac{1}{M(q)}\hat{P}(q)|\Psi(q)\rangle = 0,$$

Moving RPA equation

$$\delta\langle\Psi(q+\varepsilon)|H - \frac{\partial V}{\partial q}\hat{Q}(q)|\Psi(q+\varepsilon)\rangle = 0,$$

$$\langle\Psi(q+\varepsilon)|\hat{Q}(q)|\Psi(q+\varepsilon)\rangle|_{q=0} = \varepsilon,$$

CHF problem

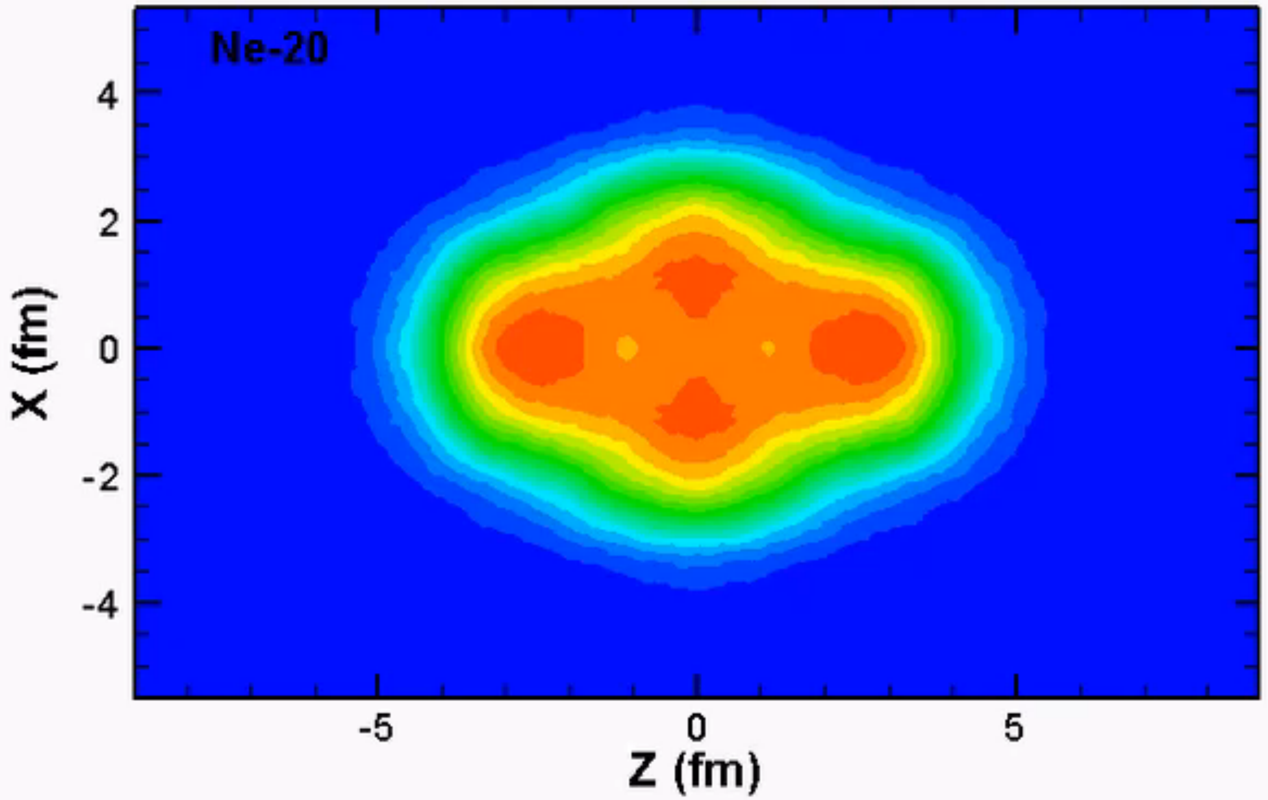
$$\Psi(q+\varepsilon)$$

Continue the iteration, we get a collective path:

$$\Psi(q), \Psi(q+\varepsilon), \Psi(q+2\varepsilon), \Psi(q+3\varepsilon), \Psi(q+4\varepsilon)......$$

When ε is small enough, the states on the trajectory keeps well the original self-consistency in the ASCC equation set.

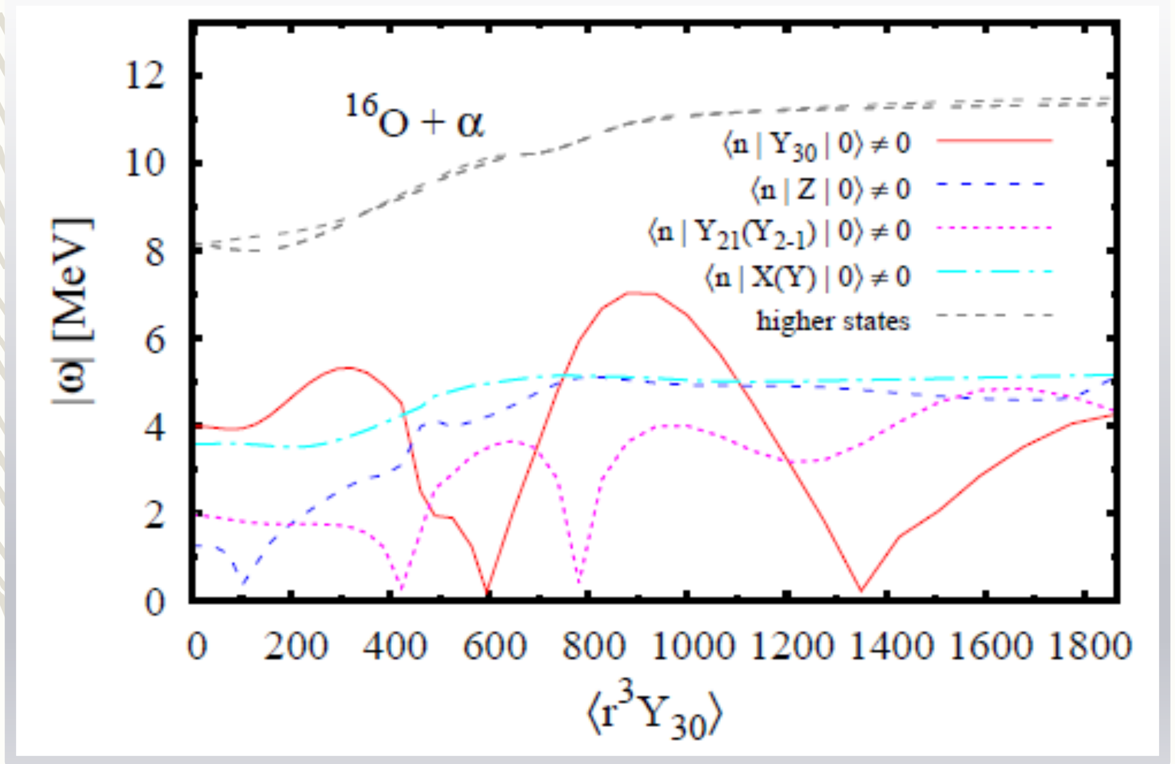
Collective motion path of fission from ^{20}Ne to ^{16}O + α

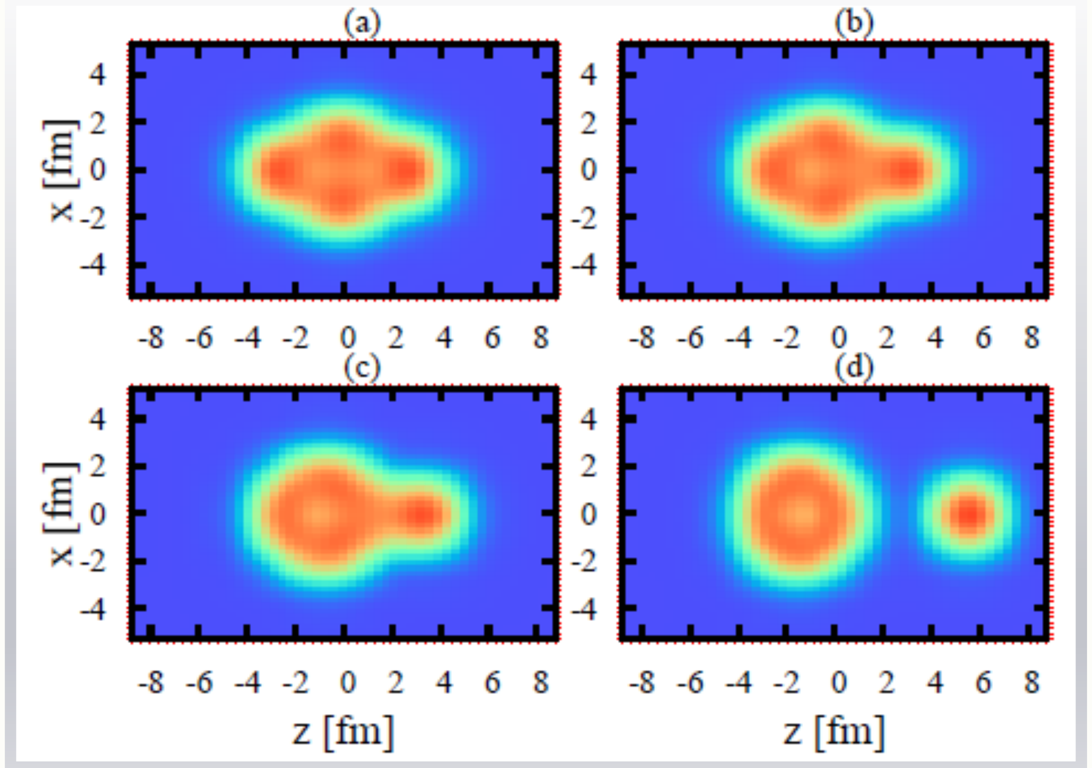


- *Starting from the ^{20} Ne at ground state, end up with ^{16}O +α*
- *The first physical RPA state with axial symmetry is used to develop the trajectory.*
- *Model space: rectangular box of 12×12×18 fm^3 with grid size 1.1 fm.*

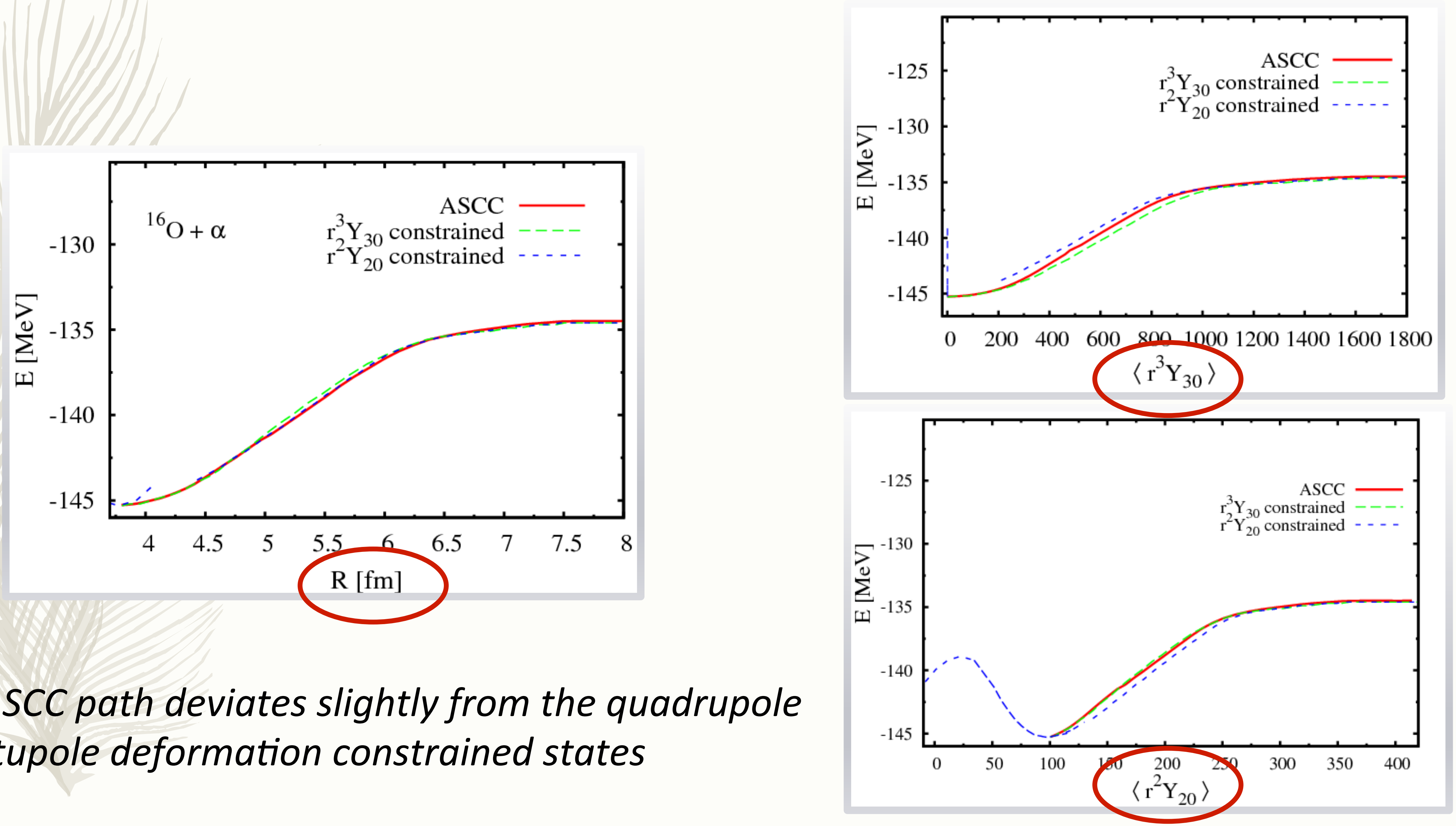
Collective motion path of $^{16}O + \alpha$

Eigen frequency of the RPA states along the ASCC collective path



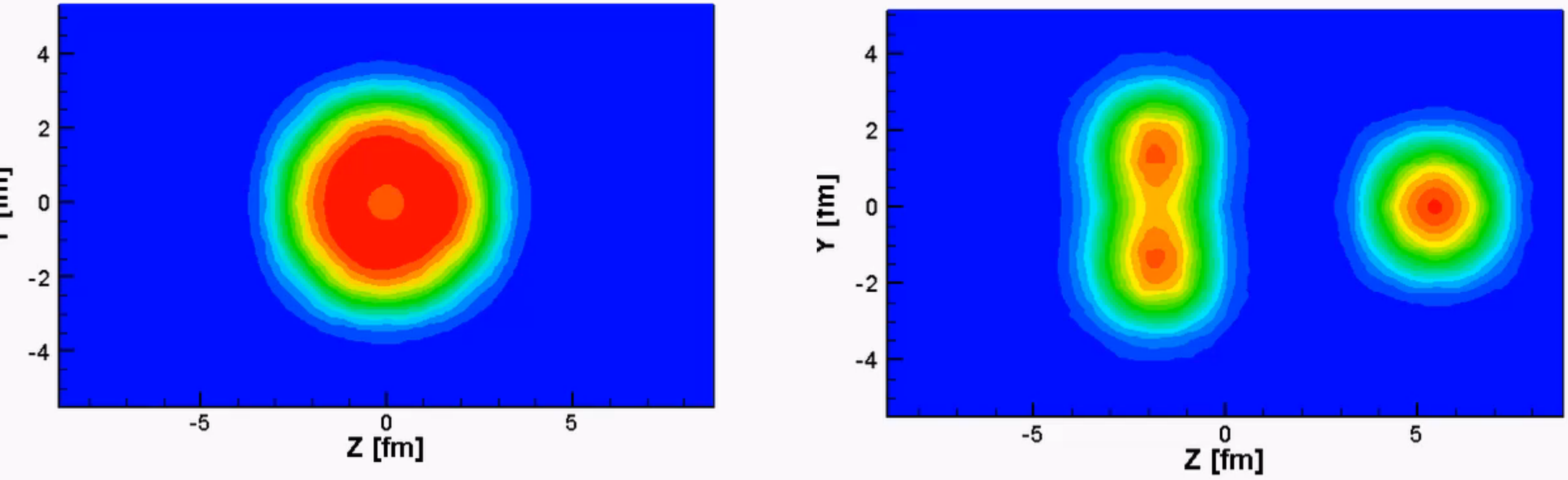


Potential of the system $^{16}O + \alpha$



The ASCC path deviates slightly from the quadrupole or octupole deformation constrained states

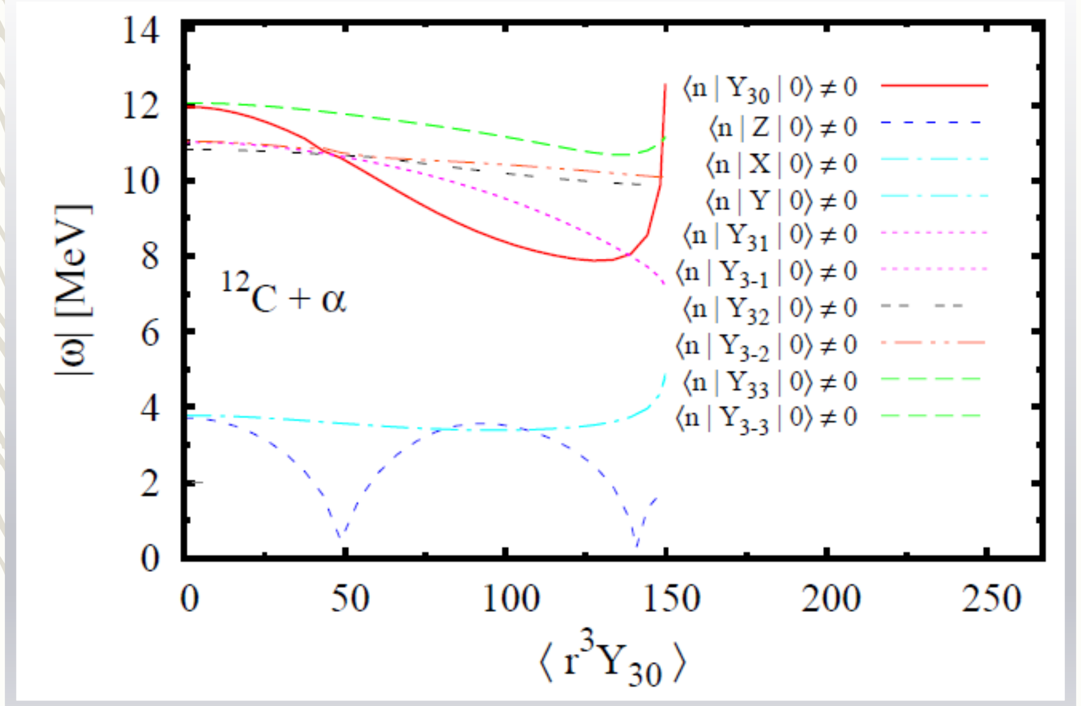
Collective motion path of fission from ^{16}O to $^{12}C + \alpha$

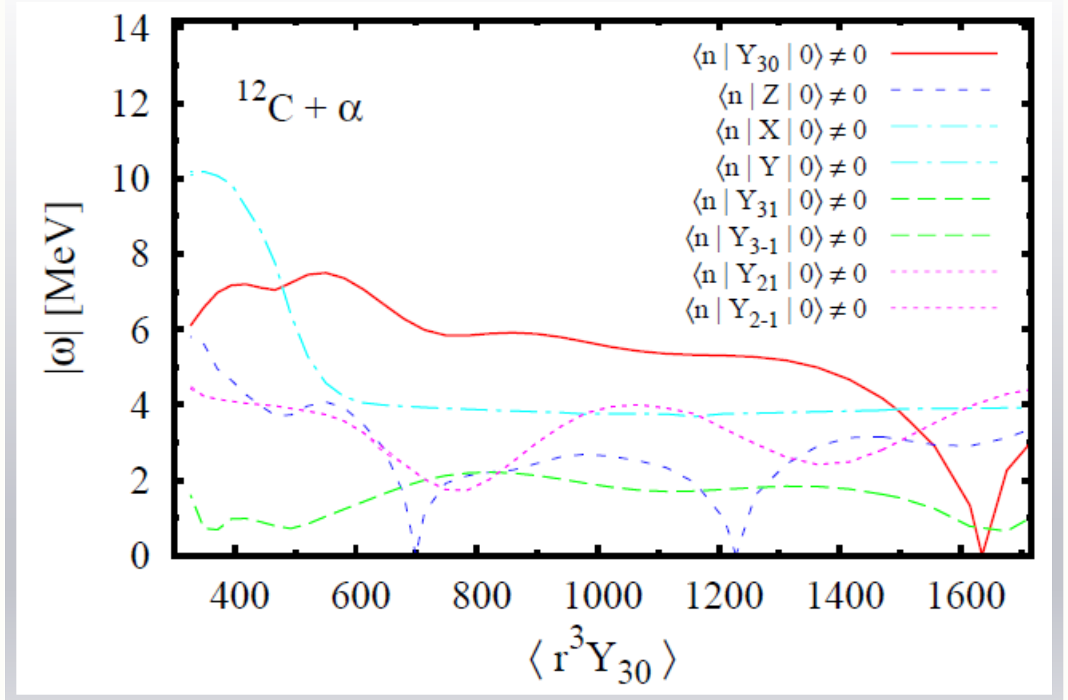


- *Starting from the ^{16}O ($^{12}C+\alpha$)*
- *The first physical RPA state with axial symmetry is used to develop the trajectory.*
- *Model space: rectangular box of $12\times12\times18$ fm^3 with grid size 1.1 fm.*

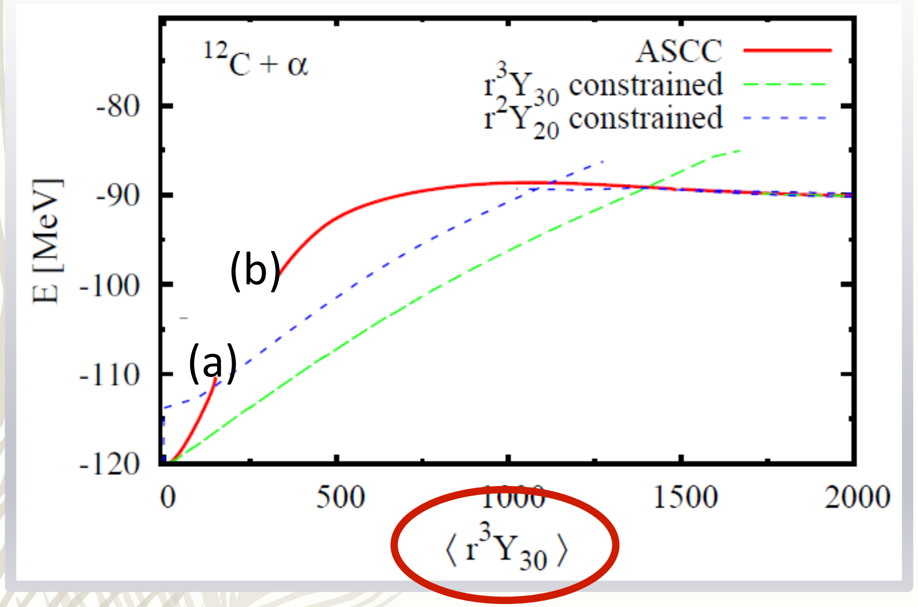
Collective motion path of $^{12}C + \alpha$

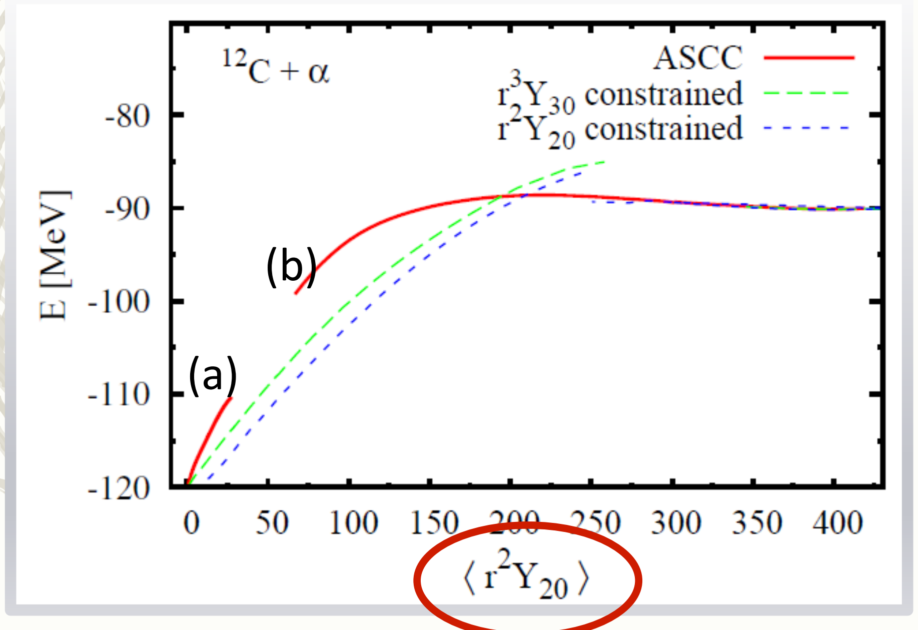
Eigen frequency of the RPA states along the ASCC collective path

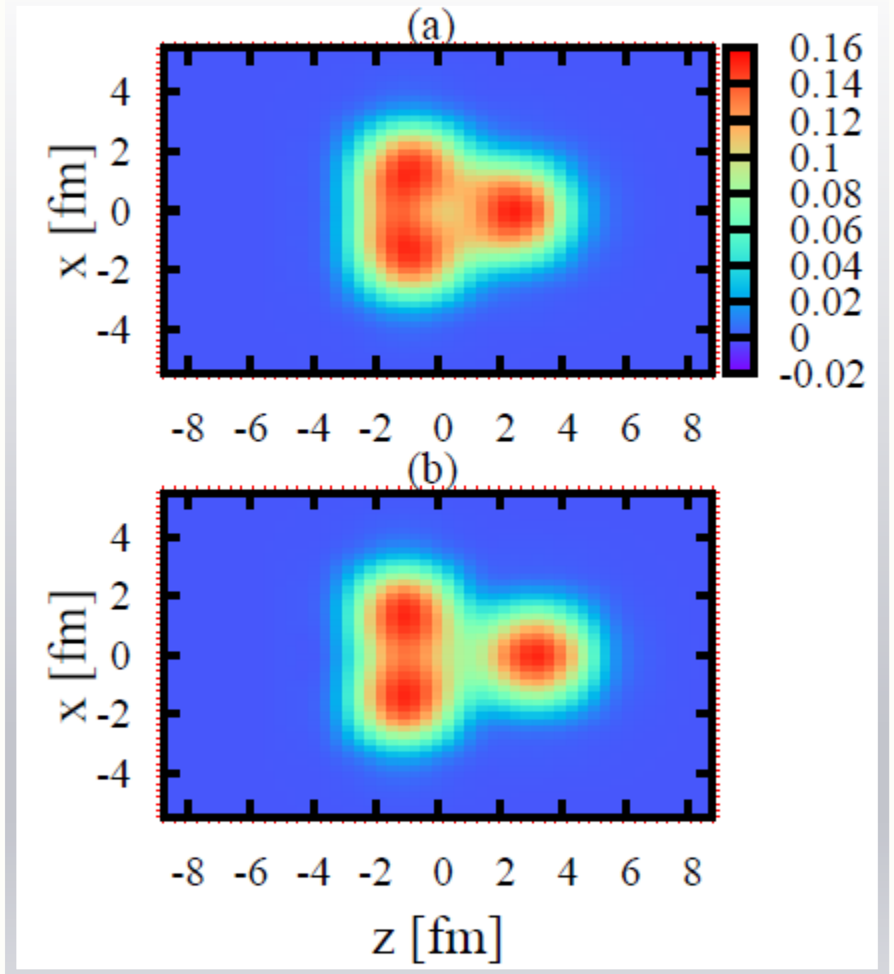




Results of the system $^{12}C + \alpha$ in large model space





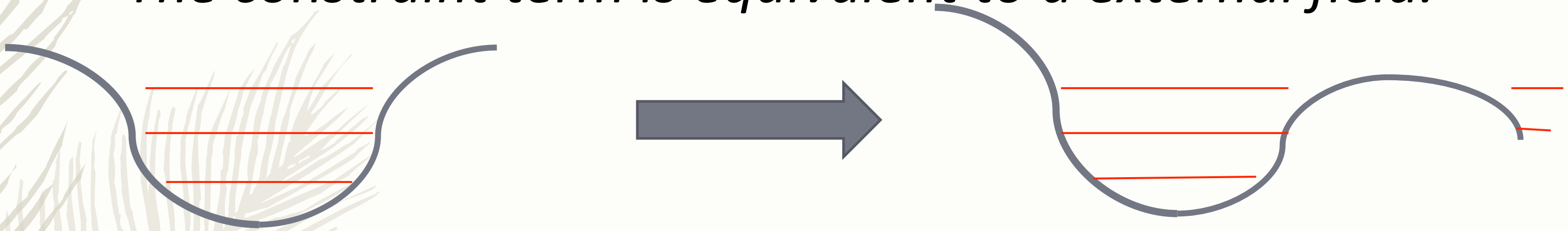


Model space: rectangular box of 12×12×18 fm³ with grid size 1.1 fm.

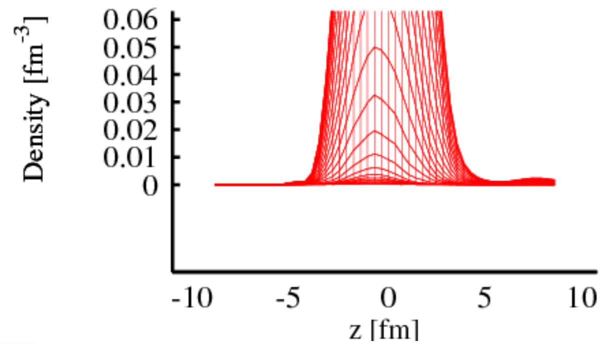
A problem in the constrained Hartree Fock calculation

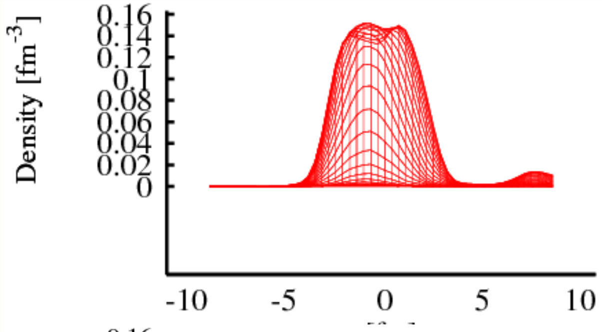
$$\delta\langle\psi|H-\lambda Q_{20}(Q_{30})|\psi\rangle=0,$$

The constraint term is equivalent to a external field.

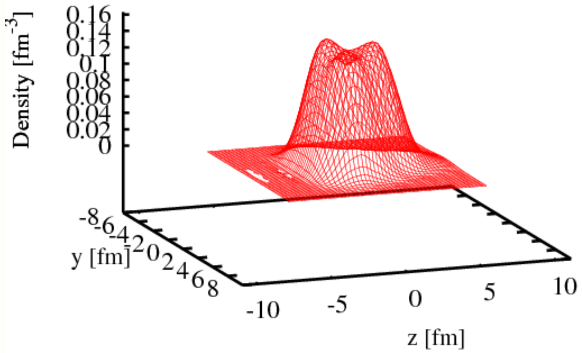


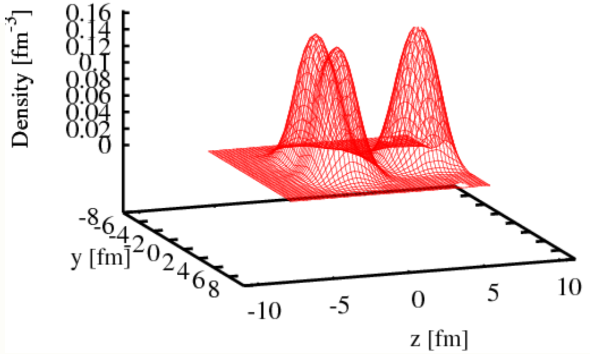
Large space :





Small space :

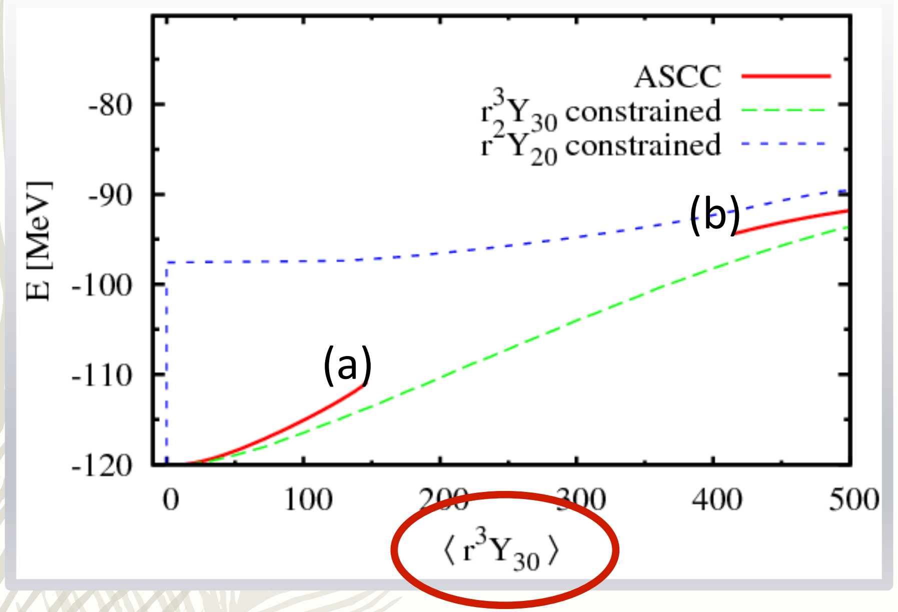


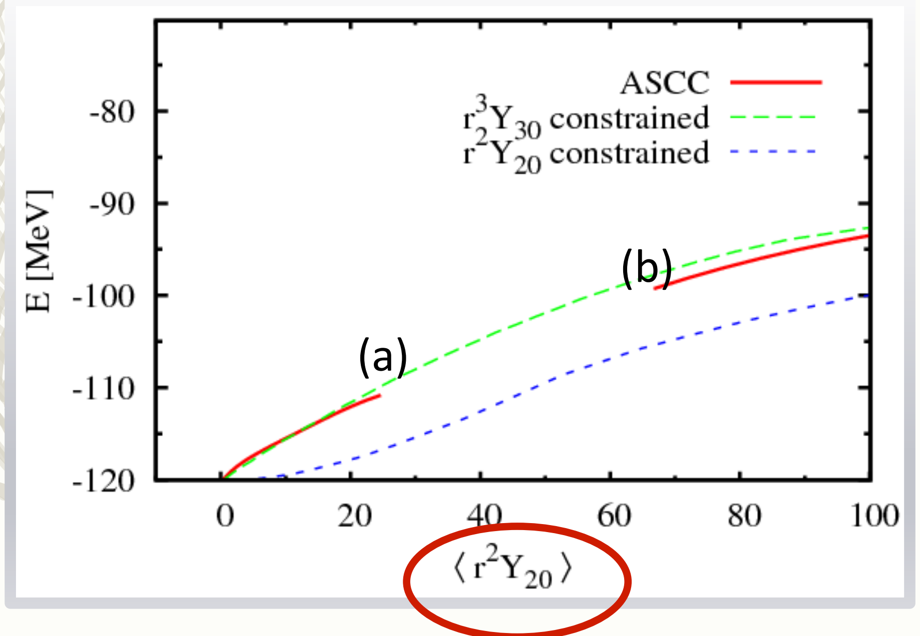


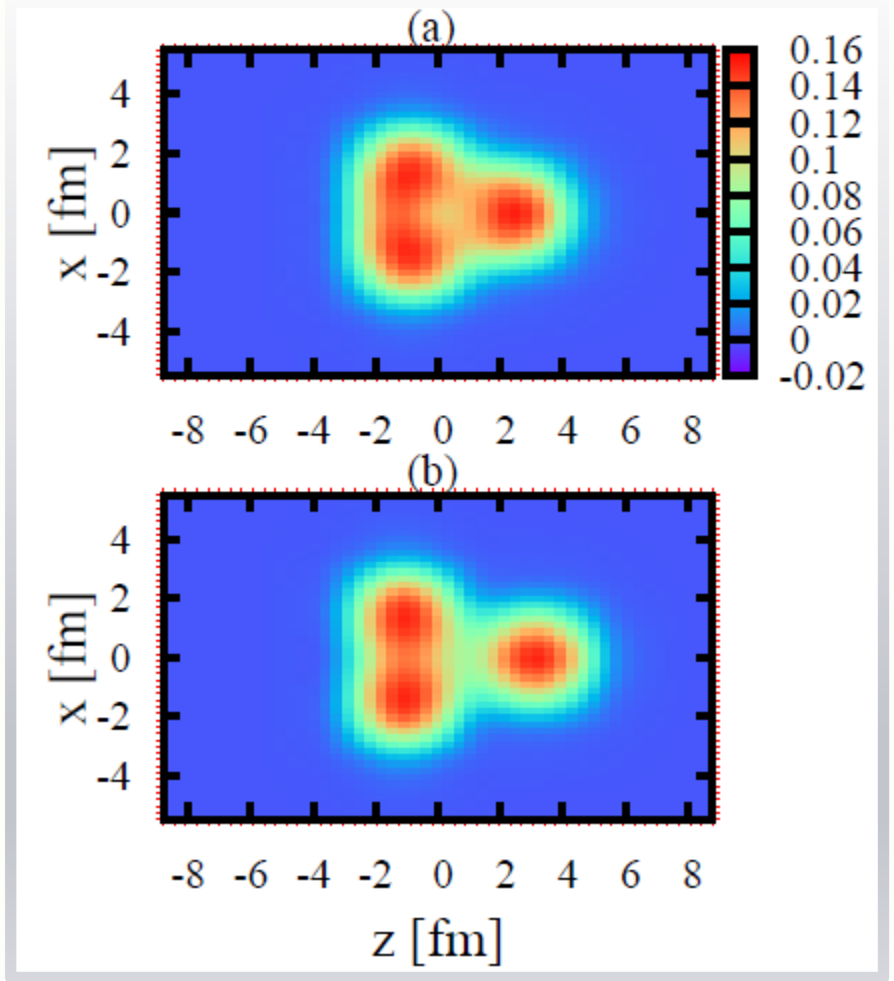
$\langle r^3Y_{30}\rangle = 300$

$\langle r^3Y_{30}\rangle = 900$

Results of the system $^{12}C + \alpha$ in small model space

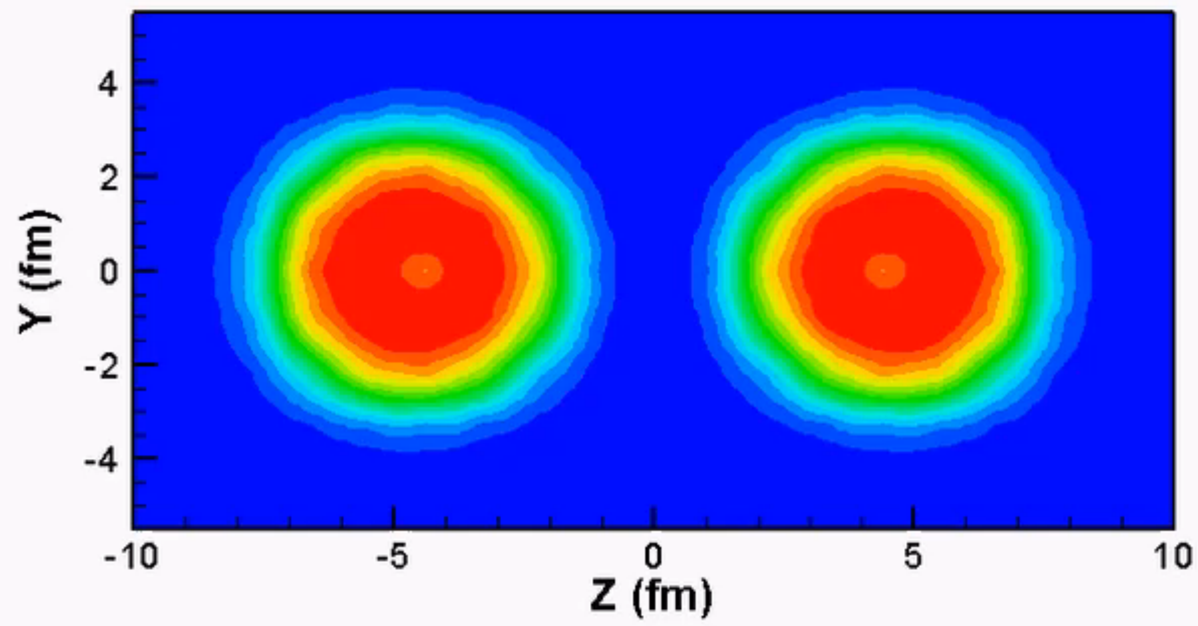






Model space: rectangular box of 12×12×14 fm³ with grid size 1.1 fm.

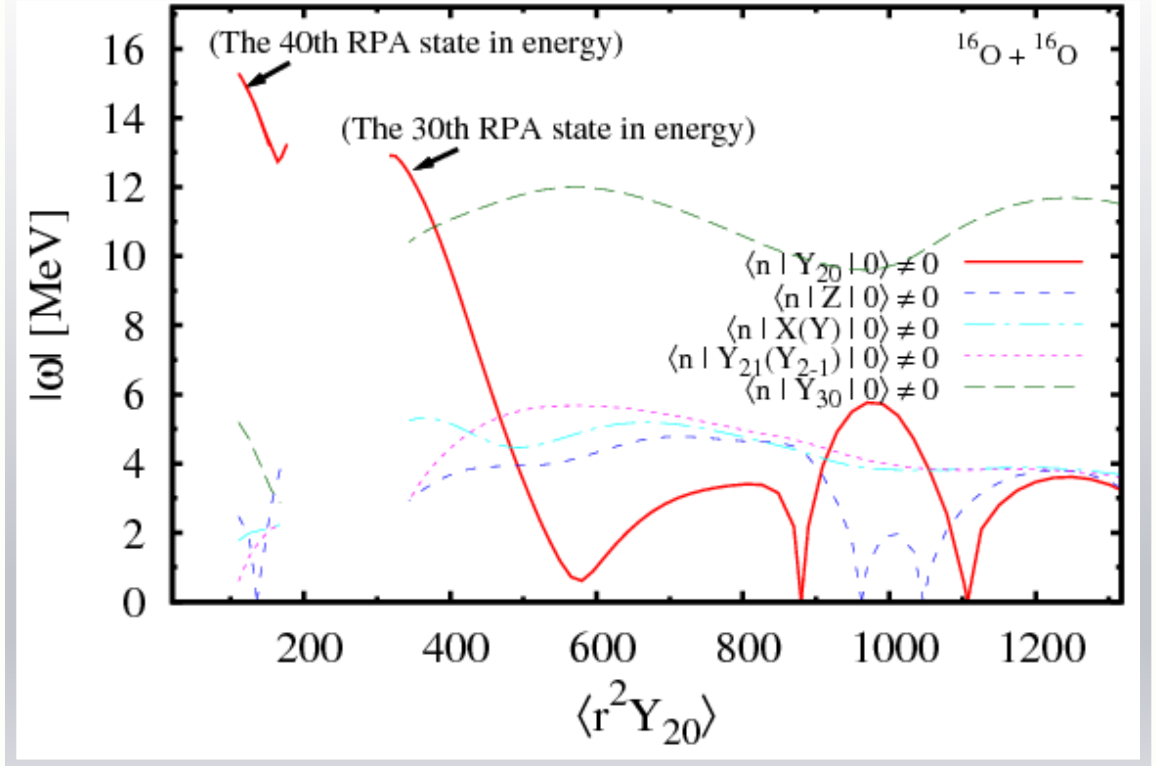
Collective motion path of scattering between $^{16}O + ^{16}O$



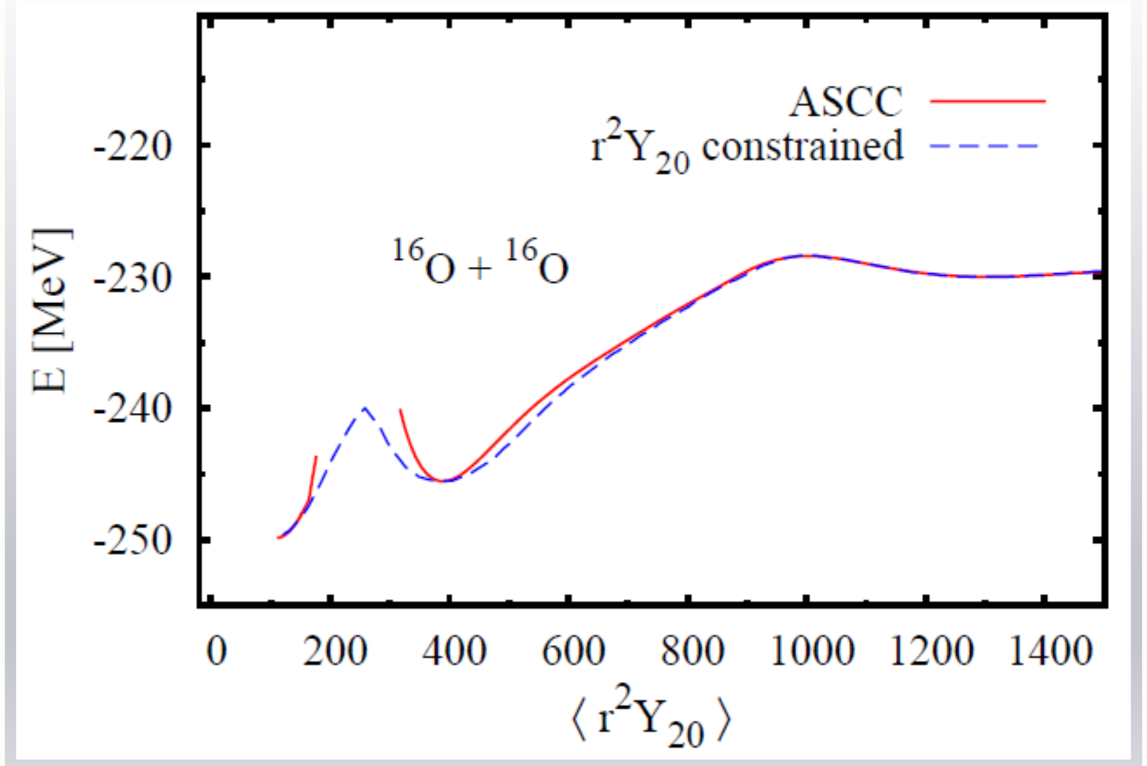
- *Starting from the separated $^{16}O + ^{16}O$ both at ground state.*
- *The first physical RPA state of quadrupole mode is used to develop the trajectory.*
- *Model space: rectangular box of $12 \times 12 \times 22$ fm^3 with grid size 1.1 fm.*

Collective motion path of $^{16}O + {}^{16}O$

Eigen frequency of the RPA states along the ASCC collective path



Potential



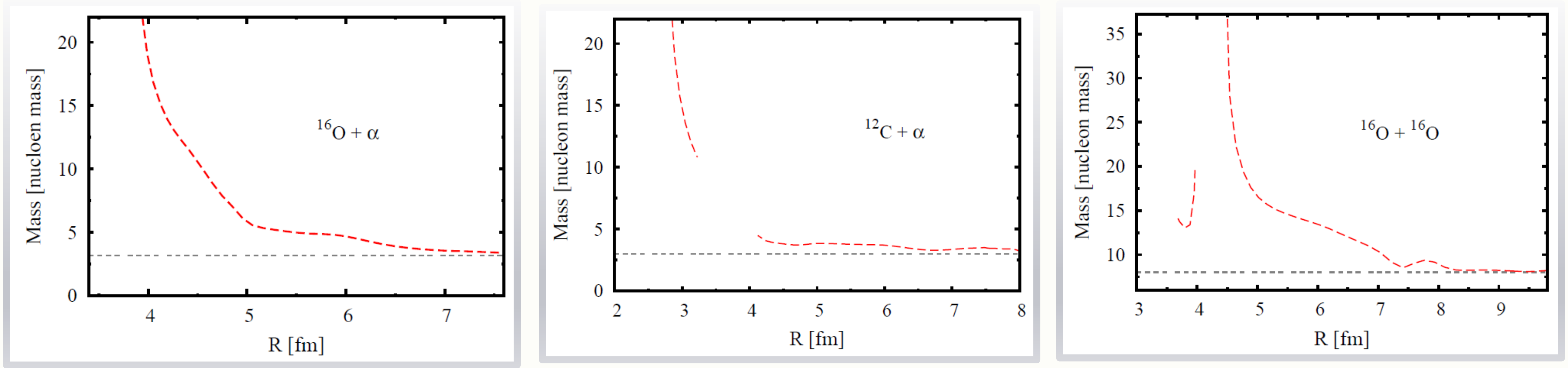
Inertial mass derived by ASCC method

Introducing the separation plane at $z = z_s$:

$$\int_{z_s}^{+\infty} \rho(r)dr = M_{\rm pro}$$

Definition of R:

$$\hat{R} \equiv z\left[\frac{\theta(z-z_s)}{M_{\rm pro}} - \frac{\theta(z_s-z)}{M_{\rm tar}}\right]$$



The reduced mass value can be well reproduced by ASCC method and Inglis cranking formula

Summary and Perspective

Thank you for your attention!

- ❑ *Based on the ASCC method, we extract the collective motion path for the system α+α, ^{12}C+α, ^{16}O+α, $^{16}O+^{16}O$,*
- ❑ *The self-consistent collective coordinate is found to be different from certain deformation parameters.*
- ❑ *The inertial mass parameters are calculated base on ASCC method.*

- ❑ *Our next plan:*

  - *To calculate the inertial mass for more heavier system.*
  - *Applying the more realistic nuclear interaction.*
  - *The mass parameter of other collective motion modes.*
  - *… …*