Self-consistent collective coordinate for reaction path and inertial mass

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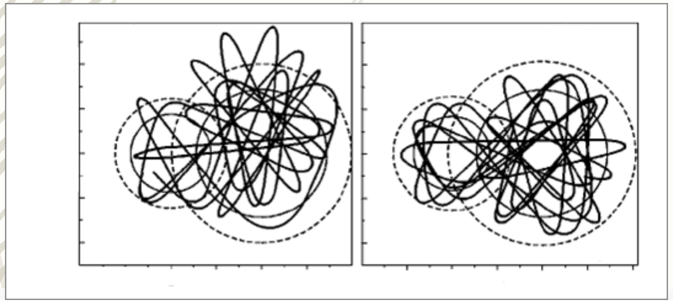
To study the **nuclear large amplitude collective motion**

Microscopic description

Time dependent density functional theory(TDDFT)



$$\Psi(t) = \frac{1}{\sqrt{A!}}\det\{\psi_1(t)\psi_2(t)\cdots\psi_A(t)\},$$

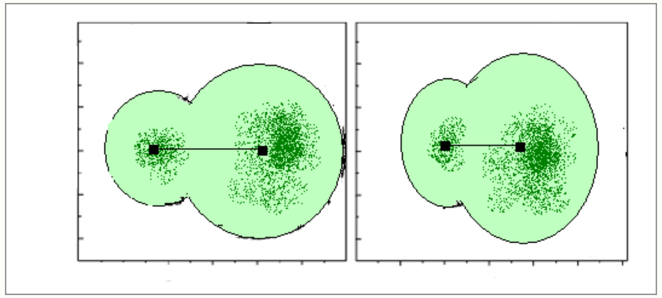
$$i\hbar\frac{\partial}{\partial t}\psi_j(r) = h(\rho)\psi_j(t).$$

- Provides us successful description for the time evolution of one-body observables;
- Can not provide us full theoretical description of collective dynamics.

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



- Definition of collective coordinates?
  microscopic or intuitive
- Inertial mass parameter?
- Collective Hamiltonian

M. Matsuo, T. Nakatsukasa, and K. Matsuyanagi, Prog. Theor. Phys. 103, 959 (2000)

Content:

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

The ASCC Method

Merit:

1. Derive the collective coordinate microscopically, which is decoupled from intrinsic DOFs.
2. Determine a collective motion path parameterized by ψ(p, q), the evolution of p and q obey the classical Hamilton's equation.
3. Obtain the inertial mass self-consistently.

Assumption:

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

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

Starting point:

The time-dependent variational principle:

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

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:

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

A weak canonical condition is imposed

$$\langle\Psi(q)|[i\hat{P}(q), \hat{Q}(q)]|\Psi(q)\rangle = 1$$

To calculate the inertial mass

1. Pick out the one desired moving-RPA solution (e.g. quadrupole state):

From many moving RPA solutions:

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

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

2. Transformation between collective coordinates from q to R

Collective Hamiltonian in q
(the solution of ASCC equations)

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

Collective Hamiltonian in R
(Defined at our convenience)

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

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

Pauli, Handbuch der Physik, Vol. XXIV (Springer Verlag, Berlin, 1933)

Numerical Details

K. Wen, T. Nakatsukasa, PRC **94**, 054618(2016)

- Coordinate-space, mixed representation

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

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

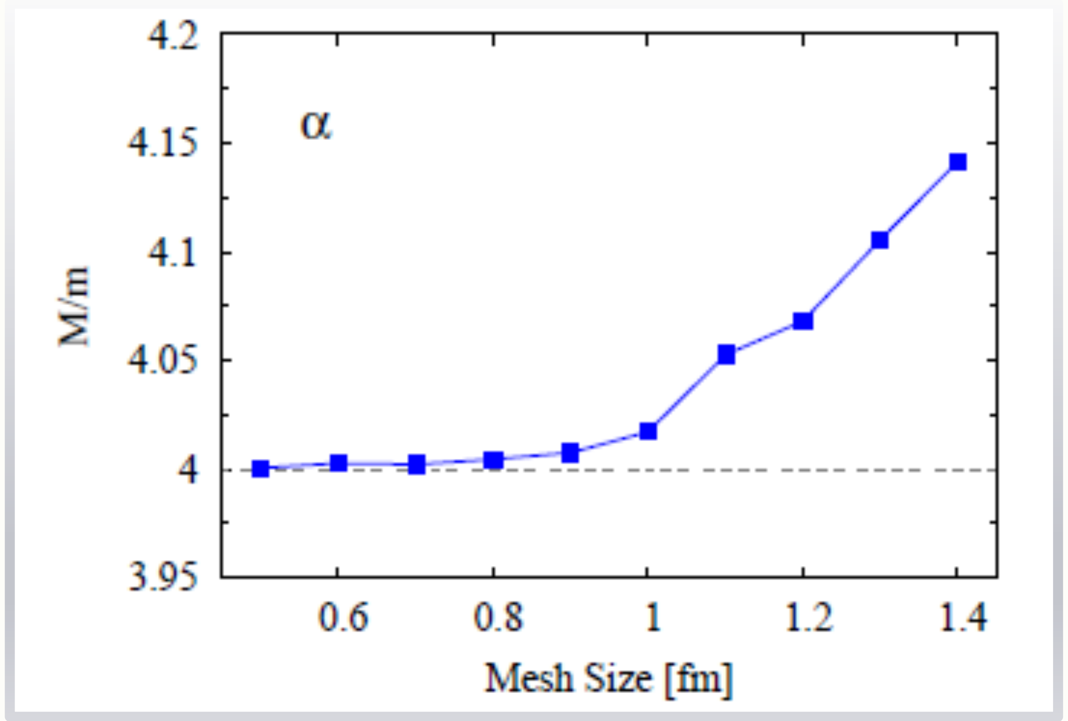
- Finite amplitude method for the moving RPA solution

T. Nakatsukasa, T. Inakura, and K. Yabana, PRC **76**, 024318(2007)

- 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:



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

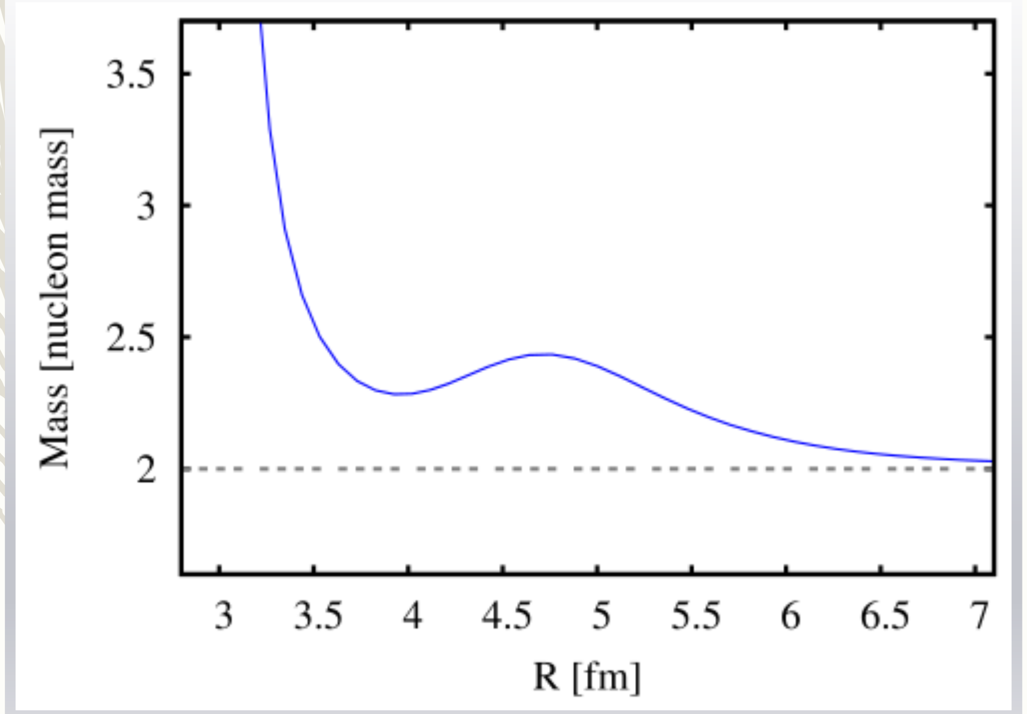
ASCC mass: fission path ^{8}Be

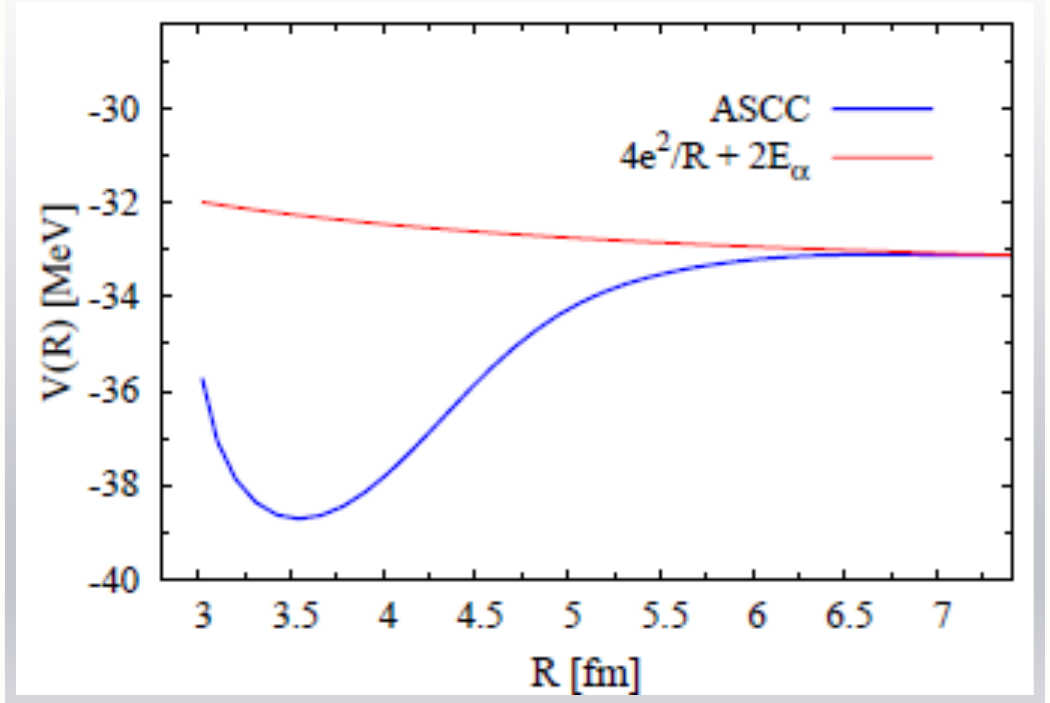
$$\delta\langle\psi(q)|\hat{H}_{\mathrm{mv}}(q)|\psi(q)\rangle = 0$$

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

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

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





Cranking Mass

Inglis cranking mass
(non-perturbative cranking mass):

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

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

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

Perturbative cranking mass:

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

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);
… …

CHF+LRPA Mass for ^{8}Be ↔ α + α

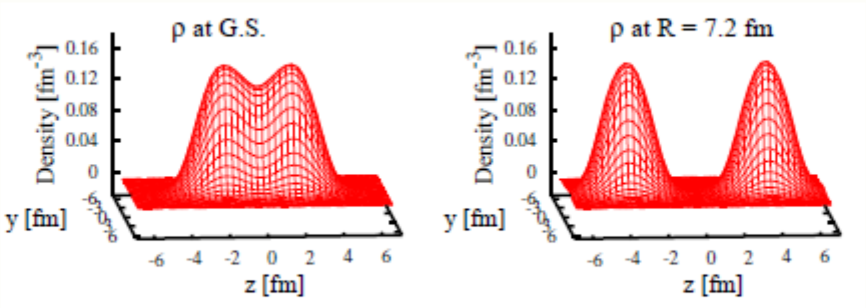
$$\delta\langle\psi(q)|[\hat{H}_{\rm mv}(q), \frac{1}{i}\hat{P}(q)] - \frac{\partial^2 V}{\partial q^2}\hat{Q}(q)|\psi(q)\rangle = 0,$$

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

$\psi(q)$ is set to be the CHF states, with different constraints:

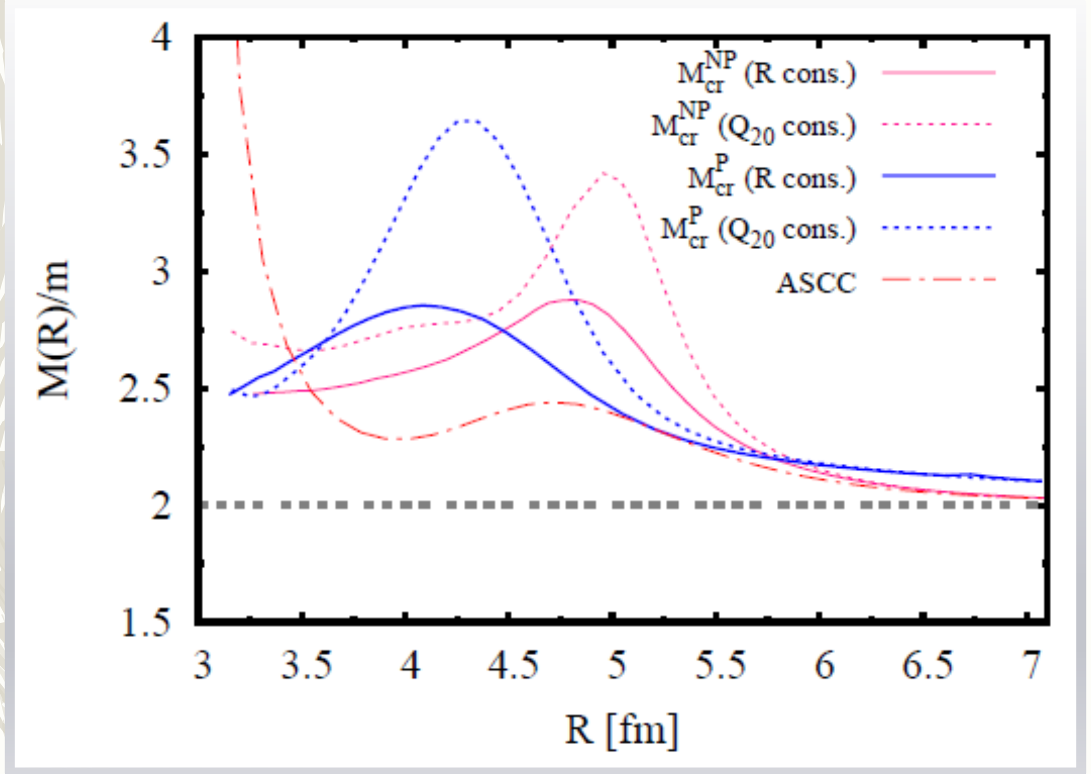
1. *Quadrupole deformation Q_{20}*
2. *Relative distance R defined as*

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

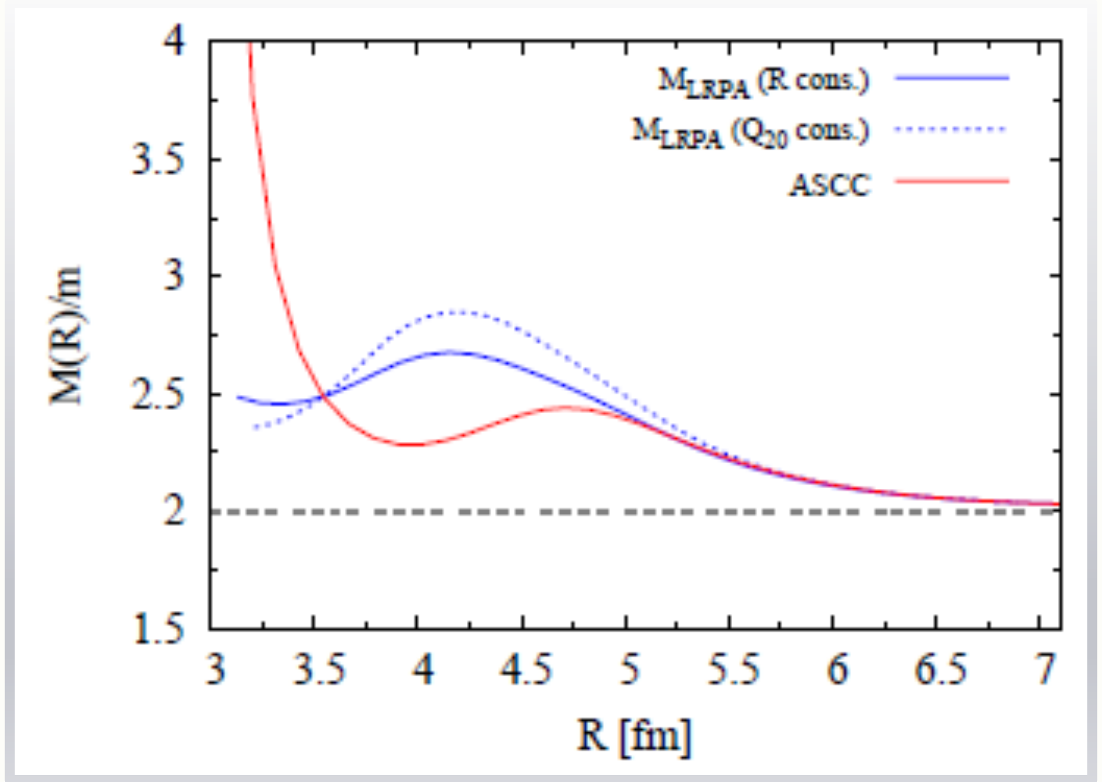


Comparison between different masses

Cranking and ASCC



CHF+LRPA and ASCC



K. Wen, T. Nakatsukasa, PRC **94**, 054618(2016)

Self-consistency of ASCC mass

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

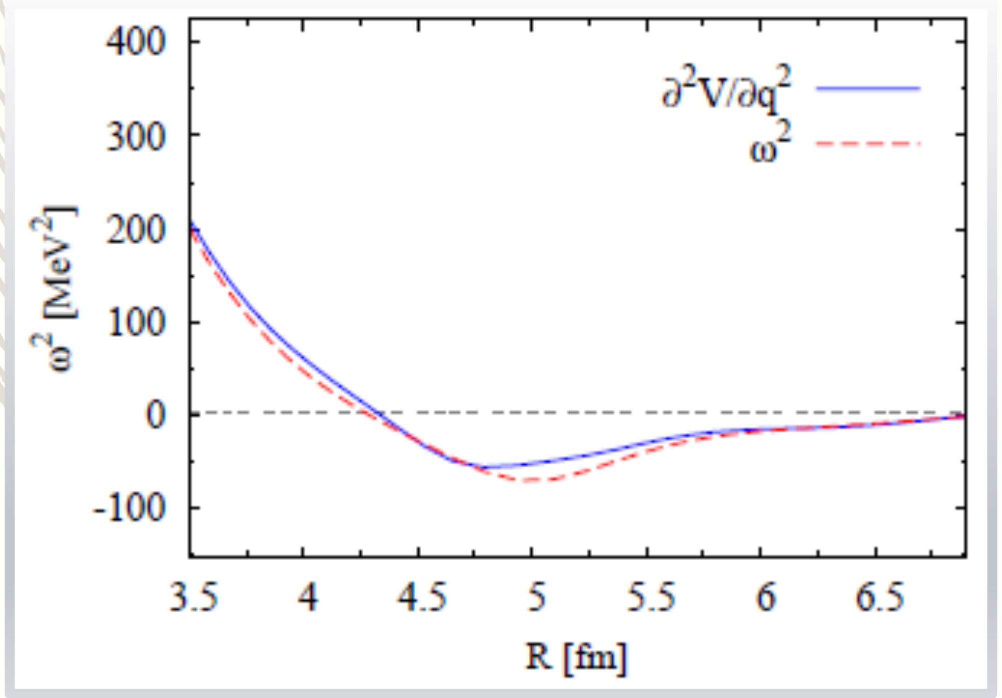
- Interpretation of RPA eigenvalue ω^2 :

$$\omega^2 = \frac{d^2 V_{\rm local}}{dq^2}$$

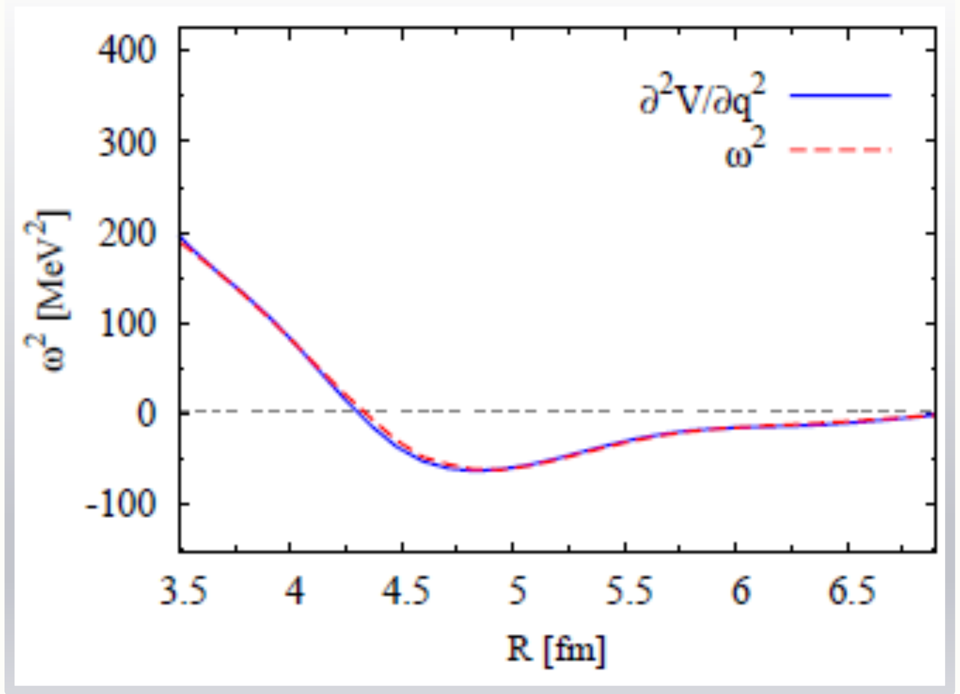
- The second order derivative of CHF potential:

$$\frac{d^2V}{dq^2} = \frac{d^2V}{dR^2}\left(\frac{dR}{dq}\right)^2 = \frac{d^2V}{dR^2}\frac{1}{M}$$

CHF+LRPA



ASCC



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- The Adiabatic Self-consistent Collective Coordinate (ASCC) Method
- The inertial mass for $^{8}Be \leftrightarrow \alpha + \alpha$.
- **The ASCC collective motion paths.**
  - $^{20}Ne \leftrightarrow {}^{16}O + \alpha$
  - $^{32}S \leftrightarrow {}^{16}O + {}^{16}O$
- 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

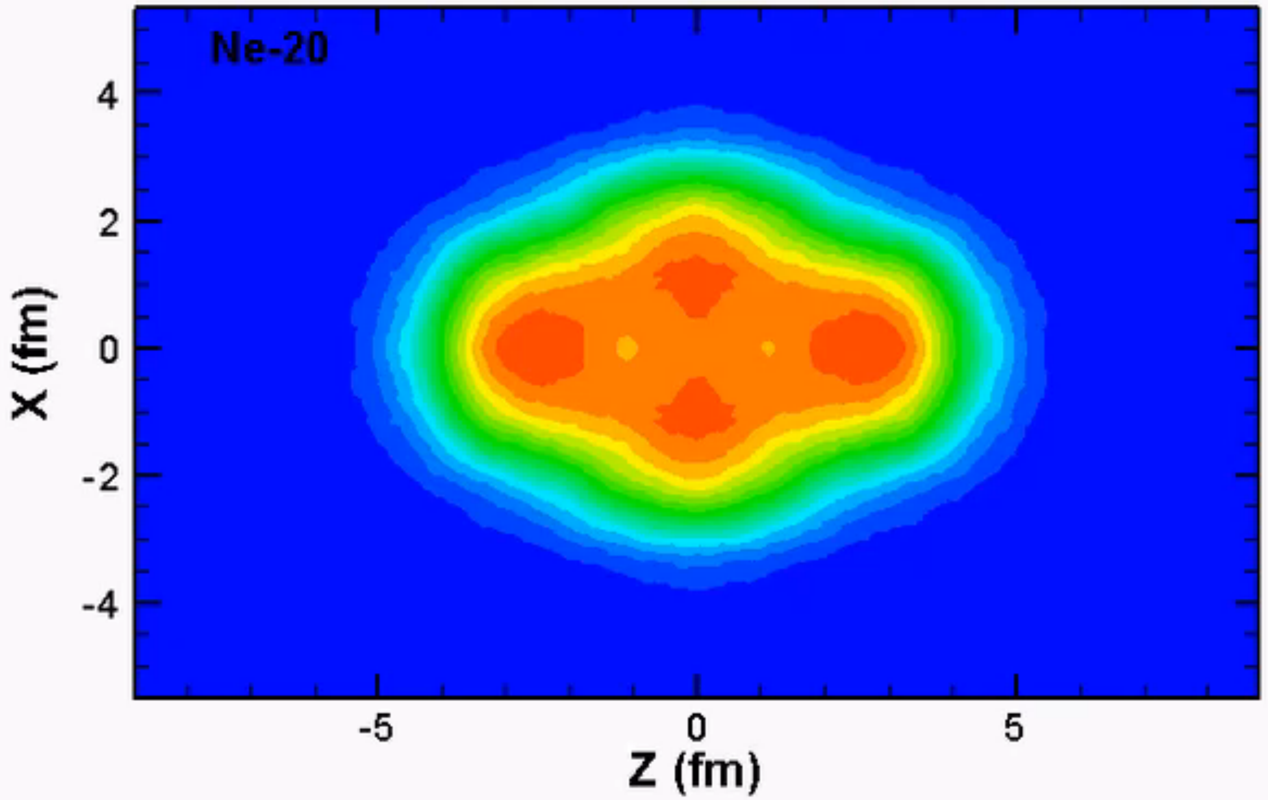
$$\Psi(q+\varepsilon)$$

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.

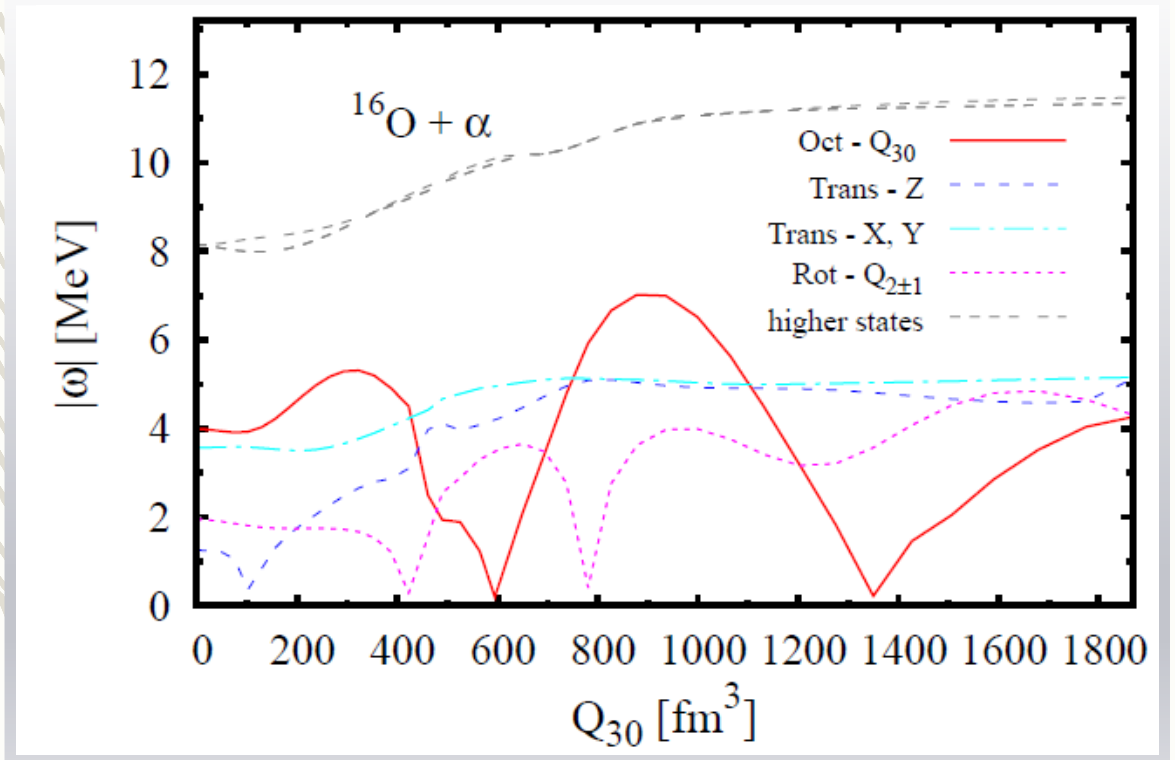
Collective motion path of fission from ^{20}Ne to ^{16}O + α

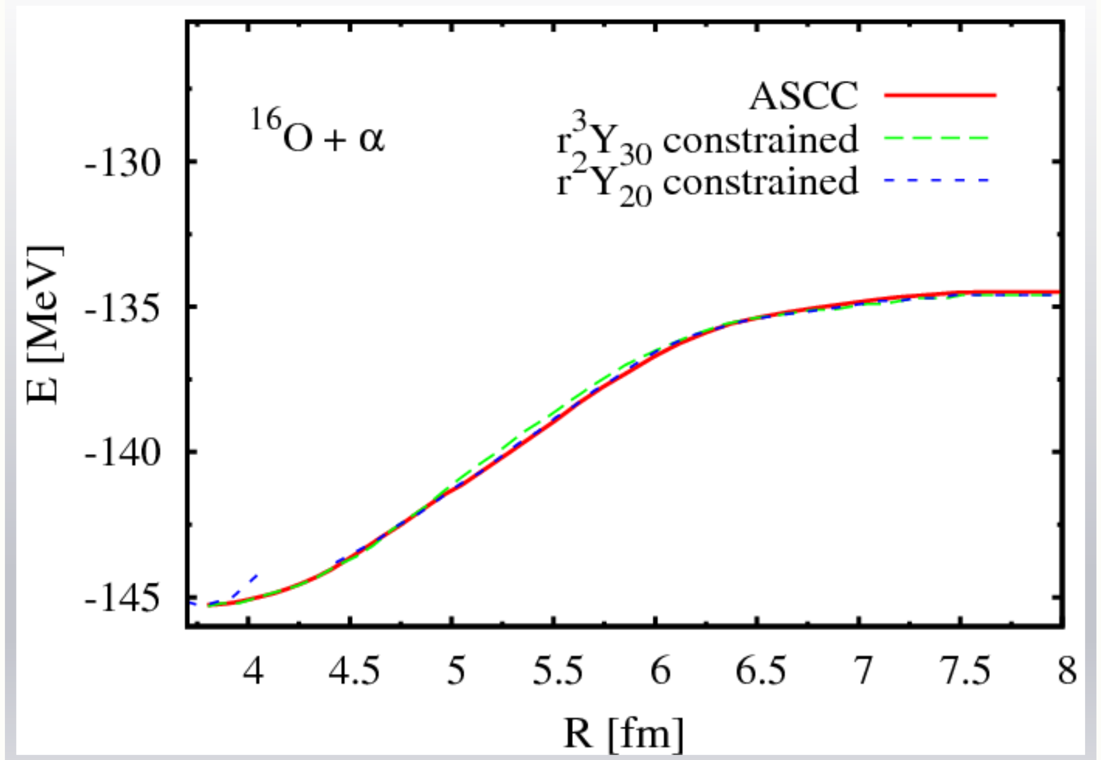


- *Starting from the ^{20} Ne at ground state, end up with ^{16}O +α*
- *The first physical moving RPA state with axial symmetry is used to develop the rajectory.*
- *Model space: rectangular box of 12×12×18 fm^3 with grid size 1.1 fm.*

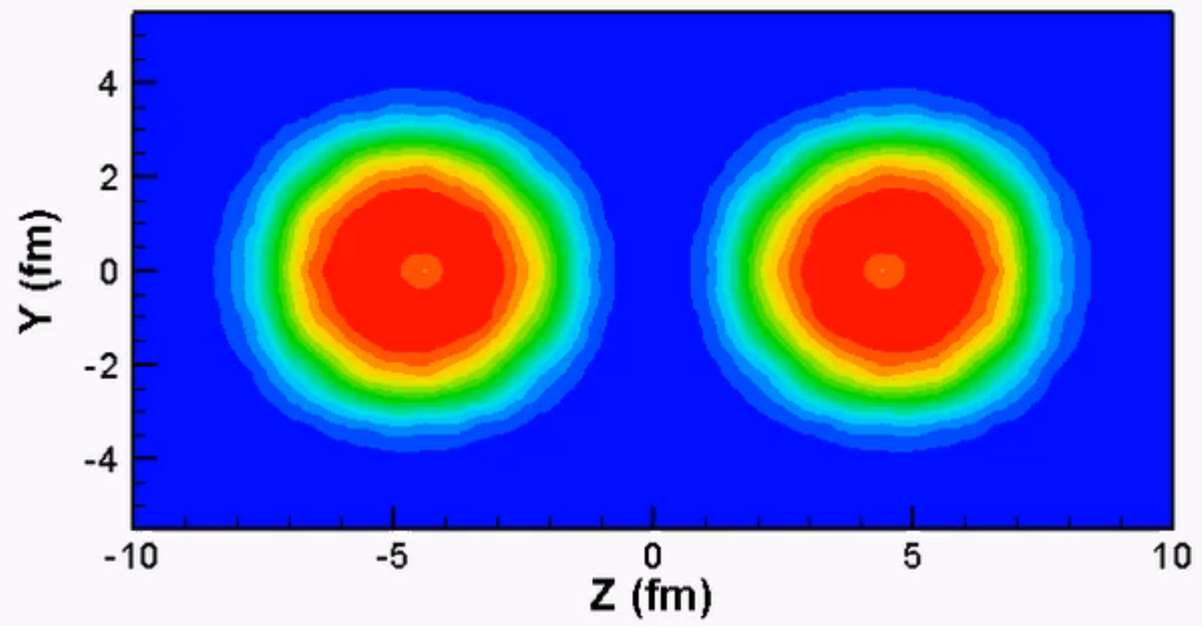
Collective motion path of $^{16}O + \alpha$

Eigen frequencies of the moving RPA states along the ASCC collective path





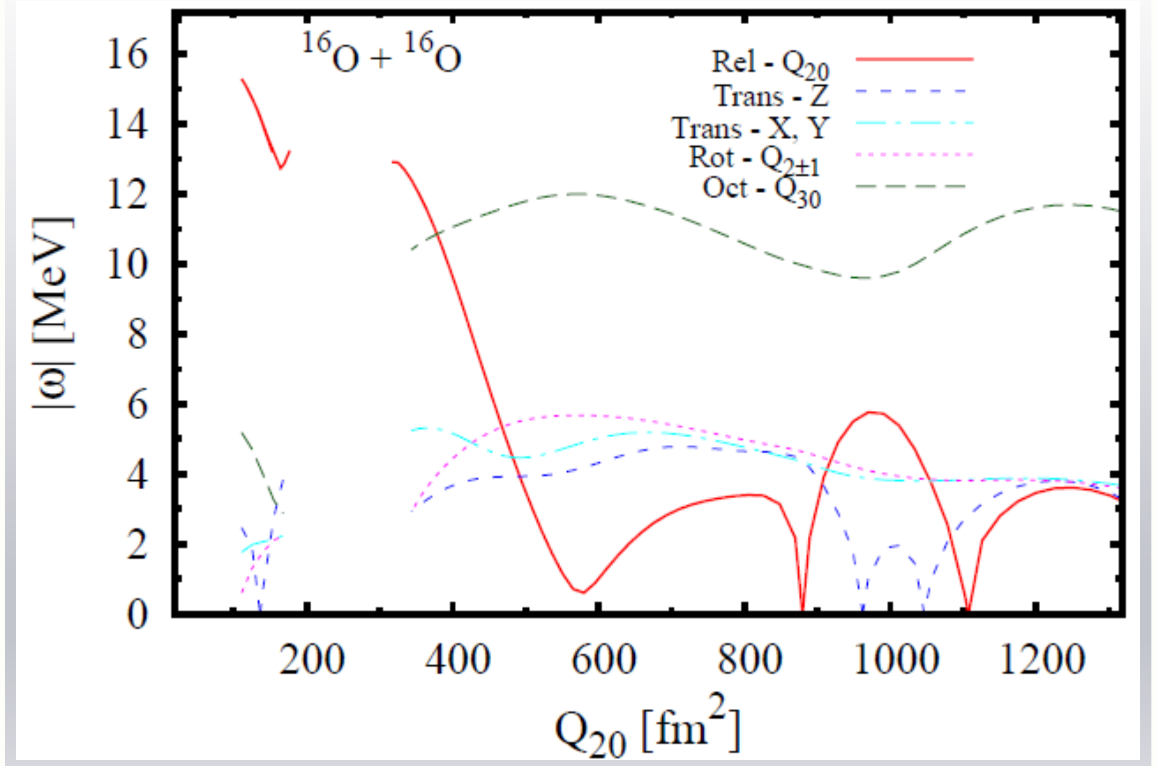
Collective motion path of scattering between $^{16}O + ^{16}O$



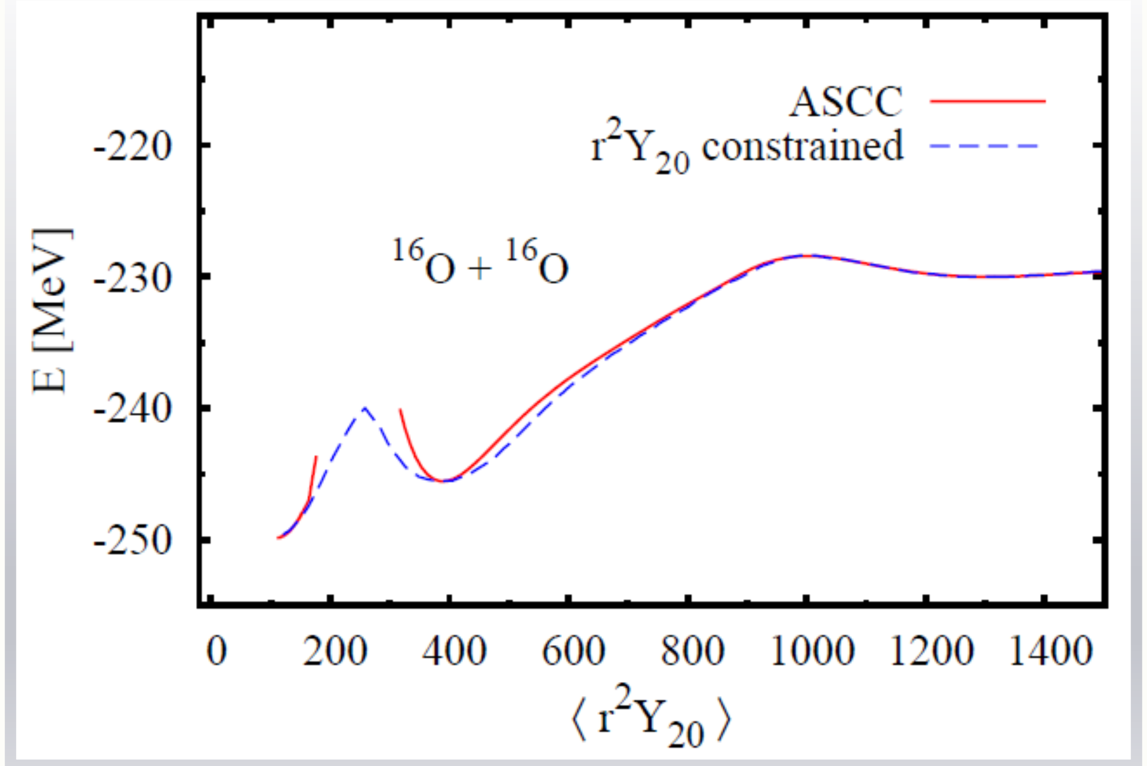
- *Starting from the separated $^{16}O + ^{16}O$, both at ground state.*
- *The first physical moving RPA state of quadrupole mode is used to develop the trajectory.*
- *Model space: rectangular box of $12 \times 12 \times 22$ fm^3 with grid size 1.1 fm.*

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

Eigen frequencies of the moving RPA states along the ASCC collective path



Potentials (CHF and ASCC)



Summary and Perspective

Thank you for your attention!

- *Based on the ASCC method, we proposed a method to extract the collective motion path.*
- *Applications have been performed for the system* α+α, ^{16}O+α, ^{16}O+^{16}O,
- *The inertial mass parameters are calculated self-consistently based on ASCC method.*

- *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.*
  - … …