Towards microscopic description of nuclear fusion reactions based on the time-dependent generator coordinate method

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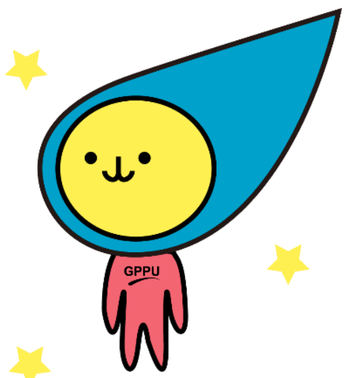

8th February 2019

GPPU 宇宙創成物理学国際共同大学院

Overview

Tunneling is essential for fusion reaction

There is no established microscopic method which can describe tunneling

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We try to construct a new method with tunneling

with Time Dependent Generator Coordinate Method (TDGCM)

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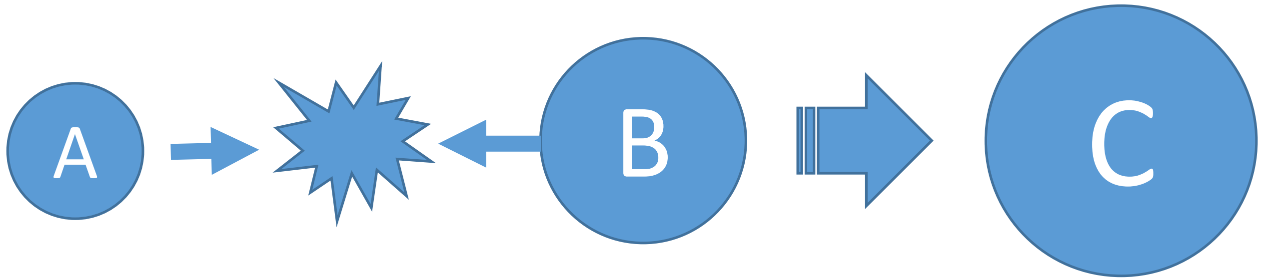
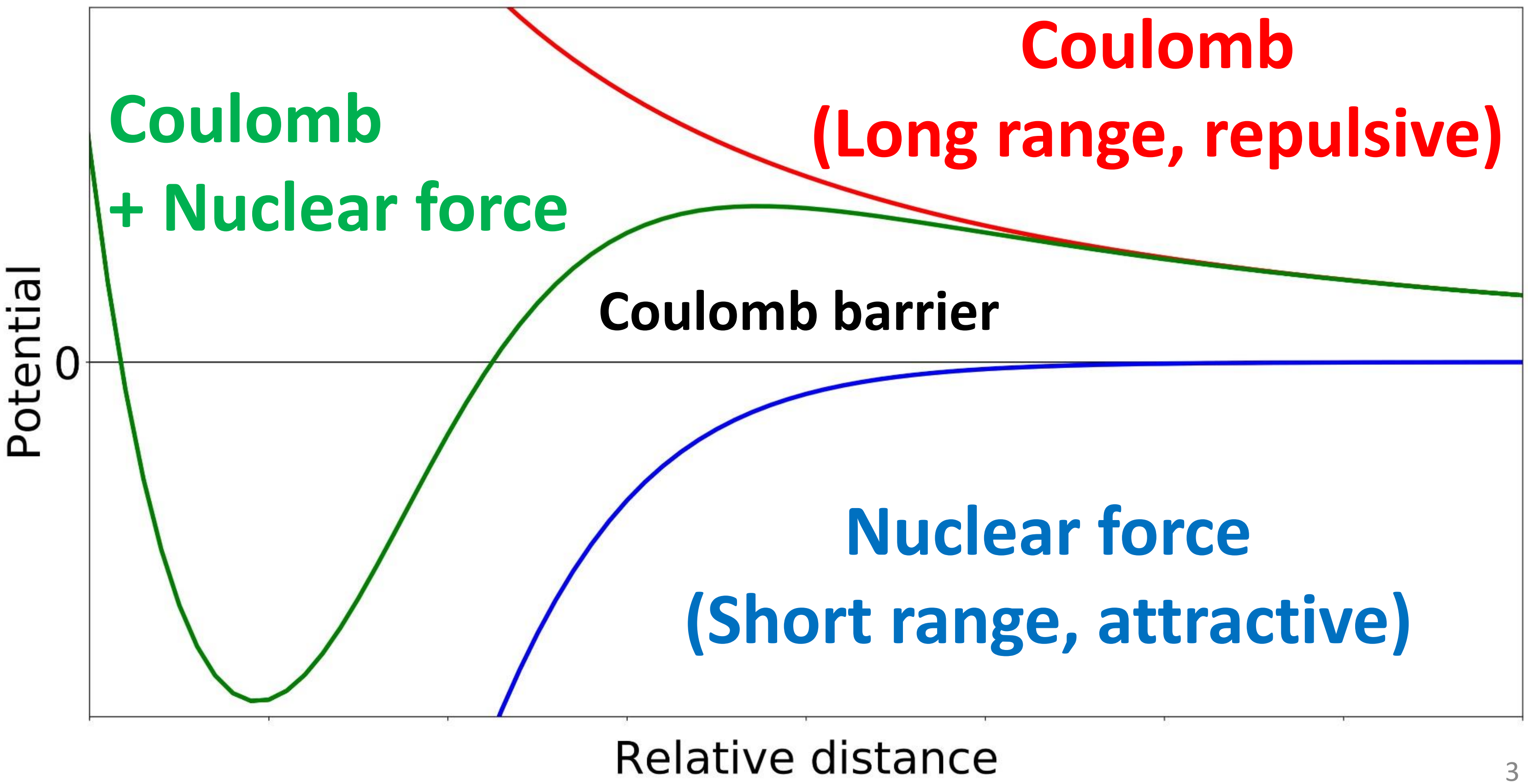
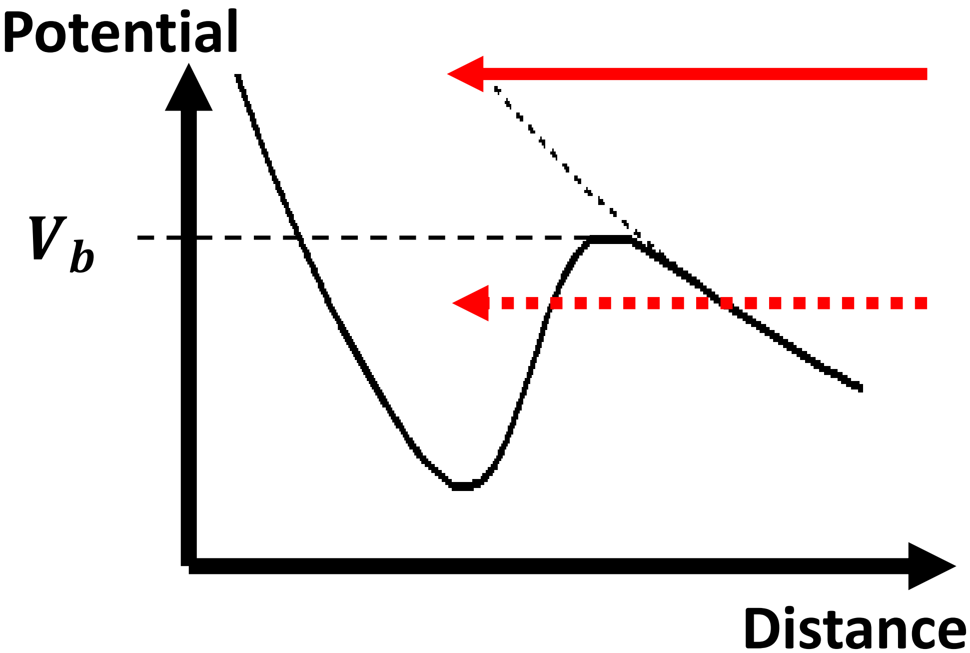
We show a limit of validity of an approximation method in TDGCM for nuclear reaction calculation

Nuclear fusion reaction





Nuclear fusion reaction



If $E > V_b$
Fusion occurs classically

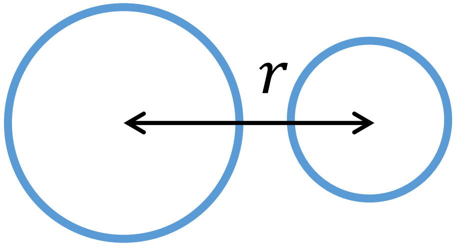
If $E < V_b$
Fusion only occurs with tunneling

Tunneling is essential for low energy fusion

$E < V_b$
for fusion in stars

Theory of fusion reactions

1. Macroscopic method

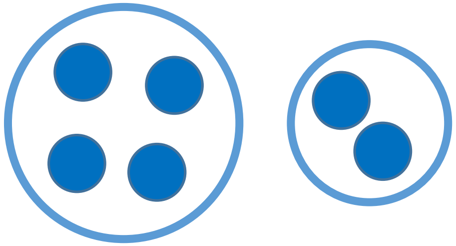


Describes fusion reaction
as a two-body problem

Low calc. cost

many
empirical parameters

2. Microscopic method



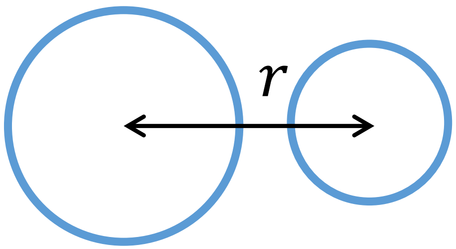
Describes fusion reaction
based on nucleon degrees of freedom

few
empirical parameters

High calc. cost

Theory of fusion reactions

1. Macroscopic method



Describes fusion reaction
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Low calc. cost

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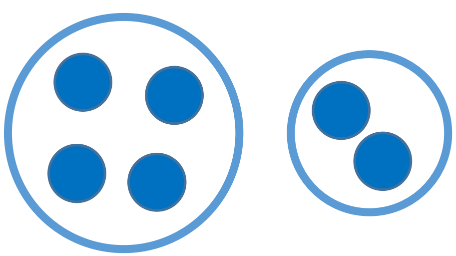
2. Microscopic method

Today's Topic



Describes fusion reaction
based on nucleon degrees of freedom

few
empirical parameters

High calc. cost

Microscopic theory

Describe nuclear reaction

based on nucleon degrees of freedom

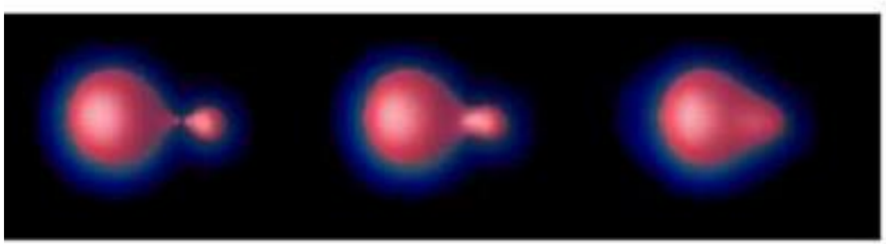
Major method: Time Dependent Hartree-Fock (TDHF)

Many-body wave function
→ Slater determinant
（Mean-field approximation）

Equations of motion for single particle wave functions

$$\Phi(t) = \mathcal{A}\{\varphi_1(t)\varphi_2(t)\dots\varphi_A(t)\}$$

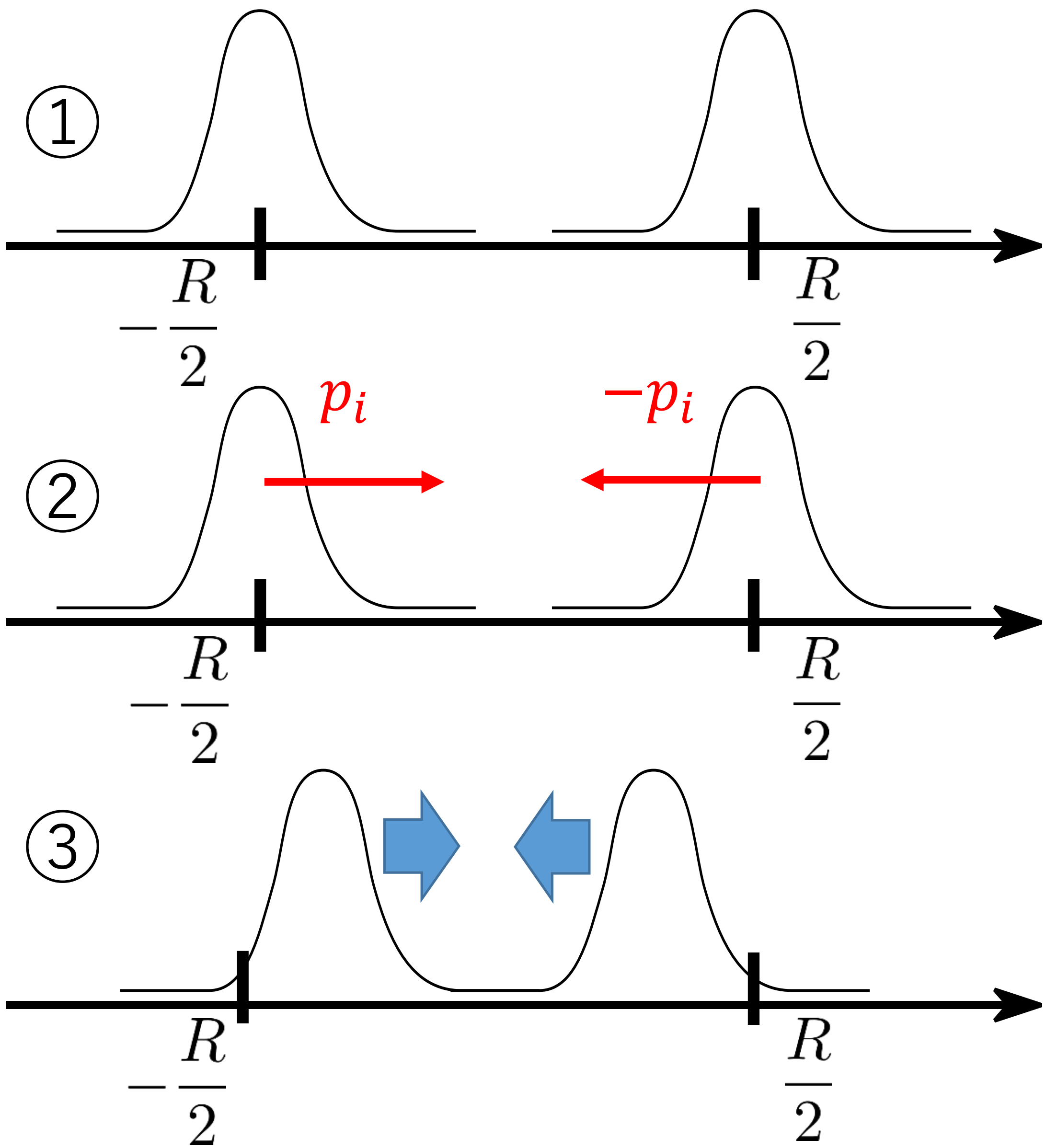
$$i\hbar\dot{\varphi}_\alpha = h[\rho]\varphi_\alpha$$



Used for nuclear reaction calc. for $E > V_b$

C. Simenel EPJA48('12)152

Nuclear Collision with TDHF



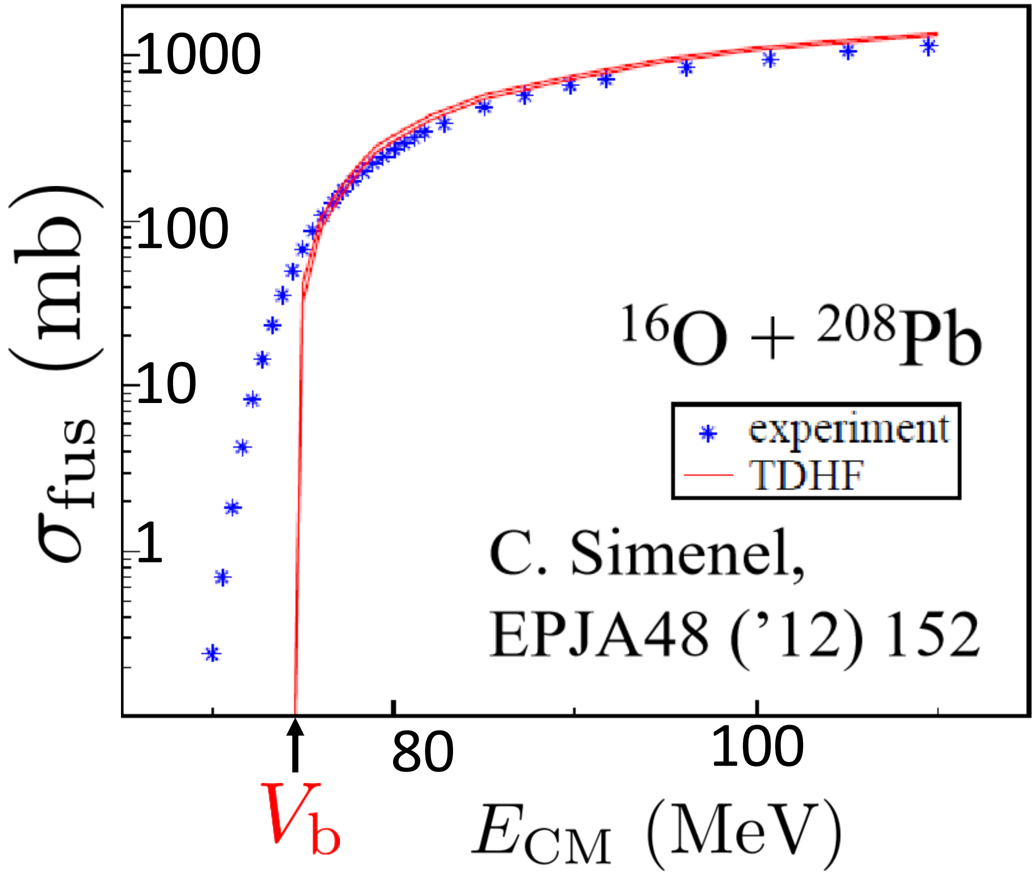
Put nuclei at left and right

Boost them toward the origin

Calculate time evolution with TDHF

$$i\hbar\dot{\varphi}_\alpha = h[\rho]\varphi_\alpha$$

Fusion cross-section



TDHF does not work below the barrier energy

Fails to describe tunneling

There is no established microscopic theory which can describe tunneling

Theory with tunneling effect

There is no established microscopic method with tunneling effect

The theory **beyond mean field** is needed

Time-Dependent Generator Coordinate Method (TDGCM)

Time-Dependent Generator Coordinate Method

Wave function of the system

→ Superposition of Slater determinants

P. G. Reinhard, R. Y. Cusson and K. Goeke
Nucl. Phys. A 398 141-188(1983)

Weight function ↓ Slater determinant ↓

$$|\Psi(t)\rangle = \int da f(a,t)\,|\Phi(a,t)\rangle$$

⟺

cf. TDHF

$$|\Psi(t)\rangle = |\Phi(t)\rangle$$

Generator Coordinate : a Macroscopic quantities (e.g. Deformation parameter)

Weight function f and Slater determinants
are determined by Time-dependent variational method

Time-Dependent Generator Coordinate Method

$$\int da' \, \langle \Phi(a,t) | H - i\partial_t | \Phi(a',t) \rangle \, f(a',t) = i \int da' \, \langle \Phi(a,t) | \Phi(a',t) \rangle \, \dot{f}(a',t)$$

$$\sum_{a'} \mathcal{H}_{aa'} f_{a'} = i \sum_{a'} \mathcal{N}_{aa'} \dot{f}_{a'}$$

$$\begin{cases} \mathcal{N}_{aa'} = \langle \Phi(a,t) | \Phi(a',t) \rangle \\ \mathcal{H}_{aa'} = \langle \Phi(a,t) | H - i\partial_t | \Phi(a',t) \rangle \end{cases}$$

: **Norm kernel**

: **Hamiltonian kernel**

Time evolution of f is determined by these $\mathcal{H}_{aa'}$ and $\mathcal{N}_{aa'}$

Time-Dependent Generator Coordinate Method

$$\sum_{a'} \mathcal{H}_{aa'} f_{a'} = i \sum_{a'} \mathcal{N}_{aa'} \dot{f}_{a'}$$

$$\begin{cases} \mathcal{H}_{aa'} = \langle \Phi(a,t) | H - i\partial_t | \Phi(a',t) \rangle \\ \mathcal{N}_{aa'} = \langle \Phi(a,t) | \Phi(a',t) \rangle \end{cases}$$

$$|\Phi(a,t)\rangle \Rightarrow |\Phi^{(\mathrm{TDHF})}(a,t)\rangle$$

instead of solving variational equation

P. G. Reinhard, R. Y. Cusson and K. Goeke
Nucl. Phys. A 398 141-188(1983)

TDHF

$$i\hbar\dot{\varphi}_i^{(a)} = h[\rho_a]\varphi_i^{(a)}$$

$$\Phi(a,t) = \mathcal{A}\{\varphi_1^{(a)}\varphi_2^{(a)} \dots \varphi_A^{(a)}\}$$

Each $|\Phi_a^{(\mathrm{TDHF})}(t)\rangle$ is independent of f(t) and $|\Phi_{b\neq a}^{(\mathrm{TDHF})}(t)\rangle$

Description tunneling with TDGCM

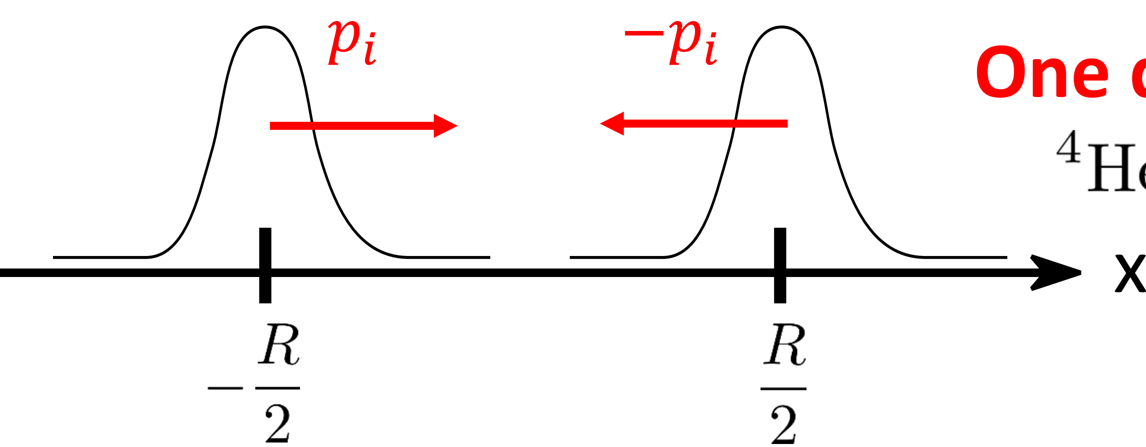
Choose initial relative momentum of the system p_i
as generator coordinate

$$|\Psi(t)\rangle = \int dp_i f(p_i, t) |\Phi_{p_i}^{(\mathrm{TDHF})}(t)\rangle$$

Calc. these quantities

Norm kernel： $\mathcal{N}(p_i, p_j) = \langle \Phi_{p_i} | \Phi_{p_j} \rangle$

Hamiltonian kernel： $\mathcal{H}(p_i, p_j) = \langle \Phi_{p_i} | H - i\partial_t | \Phi_{p_j} \rangle$



One dimensional
$^4\mathrm{He} + {}^4\mathrm{He}\ (\alpha + \alpha)$ **Collision**

Approximation in TDGCM

Gaussian Overlap Approximation (GOA)

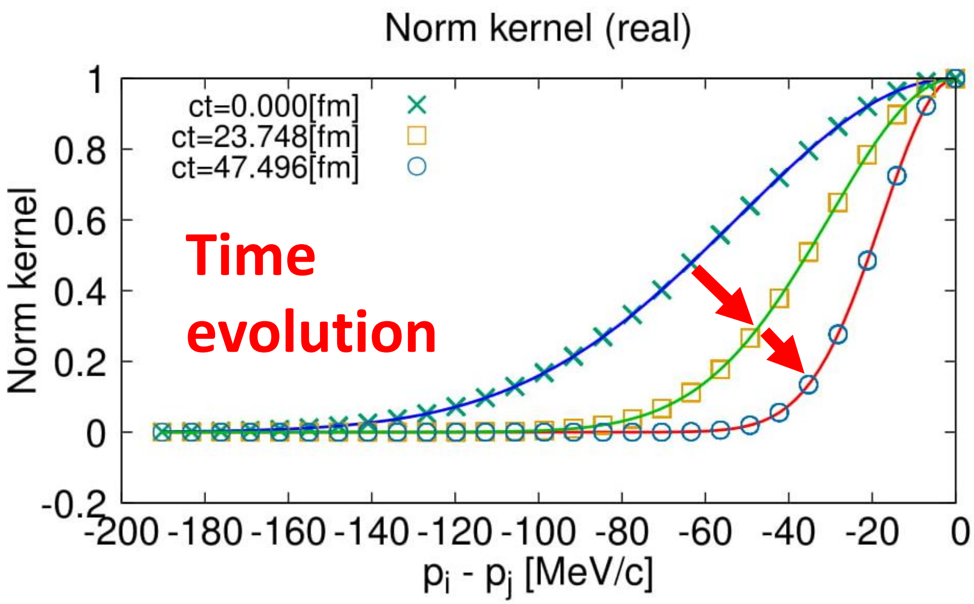
$$\mathcal{N}(p,p') \simeq e^{-(p-p')^2/4\mu}$$
$$\mathcal{H}(p,p') \simeq e^{-(p-p')^2/4\mu}\left(H_0 + H_2(p-p')^2\right)$$

Simplify $\hat{\mathcal{H}} f = i \hat{\mathcal{N}} \dot{f}$

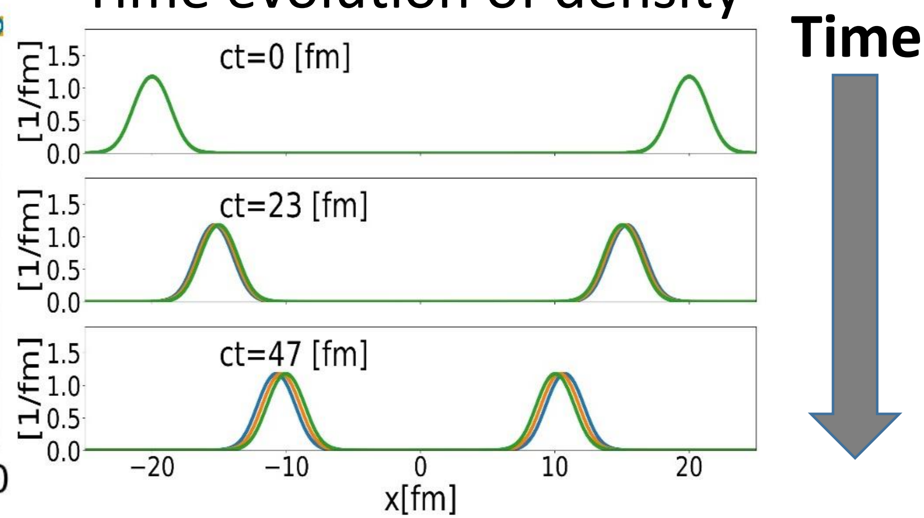
Frequently used for static GCM calculation

For nuclear reaction calculation ...

Norm kernel before collision



Time evolution of density



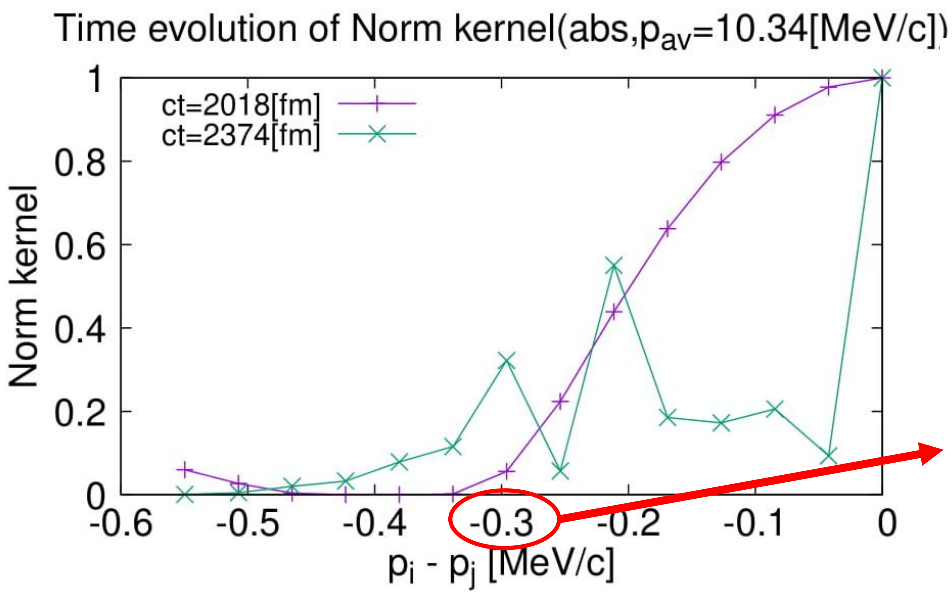
$p_i - p_j$ ：Difference of relative momentum of each system

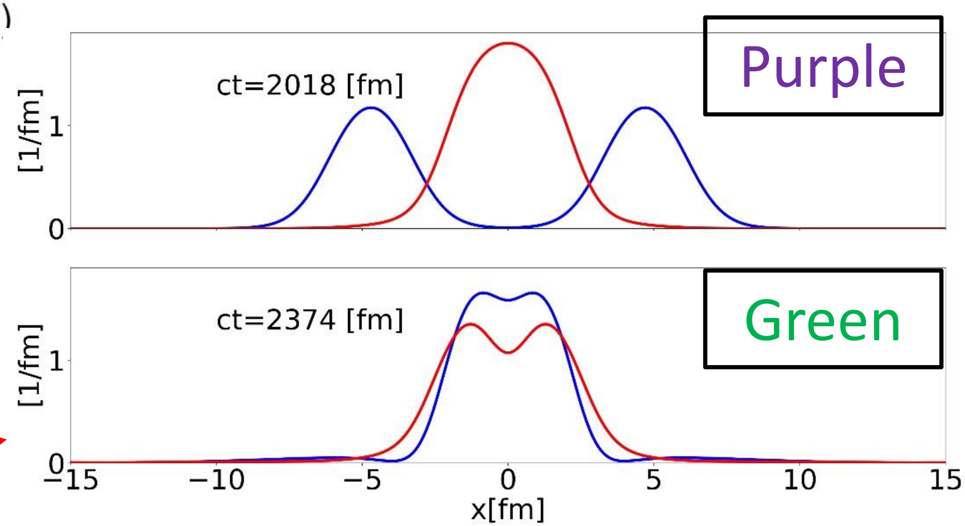
$$\mathcal{N}(p_i, p_j) = \langle \Phi_{p_i} | \Phi_{p_j} \rangle$$

Solid line：**Fit with Gaussian**

$\mathcal{N} \simeq$ **Gaussian**

Norm kernel after collision



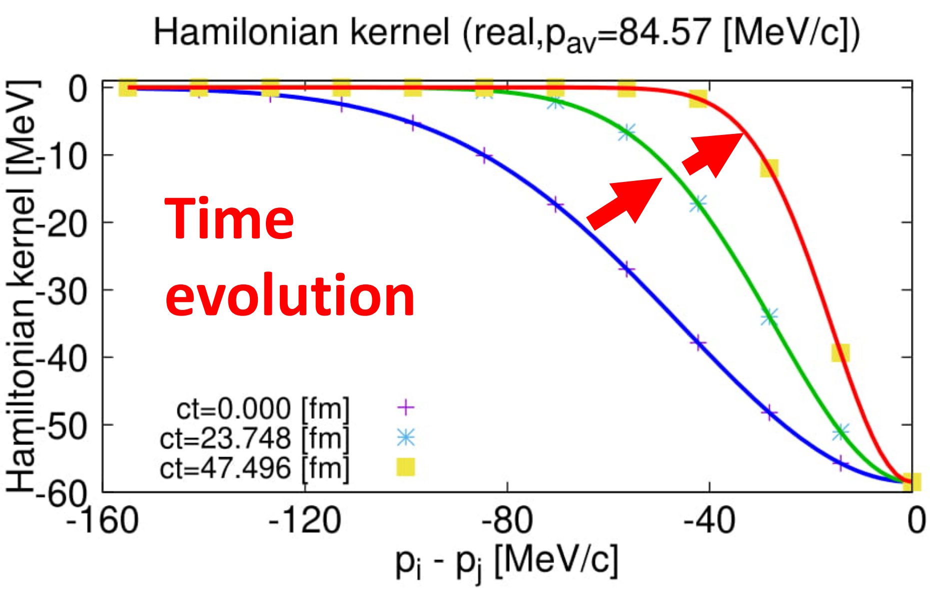


$p_j = 10.49$

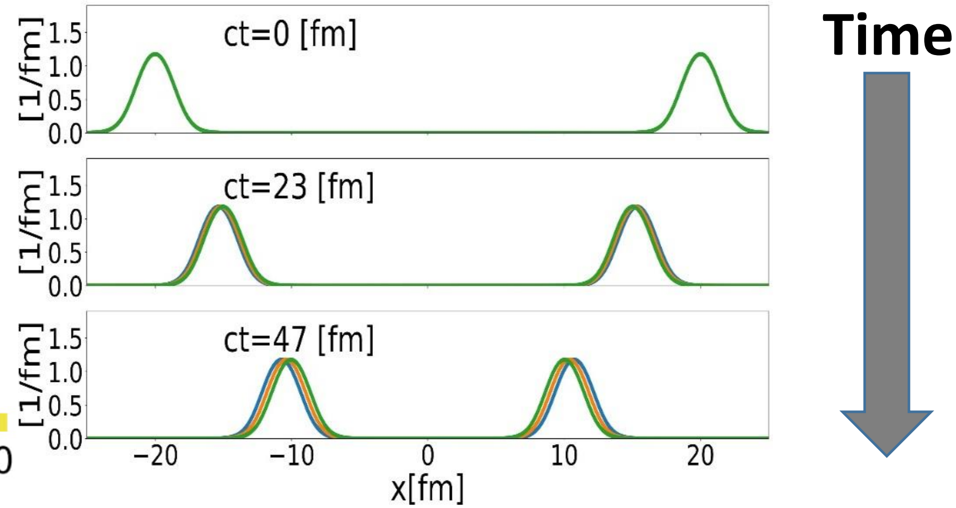
$p_i = 10.19$

Norm kernel is no longer
Gaussian form
after collision

Hamiltonian kernel before collision



Time evolution of density



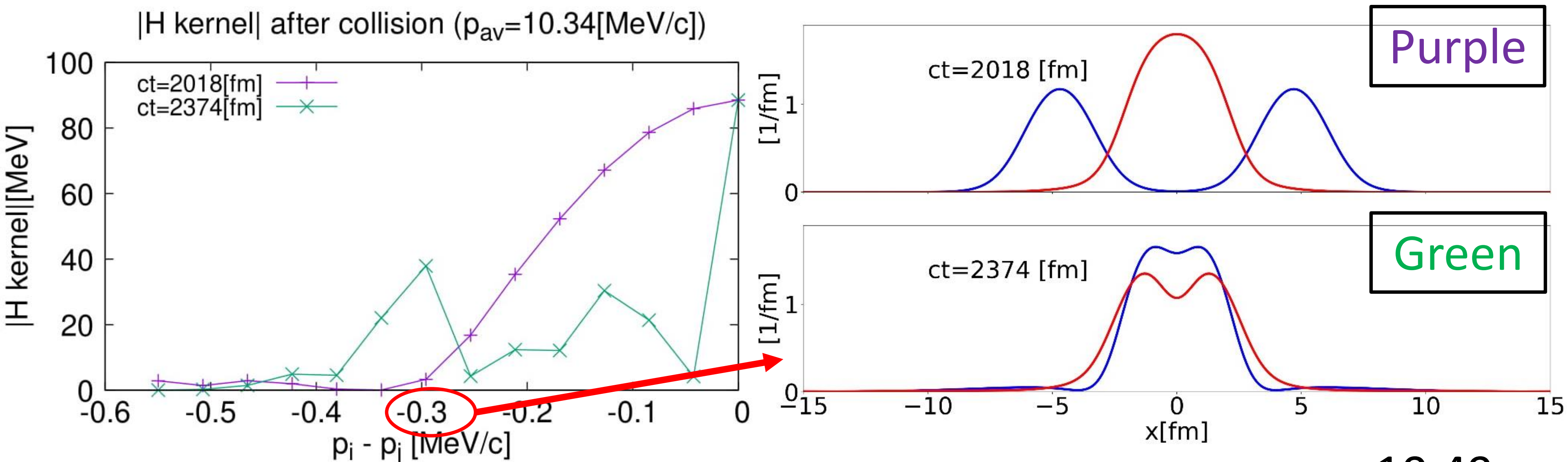
$$\mathcal{H}(p_i, p_j) = \langle \Phi_{p_i} | H - i\partial_t | \Phi_{p_j} \rangle$$

Solid line：Fit with

Gaussian × quadratic polynomial

$\mathcal{H} \simeq$ **Gaussian × quadratic polynomial**

Hamiltonian kernel after collision



$p_j = 10.49$

$p_i = 10.19$

Hamiltonian kernel is no longer

Gaussian × quadratic polynomial

after collision

Validity of Gaussian Overlap Approx.

	Norm kernel	Hamiltonian kernel
Before collision	○	○
After collision	×	×

Time evolution
after collision
is needed
to describe tunneling

⇒

GOA does not work
for nuclear reaction calculation

Conclusion

- In nuclear fusion reaction for $E < V_b$

  tunneling effect is essential

- Mean field approximation (TDHF)

  fails to describe tunneling

- **Time-Dependent Generator Coordinate Method**

  as beyond mean field

- Gaussian Overlap Approximation

  (with momentum as generator coordinate)

  does not work in nuclear reaction calculation

Next step

Calculation without Gaussian overlap approximation

↓

TDGCM can describe tunneling or not ?

Future work

Calculations which include

variation with respect to Slater determinants

$$|\Psi(t)\rangle = \int da f(a,t) |\Phi_a^{(\mathrm{TDHF})}(t)\rangle \Rightarrow |\Psi(t)\rangle = \int da f(a,t) |\Phi_a(t)\rangle$$

Full variational principle