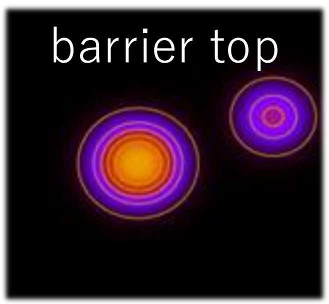
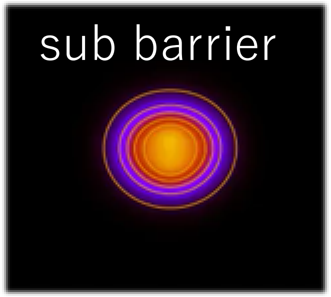
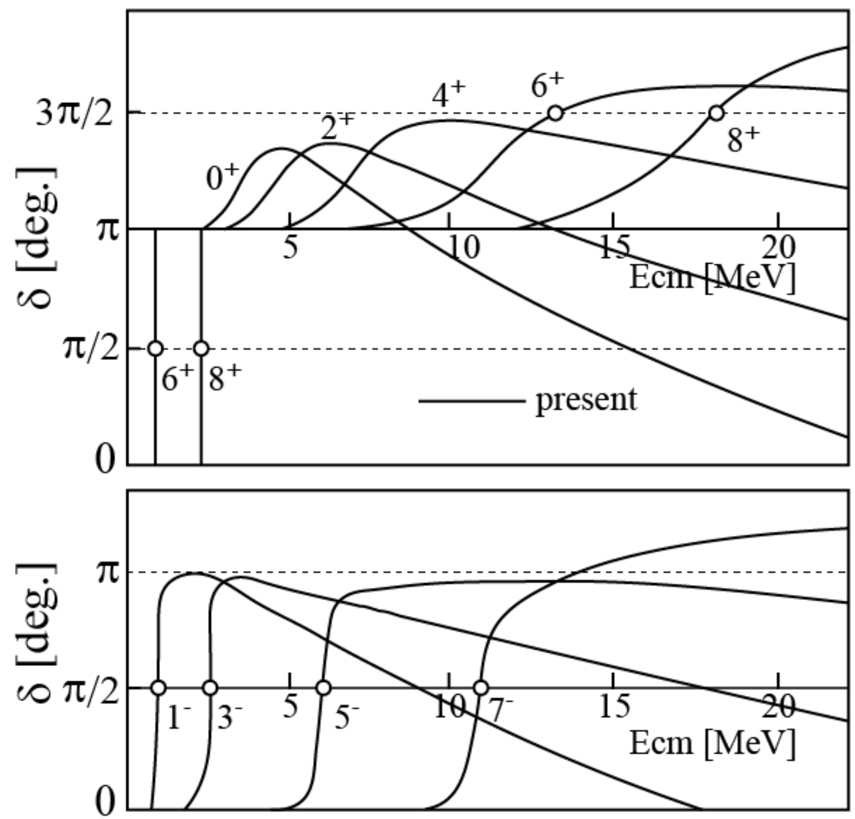
Generator Coordinate Method for low-energy scattering and tunneling

M. Kimura (RIKEN)

Phase shift analysis
by the time-dep. model



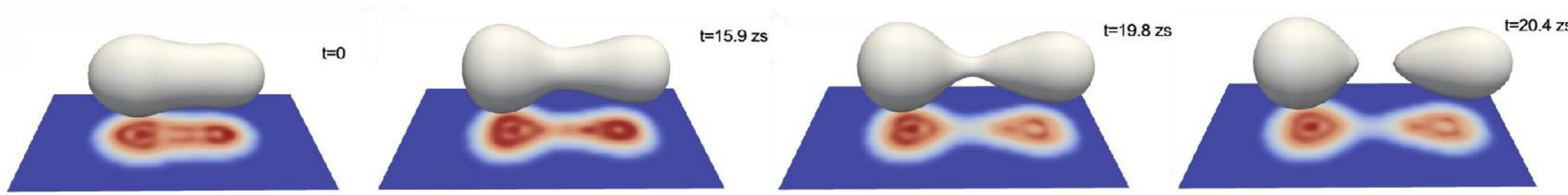




Background & Motivation

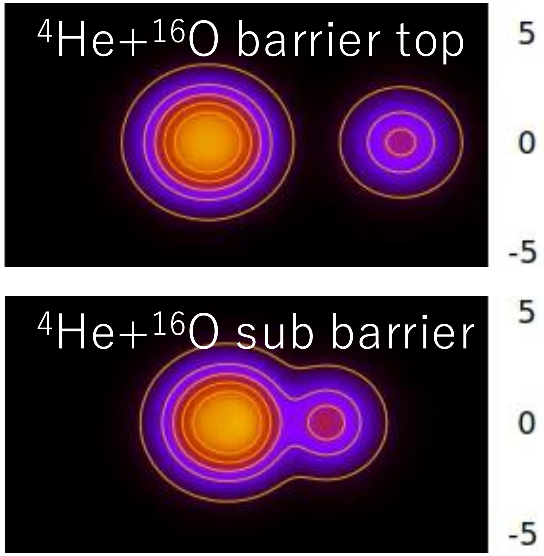
Challenge: Microscopic description of nuclear reactions and decays

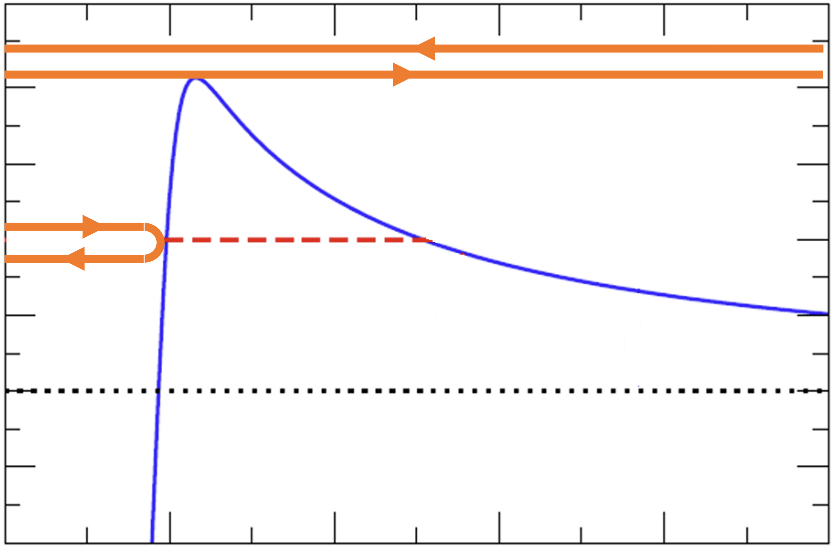
Time-Dependent many-body theory (TDHF etc)



G. Scamps and C. Simenel, Nature 564 (2018) 382

Cons: Deterministic reaction trajectory, No quantum tunneling,
too weak dissipation





Background & Motivation

A Challenge: Microscopic description of nuclear reactions and decays

(Time-Dependent) Generator Coordinate Method (GCM)

B.Li, et al., PRC108 (2023)

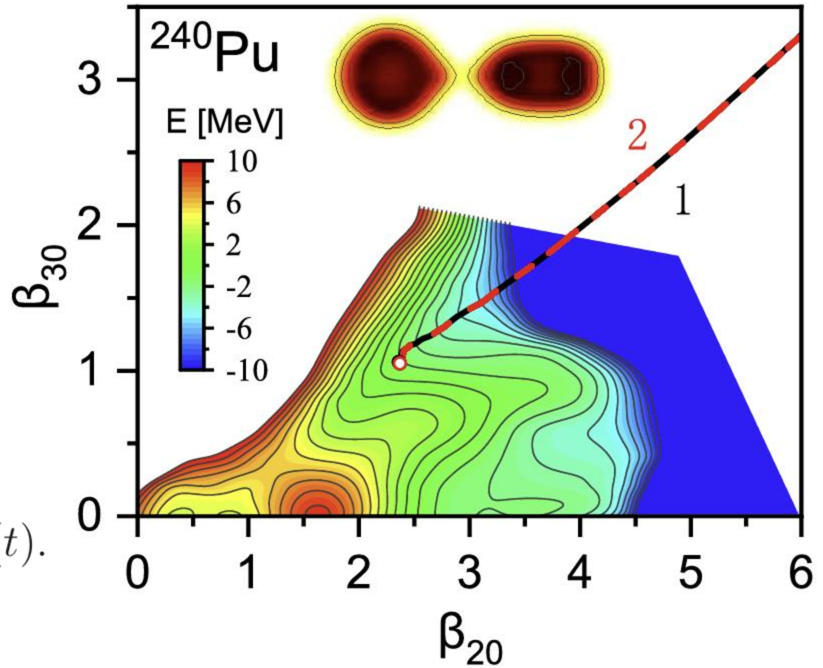
Time-Dependent GCM ansatz

$$|\Psi(t)\rangle = \int_{\boldsymbol{q}} d\boldsymbol{q}\ f_{\boldsymbol{q}}(t)|\Phi_{\boldsymbol{q}}(t)\rangle,$$

EoM for GCM amp & s.p. states

$$\sum_{\boldsymbol{q}} i\hbar\mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t)\partial_t f_{\boldsymbol{q}}(t) + \sum_{q} \mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t) = \sum_{q} \mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t).$$

$$i\hbar\partial_t|\Phi_{\boldsymbol{q}}(t)\rangle = \sum_{l_2}^{A} \hat{h}^{\boldsymbol{q}}(\boldsymbol{r},t)c^{\dagger}_{\boldsymbol{q},l_2}(t)c_{\boldsymbol{q},l_2}(t)|\Phi_{\boldsymbol{q}}(t)\rangle,$$



Cons: Still not enough to describe tunneling

Ad-hoc introduction of the generator coodinates

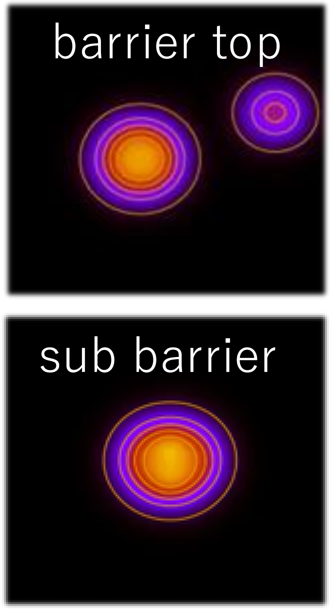
Large computational cost?

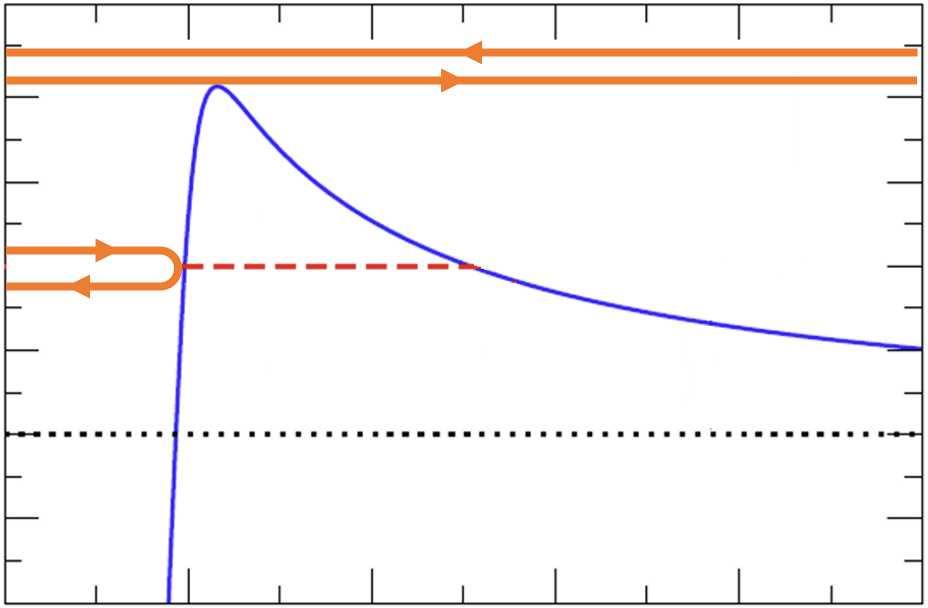
Overview of a new method

We are developing a GCM framework for the scattering problem, combined with time-dependent models

Key points

- ◯ GCM equation for the scattering problems
  derived from Kohn-Hulthen variational principle
- ◯ GCM anzats is generated by the time-dependent models
  without introducing the generator coordinate.





Kohn-Hulthen variational principle

W. Kohn, PR74 (1948); L. Hulthen, et al., Ark. Mat. Astr. Fys. 35 (1948).

○ Linear operator for scattering of nucleus A and B

$$\mathcal{L}_\ell(r, r', \xi) := H - E$$

$$= \left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2\mu r^2} + V_{\rm direct}(r) - E_{cm} \right] \delta(r, r') + V_{\rm exc.}(r, r') + H_{A+B}(\xi) - E_{A+B}$$

○ Schrödinger Eq. for nucleus-nucleus scattering

$$\mathcal{L}_\ell u_\ell := \int dr' \mathcal{L}_\ell(r, r', \xi) u_\ell(r', \xi) = 0,$$

with the boundary condition $u_\ell(r) \to \left[\phi^{(-)}(kr) - S_\ell \phi^{(+)}(kr) \right] \Phi_A \Phi_B$

Incoming Coulomb — Outgoing Coulomb

○ Action J and its variation

$$J_\ell[\widetilde{u}_\ell] := S_\ell + i\frac{\mu}{k}\langle \widetilde{u}_\ell | \mathcal{L}_\ell \widetilde{u}_\ell \rangle$$

$$\delta J_\ell[\widetilde{u}_\ell] = 2i\frac{\mu}{k}\langle \delta\widetilde{u}_\ell | \mathcal{L}_\ell \widetilde{u}_\ell \rangle = 0. \quad \Longleftrightarrow \quad \mathcal{L}_\ell \widetilde{u}_\ell = 0,$$

Thus, the scattering problem reduces to the variational problem

GCM equations for scattering problems

○ Kohn-Hulthen variational principle

$$\mathcal{L}_\ell(r, r', \xi) := H - E$$

$$\delta J_\ell[\widetilde{u}_\ell] = 2i\frac{\mu}{k}\langle\delta\widetilde{u}_\ell|\mathcal{L}_\ell\widetilde{u}_\ell\rangle = 0. \quad \Longleftrightarrow \quad \mathcal{L}_\ell\widetilde{u}_\ell = 0,$$

○ Insert GCM ansatz,

Y. Mito and M. Kamimura, PTP56, 583 (1976).

$$\widetilde{u}_l(r,\xi) = \underbrace{c_1\Phi_1 + c_2\Phi_2 + \ldots + c_N\Phi_N}_{\text{Ordinary GCM ansatz}} + \underbrace{\left[\phi^{(-)}(kr) - S_\ell\phi^{(+)}(kr)\right]\Phi_A\Phi_B}_{\text{Scatt. boundary cond.}}$$

Ordinary GCM ansatz **Scatt. boundary cond.**

we get a set of linear equations.

$$\begin{pmatrix} \langle\Phi_1|H-E|\Phi_1\rangle & \cdots & \langle\Phi_1|H-E|\Phi_N\rangle & -\langle\Phi_1|H-E|\phi^{(+)}\rangle \\ \vdots & & \vdots & \\ \langle\Phi_N|H-E|\Phi_1\rangle & \cdots & \langle\Phi_N|H-E|\Phi_N\rangle & -\langle\Phi_N|H-E|\phi^{(+)}\rangle \\ -\langle\phi^{(+)}|H-E|\Phi_1\rangle & \cdots & -\langle\phi^{(+)}|H-E|\Phi_N\rangle & -\langle\phi^{(+)}|H-E|\phi^{(+)}\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \\ S_\ell \end{pmatrix} = \begin{pmatrix} -\langle\Phi_1|H-E|\phi^{(-)}\rangle \\ \vdots \\ -\langle\Phi_N|H-E|\phi^{(-)}\rangle \\ -\langle\phi^{(-)}|H-E|\phi^{(-)}\rangle \end{pmatrix}$$

GCM equations for scattering problems

○ Ordinary GCM equation (HW equation)

- Eigenvalue problem
- Coefficient (eigenvector) c and energy E (eigen vector) are output

$$\begin{pmatrix} \langle\Phi_1|H-E|\Phi_1\rangle & \cdots & \langle\Phi_1|H-E|\Phi_N\rangle \\ \vdots & & \vdots \\ \langle\Phi_N|H-E|\Phi_1\rangle & \cdots & \langle\Phi_N|H-E|\Phi_N\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} = 0$$

○ GCM equation for scatt. problem

- Linear equations
- Coefficient c and S-matrix S_ℓ (solution of linear eqs.) are output
- E is input ($E = E_A + E_B + E_{cm}$)

$$\begin{pmatrix} \langle\Phi_1|H-E|\Phi_1\rangle & \cdots & \langle\Phi_1|H-E|\Phi_N\rangle & -\langle\Phi_1|H-E|\phi^{(+)}\rangle \\ \vdots & & \vdots & \\ \langle\Phi_N|H-E|\Phi_1\rangle & \cdots & \langle\Phi_N|H-E|\Phi_N\rangle & -\langle\Phi_N|H-E|\phi^{(+)}\rangle \\ -\langle\phi^{(+)}|H-E|\Phi_1\rangle & \cdots & -\langle\phi^{(+)}|H-E|\Phi_N\rangle & -\langle\phi^{(+)}|H-E|\phi^{(+)}\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \\ S_\ell \end{pmatrix} = \begin{pmatrix} -\langle\Phi_1|H-E|\phi^{(-)}\rangle \\ \vdots \\ -\langle\Phi_N|H-E|\phi^{(-)}\rangle \\ -\langle\phi^{(-)}|H-E|\phi^{(-)}\rangle \end{pmatrix}$$

GCM anzats

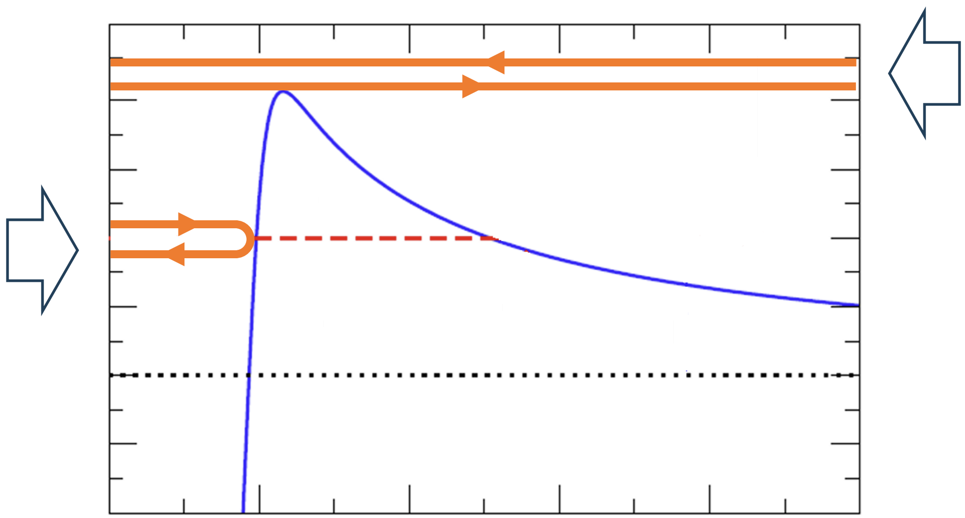
How can we prepare GCM anzats?

$$\widetilde{u}_l(r,\xi) = \underline{c_1\Phi_1 + c_2\Phi_2 + \ldots + c_N\Phi_N} + \left[\phi^{(-)}(kr) - S_\ell \phi^{(+)}(kr)\right] \Phi_A \Phi_B$$

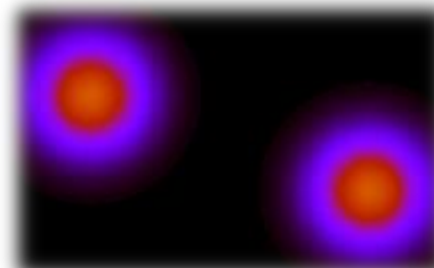
GCM ansatz (wave functions along time-dev.)

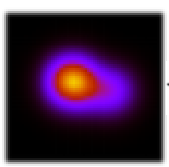
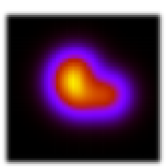
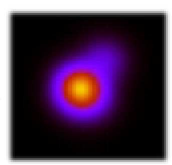
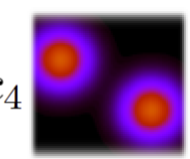
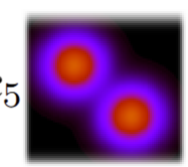
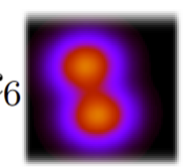
We generate basis functions along the reaction path by time-dep. models

Time-Evo.
below barrier



Time-Evo.
above barrier



$\widetilde{u}_l(r,\xi) = c_1$  $+ c_2$  $+ c_3$  $+ c_4$  $+ c_5$  $+ c_6$  $+ \ldots$

$$+ \left[\phi^{(-)}(kr) - S_\ell \phi^{(+)}(kr)\right] \Phi_A \Phi_B$$

Time-Dep. Molecular Dynamics (and TDHF)

Model wave function (time-dependent wave packets)

Each nucleon is described by time-dependent Gaussian wave packets

$$\phi(\boldsymbol{Z}_i(t)) = \exp\left\{-\nu(\boldsymbol{r} - \boldsymbol{Z}_i(t))^2\right\}(\alpha_i(t)\left|\uparrow\right\rangle + \beta_i(t)\left|\downarrow\right\rangle)$$

Many-body system is described by the Slater determinant of the time-dependent wave packets,

$$\Phi(t) = \mathcal{A}\left\{\phi(\boldsymbol{Z}_1(t)), ..., \phi(\boldsymbol{Z}_A(t))\right\}$$

Time-dependent parameters of the model

$\boldsymbol{Z}_i(t)$: Centroids of wave packets (position and momentum of a nucleon)

$\alpha_i(t)$ $\beta_i(t)$: Spin direction of a nucleon

Hamiltonian

Microscopic Hamiltonian with effective NN interactions (Minnesota & Gogny)

$$H = \sum_{i=1}^{A} t(i) - t_{cm} + \sum_{i<j}^{A} v(ij)$$

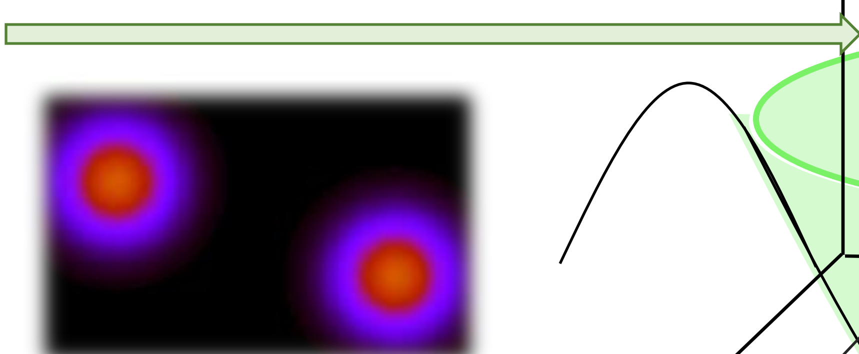
Time-Dep. Molecular Dynamics (and TDHF)

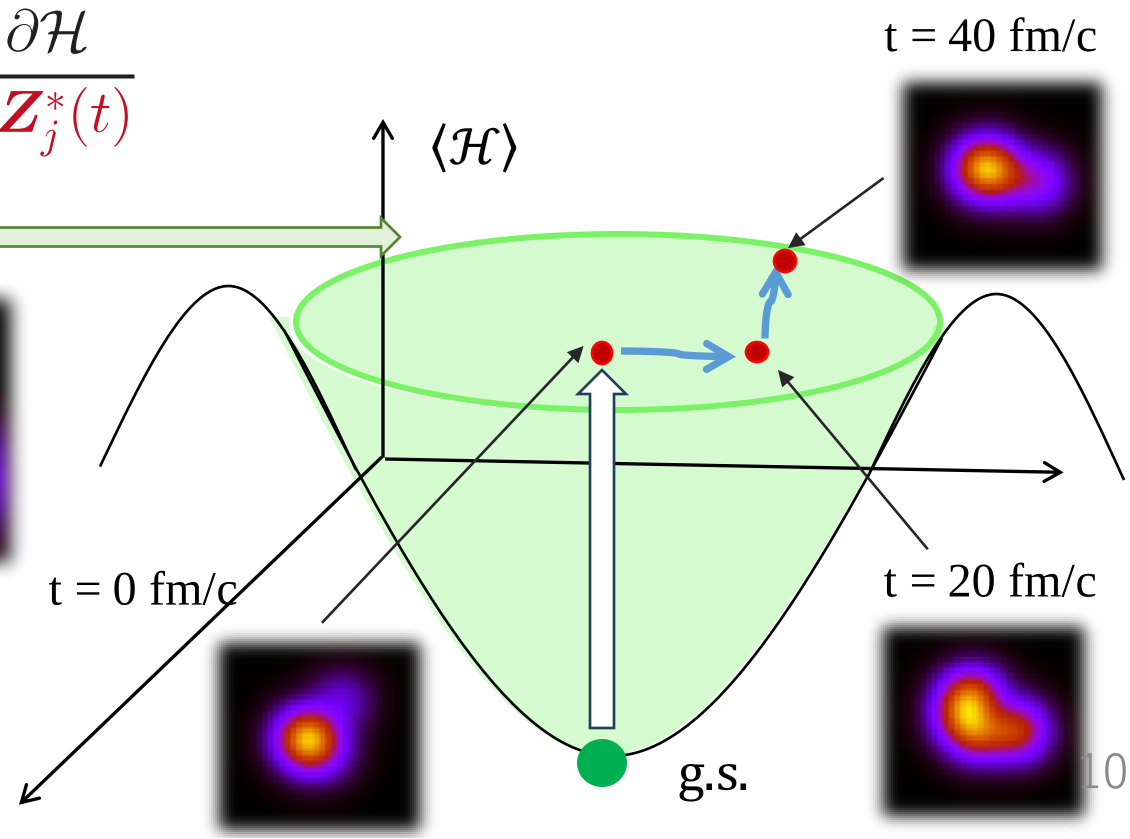
Time-dependent variational principle

$$\delta \int dt \, \frac{\langle \Phi(t) | i\hbar d/dt - H | \Phi(t) \rangle}{\langle \Phi(t) | \Phi(t) \rangle} = 0$$

Equation of motion for nucleon wave packets

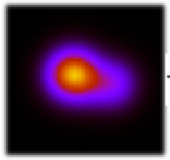
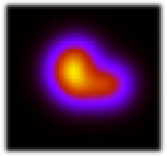
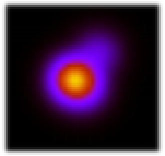
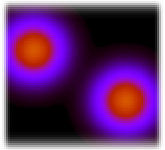
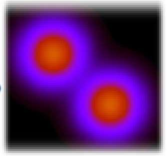
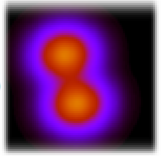
$$\Rightarrow \quad i\hbar \frac{d\mathbf{Z}_i(t)}{dt} = \sum_j C_{ij}^{-1} \frac{\partial \mathcal{H}}{\partial \mathbf{Z}_j^*(t)}$$



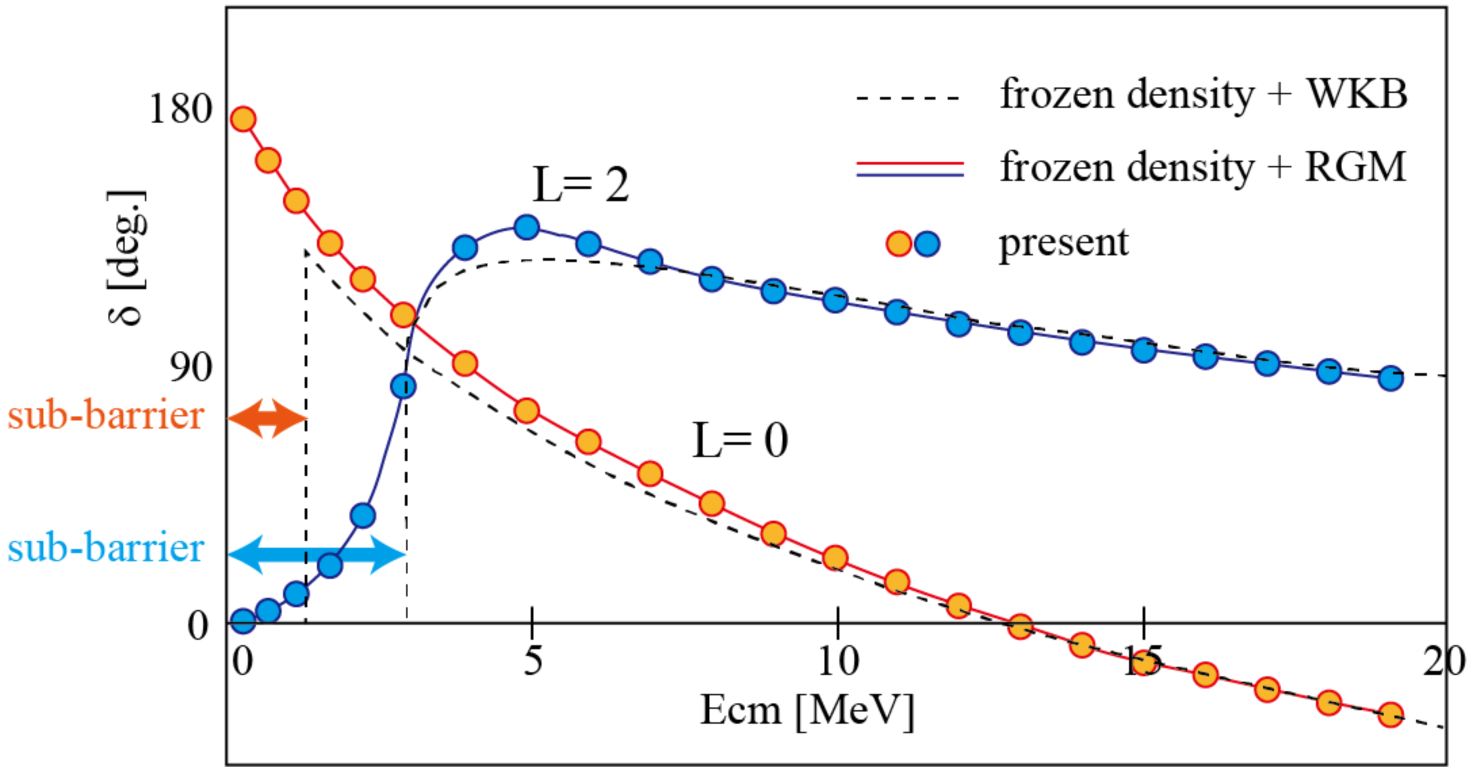


Numerical example ($^4He+^4He$)

- ○ 50 ∼ 100 basis are superposed after AMP
- ○ ^{4}He+^{4}He scattering phase shifts are reasonably described
- ○ Phase shift below the Coulomb barrier is

$\tilde{u}_l(r,\xi) = c_1$  $+\, c_2$  $+\, c_3$  $+\, c_4$  $+\, c_5$  $+\, c_6$  $+ \dots$

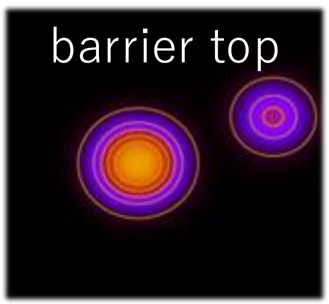
$$+ \left[\phi^{(-)}(kr) - S_\ell \phi^{(+)}(kr)\right] \Phi_A \Phi_B$$

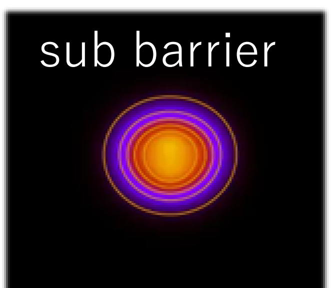


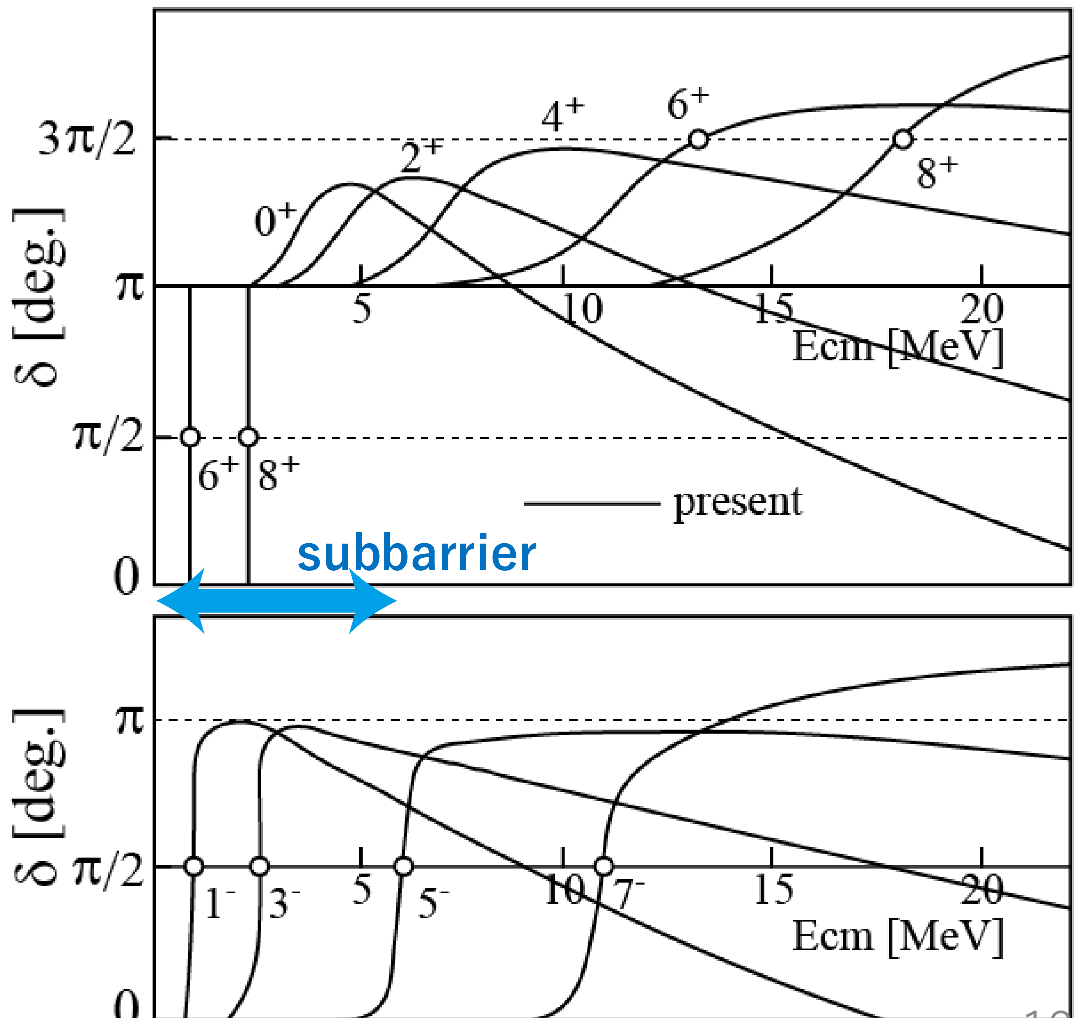
Numerical example ($^{4}He+^{16}O$)

$^{4}He+^{16}O$ scattering shows more complicated behavior due to the presence of the bound state

- ○ Sharp 6^+, 8^+ resonances
- ○ Other states start from π (Levinson's theorem)
- ○ Sharp resonances in the negative-parity (1^-, 3^-, 5^-, 7^-)

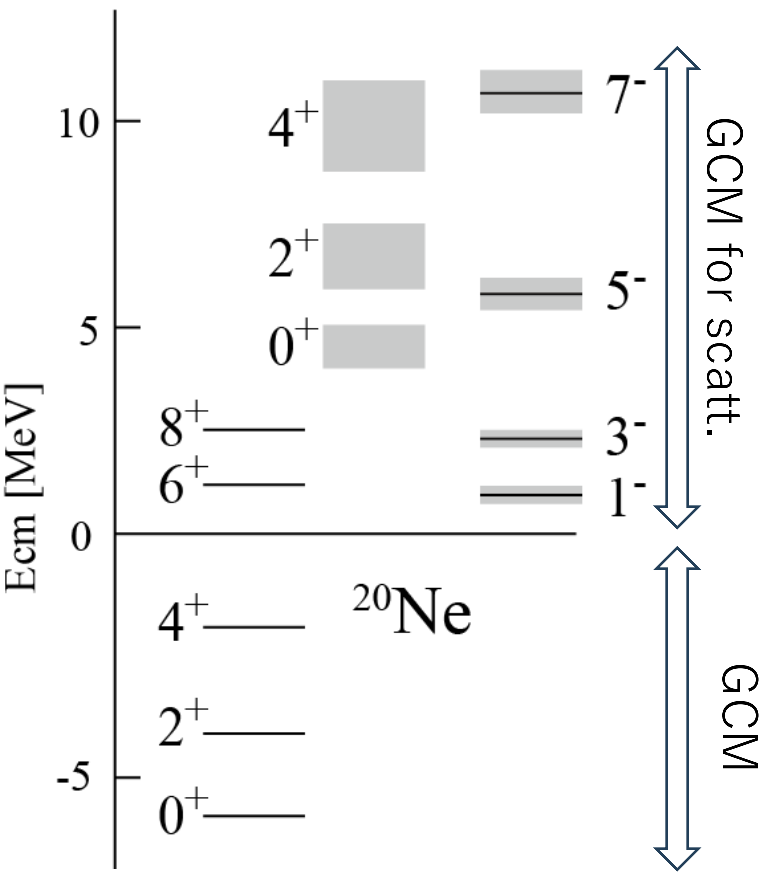


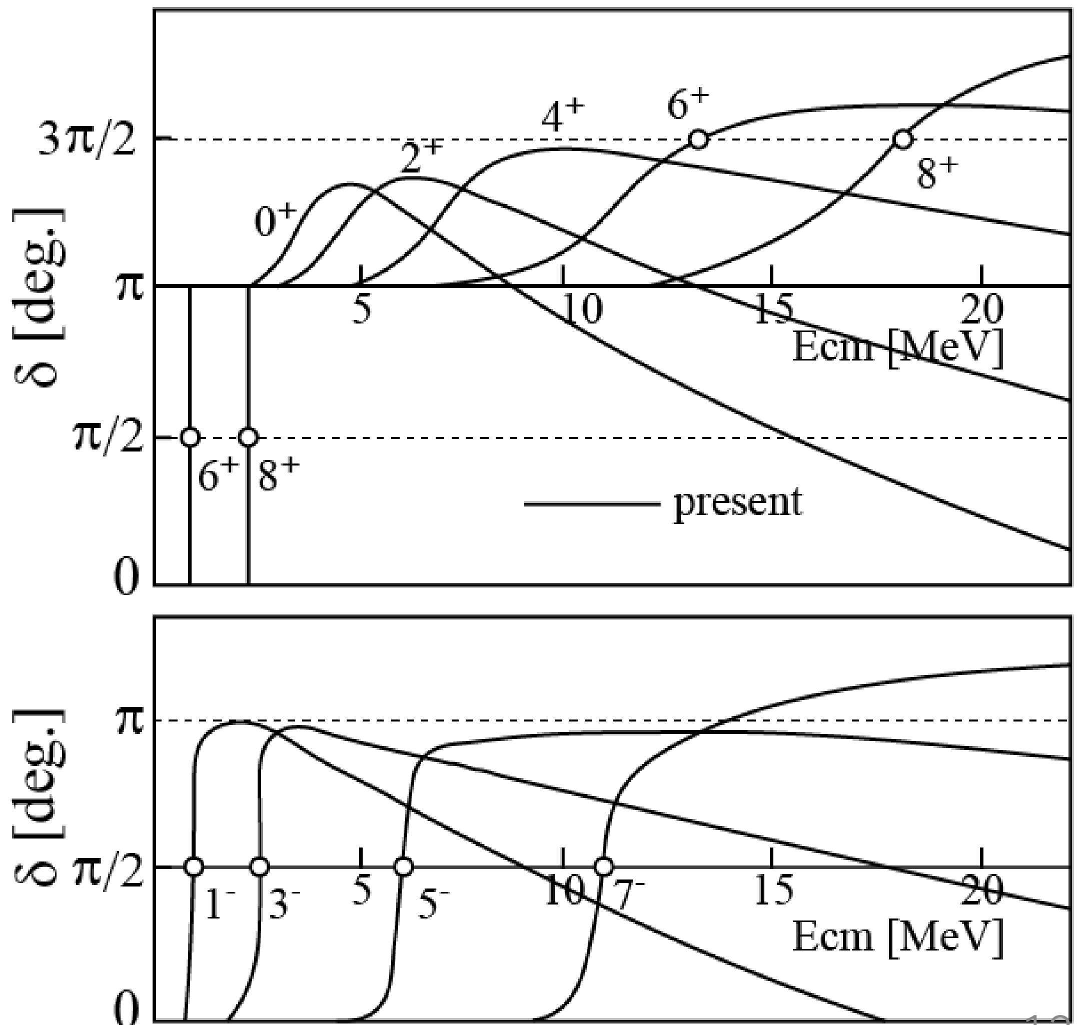




Numerical example ($^4He+^{16}O$)

○ From the phase shift analysis, we have identified the resonances
○ The bound states are also calculated by ordinary GCM





Summary and Outlook

GCM framework for low-energy scattering

○ Kohn-Hulthen variational principle

○ GCM anzats generated by the time-dependent models

Numerical examples

○ Phase shift analysis of ^{4}He+^{4}He and ^{4}He+^{16}O

○ Reasonable description of quantum tunneling

○ Unified description of the bound, resonant and scattering states by GCM

Outlook

○ Extension to the inelastic and transfer reactions

○ Application to the astrophysical reactions of light nuclei

○ TDHF-based calculation for heavier systems

○ Application to the alpha decay and induced fission of heavier nuclei