University of Tsukuba
筑波大学

A Study on the

Fluctuation-Dissipation Dynamics in Nuclear Fusion Reactions

Based on Quantum Molecular Dynamics Simulations

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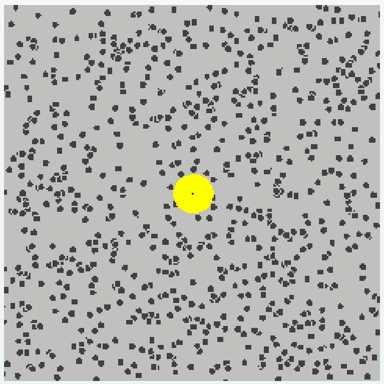
Talk on the 22nd ASRC International Workshop, Dec 5th, 2014

To describe the low-energy nuclear fusion process

Langevin type equation applied

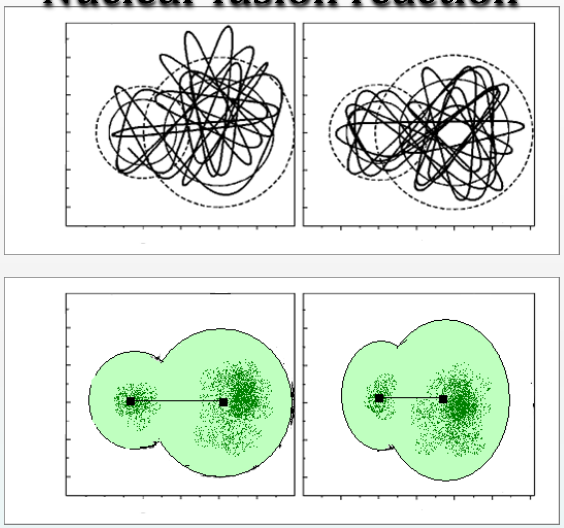
Motion of Pollen particle (Brownian motion)



$$m\frac{du}{dt} = -m\gamma u + \delta F(t)$$

Langevin, P. (1908). "On the Theory of Brownian Motion". C. R. Acad. Sci. (Paris) 146: 530–533.
...

Nuclear fusion reaction



$$\frac{du(t)}{dt} = -\int_{-\infty}^{t} \gamma(t-t')u(t')dt' + \frac{1}{\mu}\delta F(t) - \frac{1}{\mu}\frac{dV(R)}{dR}$$

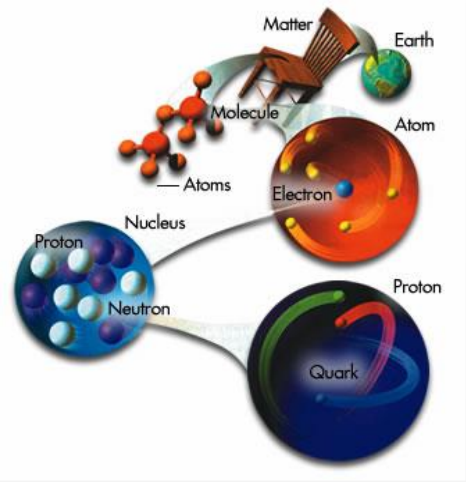
W. J. Swiatecki et al.,Acta Phys. Pol. B 34, 2049 (2003);
G. G. Adamian et al., Phys. Rev. C 78, 044605 (2008)
...

- The relevant degree of freedom

develops under the environment of

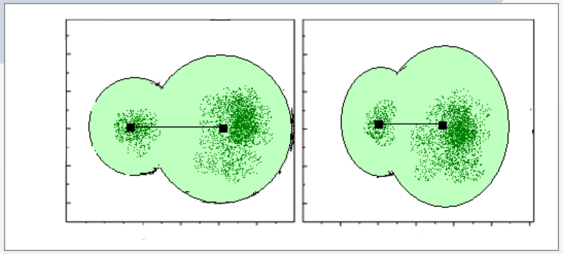
- Irrelevant degree of freedom

In Nuclear Fusion Reaction



Macroscopic

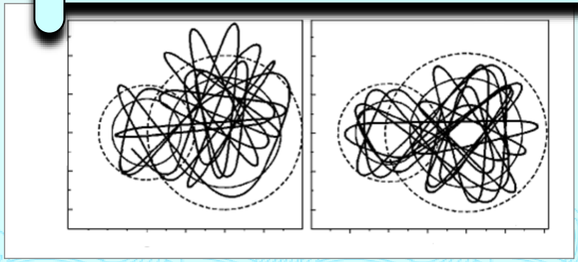
Generalized Langevin Equation



Microscopic

numerical calculations:

P. Bonche et al., Phys. Rev. C 13, 1226 (1976).
J. Aichelin, Phys. Rep. 202, 233 (1991).
...



How the macroscopic Langevin-type dynamics emerges out of the microscopic one?

Quantum molecular dynamics model

- The trial wave function for each nucleus is restricted within a parameter space $\{r_j, p_j\}$:

$$\phi_i(\mathbf{r}) = \frac{1}{(2\pi\sigma_r^2)^{3/4}} \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{4\sigma_r^2} + \frac{i}{\hbar}\mathbf{r}\cdot\mathbf{p}_i\right],$$

The total wave function is the direct product of the coherent states.

- This model focus on the evolution of ***phase space density function*** after Wigner transformation.

$$f(\mathbf{r},\mathbf{p}) = \sum_i \frac{1}{(\pi\hbar)^3} \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2\sigma_r^2} - \frac{2\sigma_r^2}{\hbar^2}(\mathbf{p}-\mathbf{p}_i)^2\right].$$

- The time evolution of the trial wave function under an effective potential is governed by the ***time-dependent variational principle***:

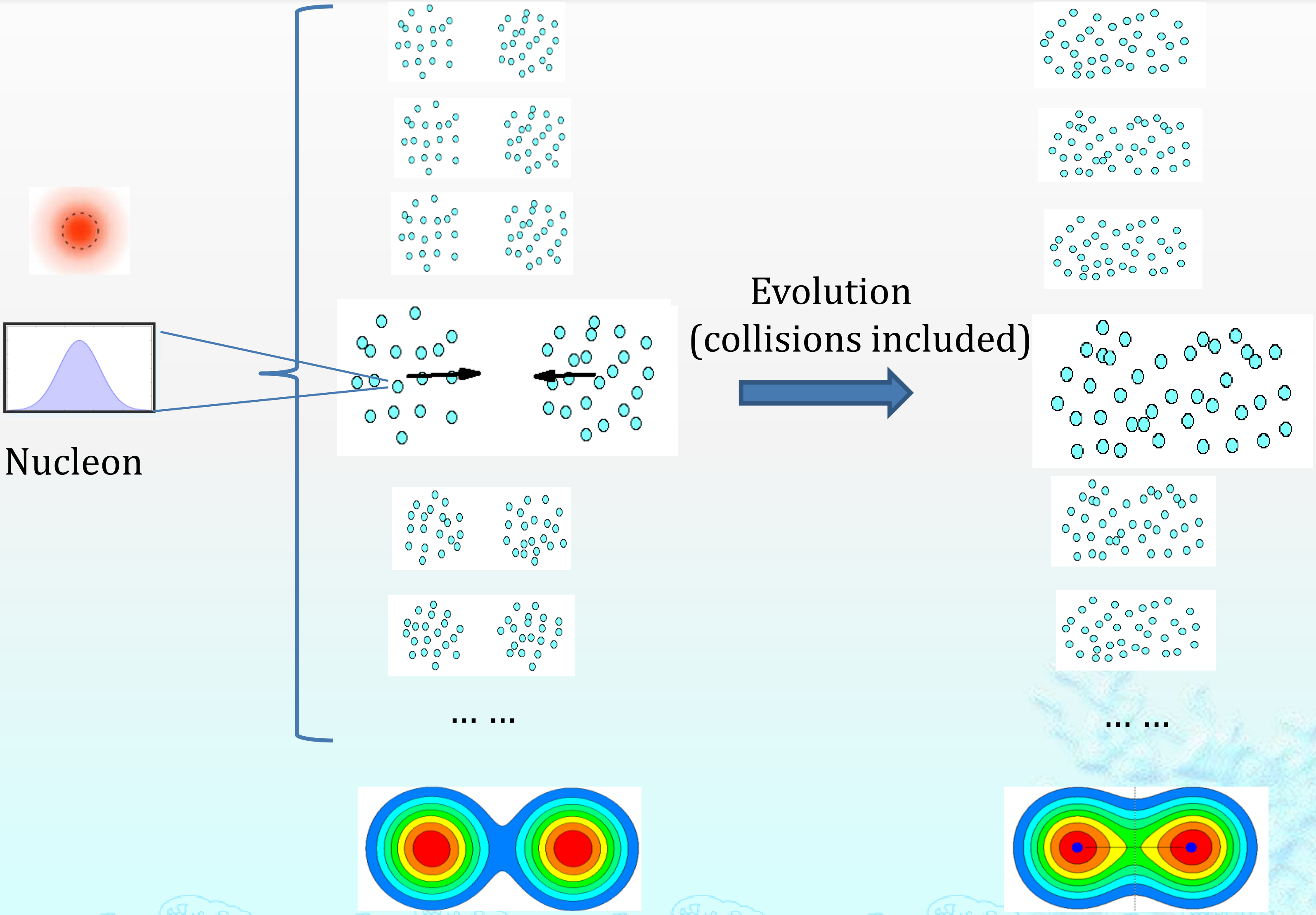
$$\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{r}}_i} = \frac{\partial\mathcal{L}}{\partial\mathbf{r}_i} \to \dot{\mathbf{p}}_i = -\frac{\partial\mathcal{H}}{\partial\mathbf{r}_i},$$

$$\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{p}}_i} = \frac{\partial\mathcal{L}}{\partial\mathbf{p}_i} \to \dot{\mathbf{r}}_i = \frac{\partial\mathcal{H}}{\partial\mathbf{p}_i}.$$

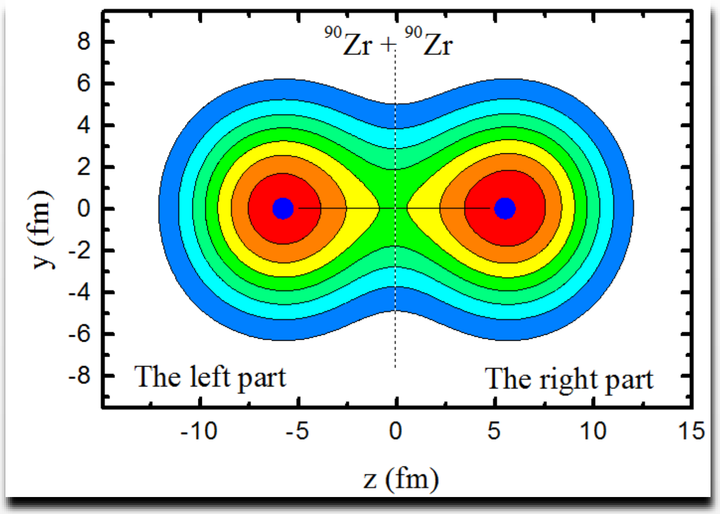
- ***Monte Carlo sampling procedure*** is performed.

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

Quantum molecular dynamics model



Macroscopic reduction procedure



By introducing a **separating plane**, we define the collective variables, which gives us the **average property.**

Example: Reaction system ^{90}Zr + ^{90}Zr; Head on collision $b = 0$ fm; *10000* events; $E_{cm} = 195$ MeV.

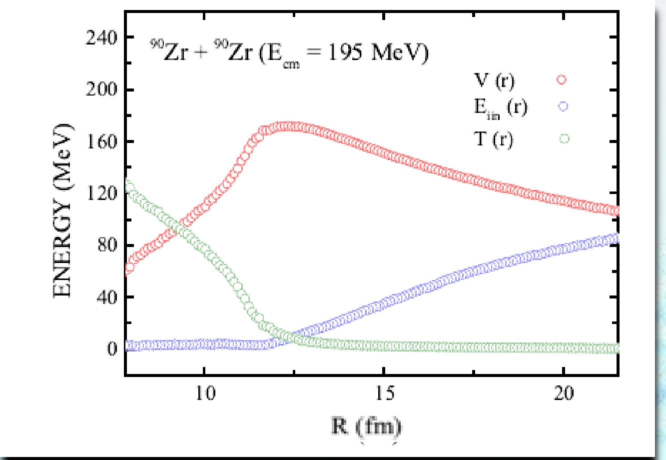
- Collective energy:

$$V(R) = E_{\text{tot}}(R) - E_{\text{left}}(R) - E_{\text{right}}(R),$$

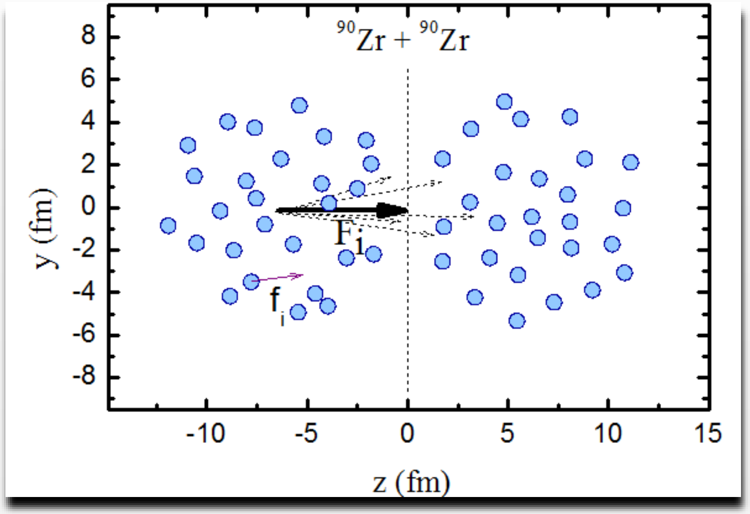
$$E_{\text{coll}}(R) = P^2/2\mu + V(R).$$

- Intrinsic energy:

$$E_{\text{intr}}(R) \equiv E_{\text{tot}}(R) - E_{\text{coll}}(R)$$



Macroscopic reduction procedure



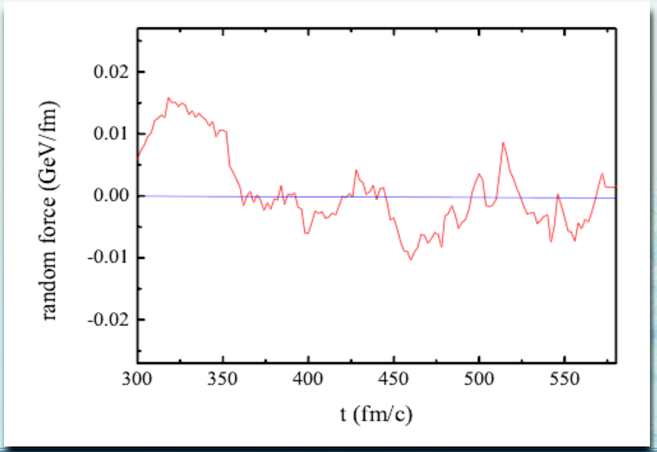
Besides the average property, the ImQMD simulations provide us the information of fluctuation.
——Random Force

What is different in QMD

- Fluctuating force in the Langevin equation:

$$\delta F(x)_i \equiv F_i(x) - \langle F(x) \rangle, \quad x = t \text{ or } R,$$

$$F_i(x) \equiv \sum_{j=1}^{A} f_i^j(x), \quad \langle F(x) \rangle \equiv \frac{1}{n} \sum_{i=1}^{n} F_i(x)$$



The development of the distribution of the random force

One may divide the whole process into three regions:

Region 1:

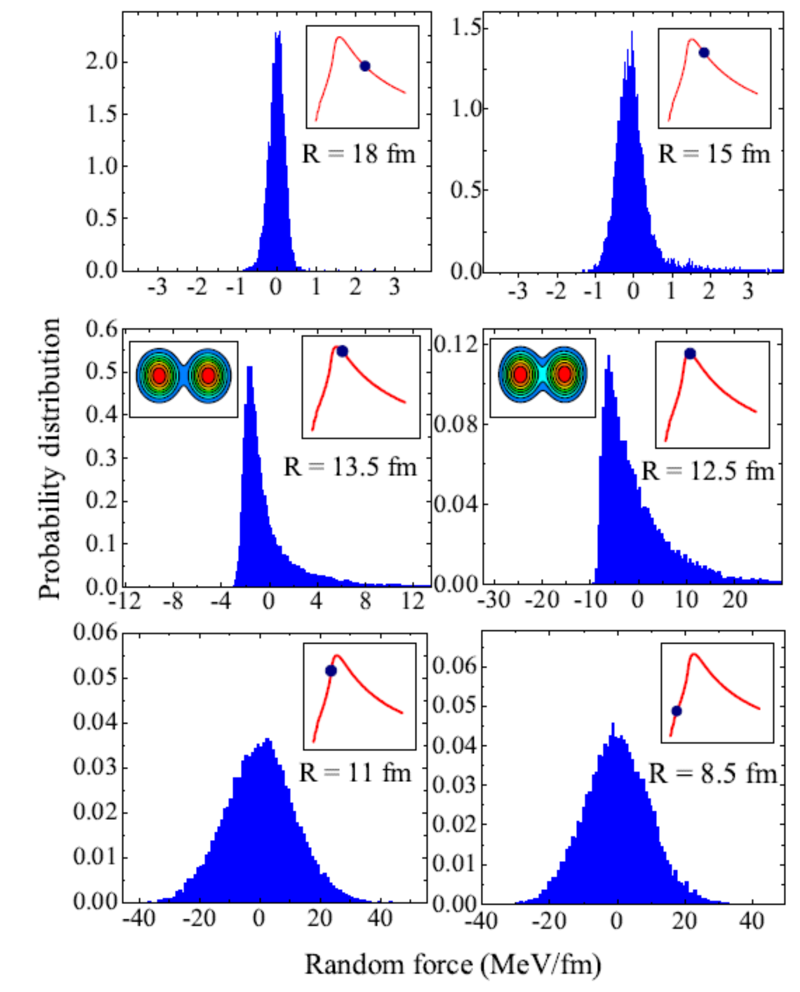
Approaching phase up to a touching point where the width of random force has Gaussian form with rather stable and narrow width.

Region 2:

From the touching to a barrier top where the width increases rapidly up to a value of almost two order of magnitude larger than that in Region 1, i.e., up to FWHM≈ 1.50×10^{-2} GeV/fm.

Region 3:

From the barrier top to fusing phase.

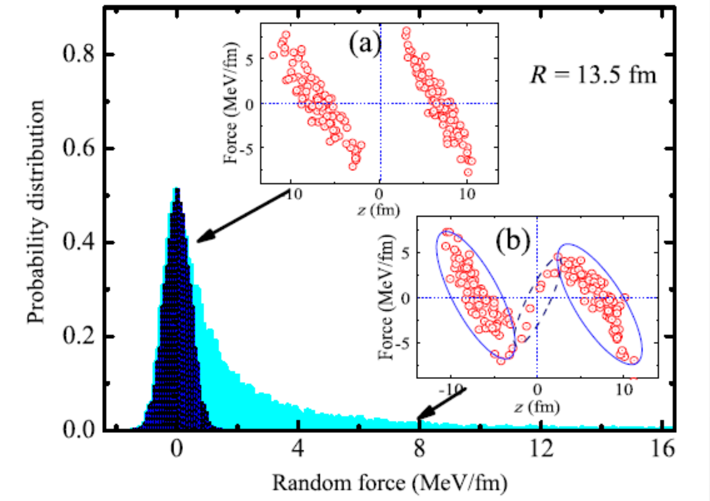


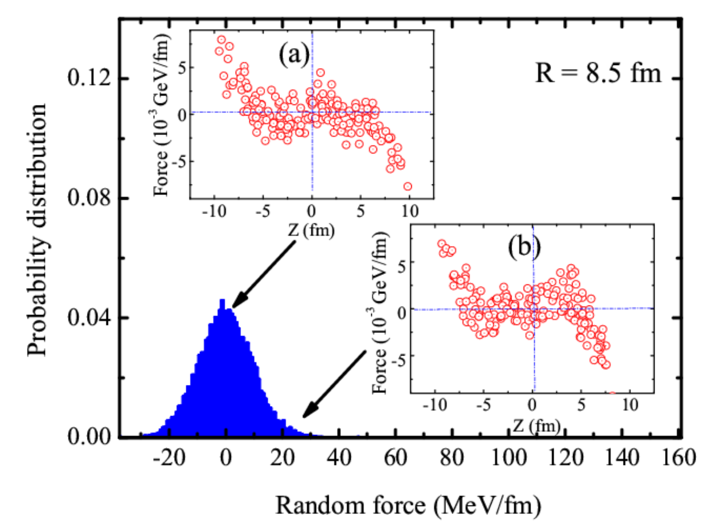
Wen, Sakata, Li, Wu, Zhang, Zhou, PRL 111, 012501(2013)

Why the non-Gaussian happened in region 2?

- In region 2, we first divide the non-Gaussian distribution into two parts
  - (a): Events in the symmetric Gauss, the whole nucleons are well divided into two separated groups so as to keep a stable mean-field.
  - (b): Events in the asymmetric tail, a small third group of exchanging nucleon appears.

- In region 3, it becomes very difficult to distinguish the event in the symmetry Gauss from that in the asymmetric tail.





Wen, Sakata, Li, Wu, Zhang, Zhou, PRL 111, 012501(2013)

Fluctuation-dissipation relation

Fluctuation-dissipation relation links the macroscopic quantity describing the energy dissipation of the collective subsystem to the microscopic characteristic of fluctuations.

- From normal Langevin equation:

$$m\frac{du}{dt} = -m\gamma u + \delta F(t) \;, \quad \Rightarrow \quad \langle \delta F(t_1)\delta F(t_2)\rangle = 2m\gamma kT\delta(t_2 - t_1).$$

- From the generalized Langevin equation:

$$\frac{dp}{dt} = -\int_{-\infty}^{t} \gamma(t-t')p(t')dt' + \frac{\partial V}{\partial R} + \delta F(t) \;, \quad \Rightarrow \quad \langle \delta F(t_1)\delta F(t_2)\rangle = m\gamma kT\gamma(t_2 - t_1).$$

- From the Langevin equation of Mori tpye:

$$\frac{dA}{dt} - i\Omega \cdot A(t) + \int_0^t d\tau\varphi(\tau) \cdot A(t-\tau) = f(t). \quad \Rightarrow \quad \varphi(\tau) = \langle f(\tau)f^*(0)\rangle \cdot \langle AA^*\rangle^{-1}.$$

What kind of relation can we find from the micscopic ImQMD simulation?

The fluctuation-dissipation relation extracted from ImQMD

- **The friction** is calculated assuming the work done by the friction force has completely converted into the intrinsic energy.

$$\gamma_0(R) \equiv \frac{\langle F_{\rm fric}(R)\rangle}{\langle P\rangle_R}, \qquad F_{\rm fric}(R) \equiv dE_{\rm intr}(R)/dR,$$

$$E_{\rm intr}(R) \equiv E_{\rm tot}(R) - E_{\rm coll}(R),$$

where

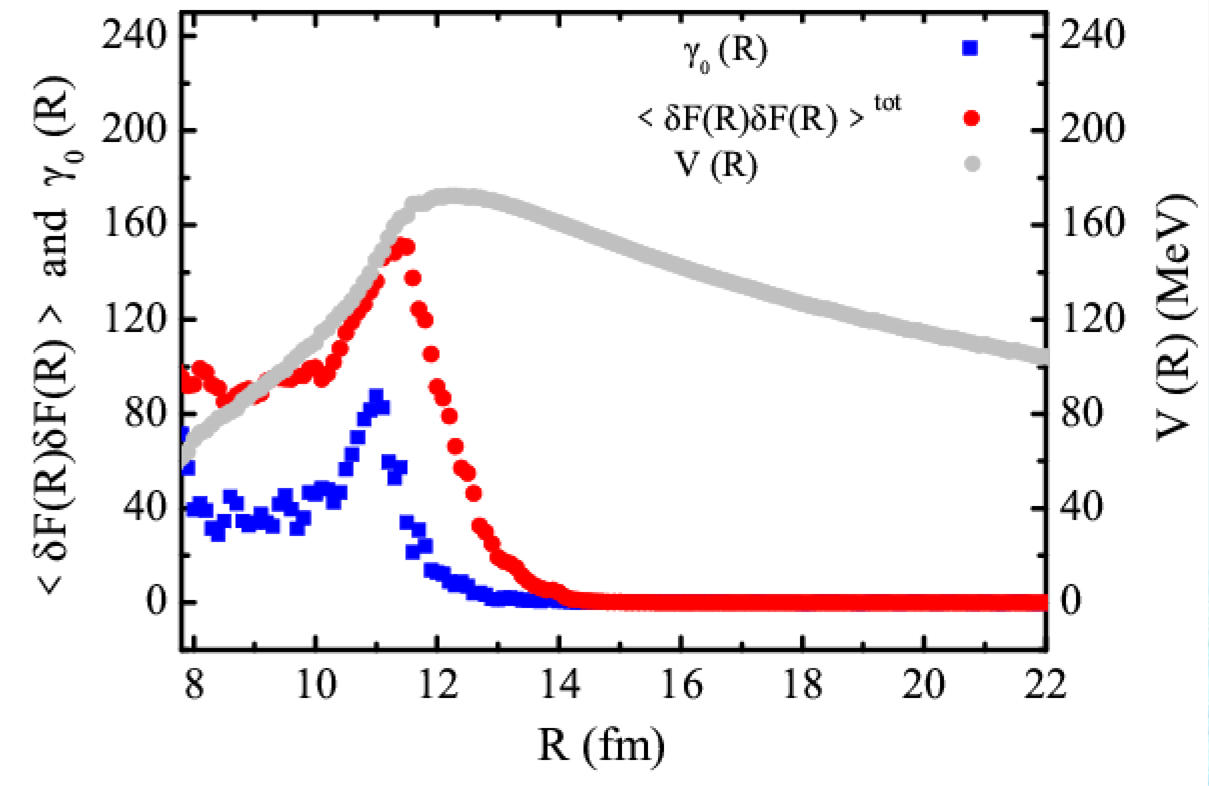
$$\langle P\rangle_R \equiv \frac{1}{n}\sum_{i=1}^{n} P_i(t_i)\big|_{\{t_i|R_i(t_i)=R\}},$$

- In order to compare the friction with the **strength of random force** at given relative distance r, we calculate.

$$\langle \delta F(R)\delta F(R)\rangle \equiv \frac{1}{n}\sum_{i=1}^{n} \delta F_i(t_i)\delta F_i(t_i)\big|_{\{t_i|R_i(t_i)=R\}}.$$

The fluctuation-dissipation relation extracted from ImQMD

- Both of the friction and the strength of the random force take almost the same shape and their peaks locate at the same point. The pink diamond is calculated by elimination the asymmetric tail.



Wen, Sakata, Li, Wu, Zhang, Zhou, PRL 111, 012501(2013)

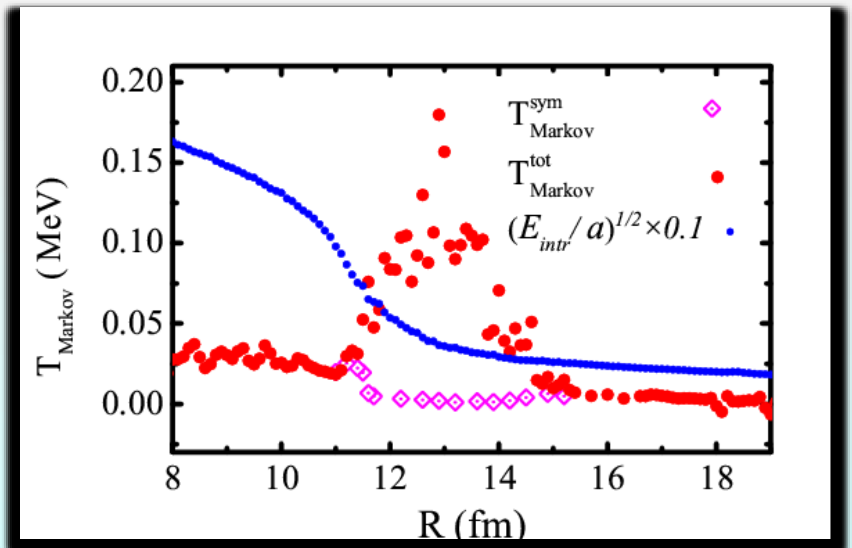
The effective temperature

If Markov approximation is assumed.

$$T_{\mathrm{Markov}} = \frac{\langle \delta F(R)\delta F(R)\rangle}{2\mu k_B \gamma(R)}$$

There appears a bump in T_{eff} ;

T_{markov} is found to be too small.

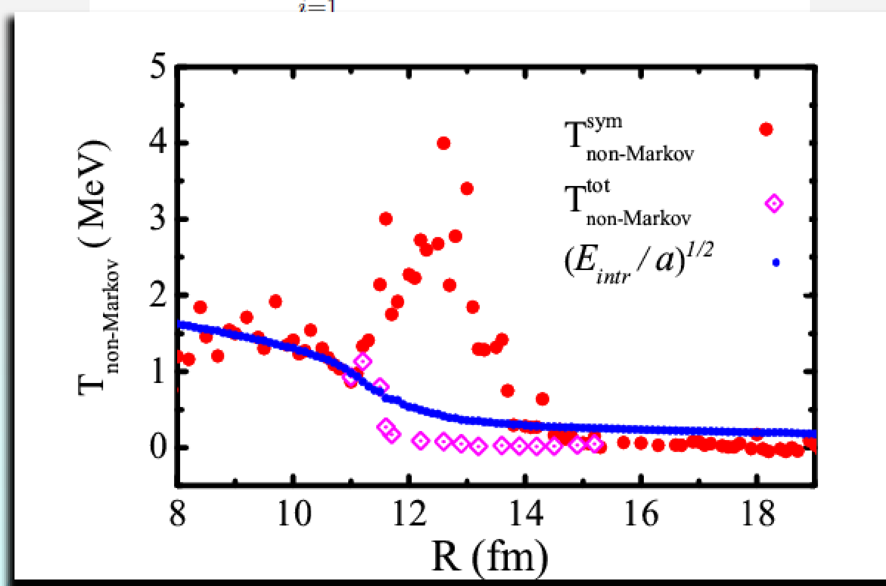


When Non-Markovian effects is taken into account.

$$\langle \delta F(t)\delta F(t-t')\rangle = \mu T \gamma(t-t')$$

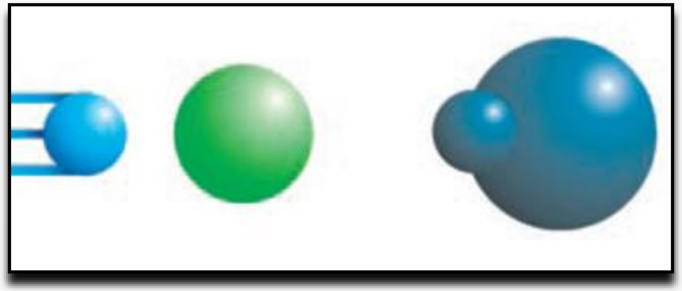
$$T_{\mathrm{non-Markov}}(R) = \frac{1}{\mu\gamma_0(R)}\int_0^\infty d\tau\,\sigma(R,\tau).$$

$$\sigma(R,\tau) \equiv \frac{1}{n}\sum_{i=1}^{n} \delta F_i(t_i)\delta F_i(t_i-\tau)\big|_{\{t_i|R(t_i)=R\}}\,.$$



Wen, Sakata, Li, Wu, Zhang, Zhou, PRL 111, 012501(2013)

When we increase the incident energy



What kind of dynamical change will it be in the fluctuation-dissipation dynamics?

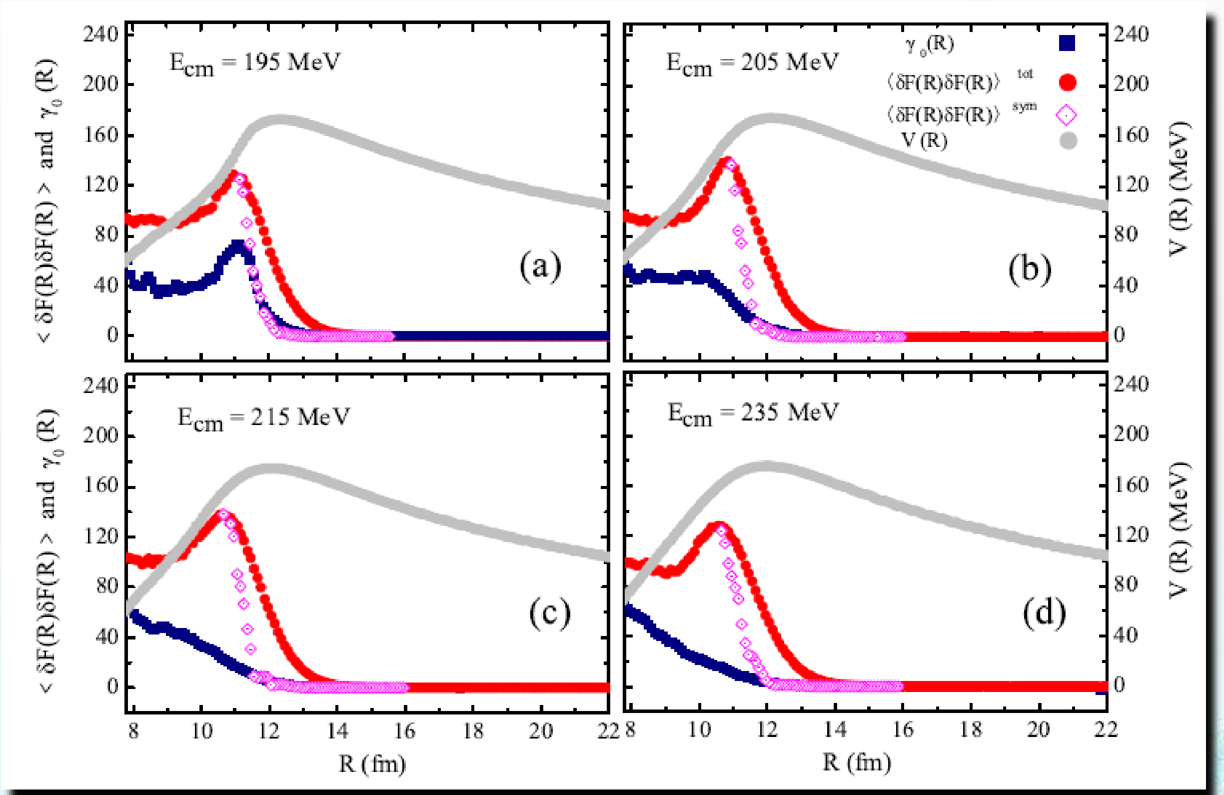
What is the microscopic reason of the dynamical change?

What is the ***mechanism of dissipation*** in fusion reaction ?

Wen, Sakata, Li, Wu, Zhang, Zhou, Phys. Rev. C **90**, 054613

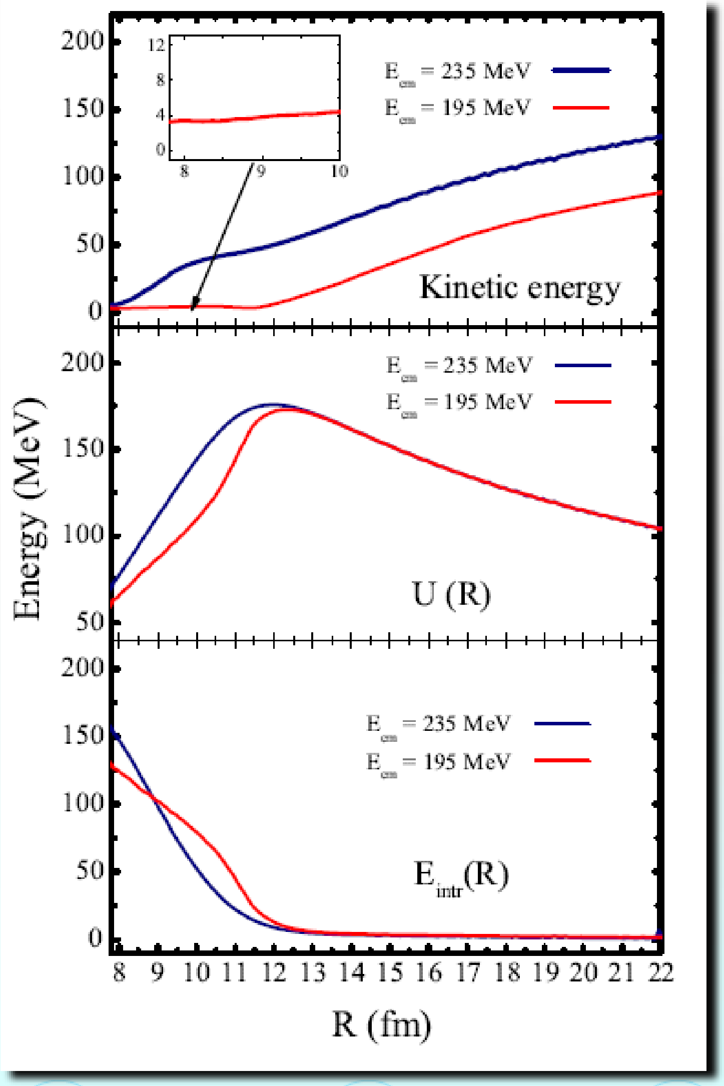
Incident Energy Dependence of Fluctuation and Dissipation

- The approximate linear relation between fluctuation and dissipation obtained at the energy just above the Coulomb barrier fades out when the incident energy increases.



- *When E_{cm} increases, the friction parameter exhibits sizable energy dependence while the strength of the random force does not change much.*

Incident Energy Dependence of Kinetic, Potential, and Intrinsic Energy



One of the reasons why the fluctuation-dissipation relation fade out at higher bombarding energy.

The collective potential U(R) exhibits sensitive energy dependence at E_{cm} near the Coulomb barrier

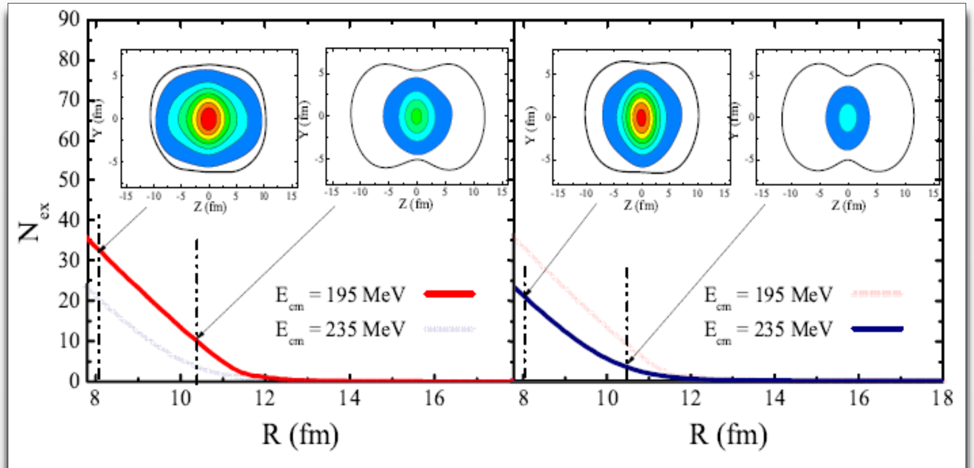
K. Washiyama et. al., Phys. Rev. C, 78:024610, 2008.

Dissipation Mechanism

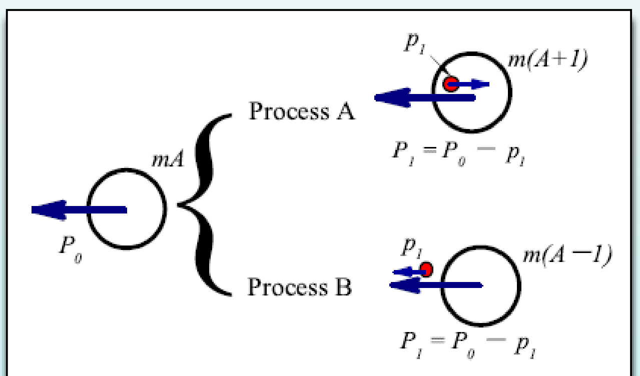
—What we are going to explore.

Microscopic reason of Energy Dissipation (I)

Nucleon Exchange



Nucleon Exchange will cause dissipation



After N nucleons exchange, we may calculate loss of collective kinetic energy by

$$T_R^{(i)} = \frac{P_i^2}{2mA_i}, \quad P_i = P_{i-1} - p_i, \quad A_i = A_{i-1} + \pi_i$$

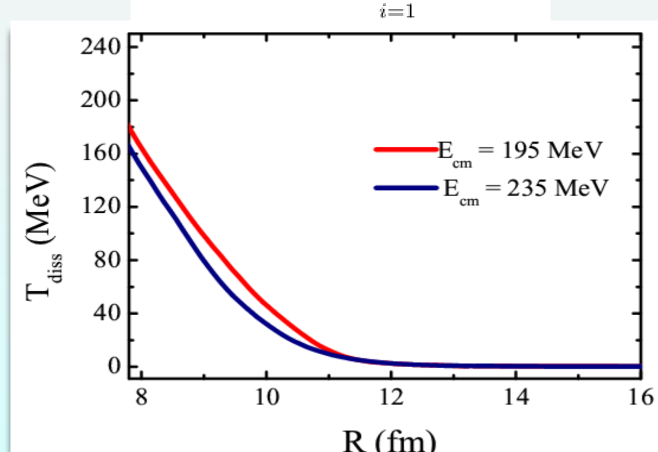
$$\pi_i = \begin{cases} +1; \text{ nucleon from the left involved,} \\ -1; \text{ nucleon from the right involved,} \end{cases}$$

$$i = 1, 2, \cdots, \quad A_0 = A,$$

$$T_{\rm diss}(R) = \frac{P_0^2}{2mA} - \frac{P_{N{\rm ex(R)}}^2}{2mA_{N{\rm ex(R)}}},$$

$$P_{N{\rm ex(R)}} = P_0 - \sum_{i=1}^{N{\rm ex(R)}} p_1,$$

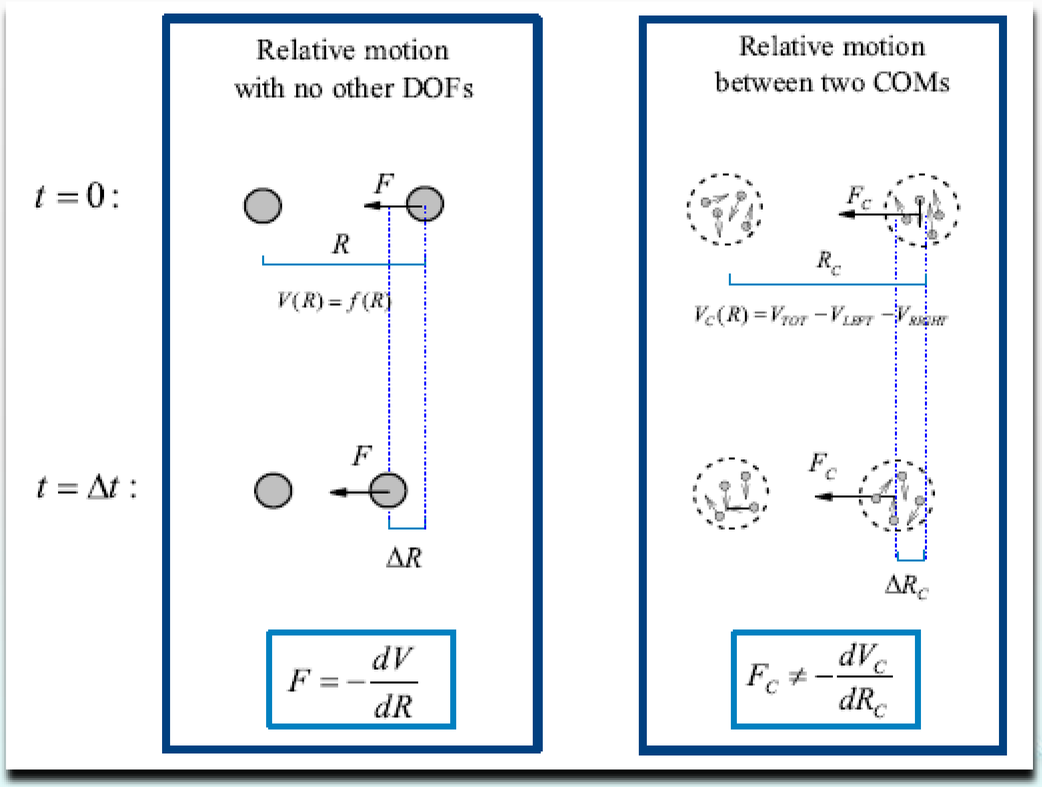
$$A_{N{\rm ex(R)}} = A_0 + \sum_{i=1}^{N{\rm ex(R)}} \pi_i.$$



Wen, et. al., in preparation.

Microscopic reason of Energy Dissipation (II)

Starting point: How the "non-conservative" force turns out?



"Non-conservative" forces can arise in classical physics due to neglecting degrees of freedom.

Wen, et. al., in preparation.

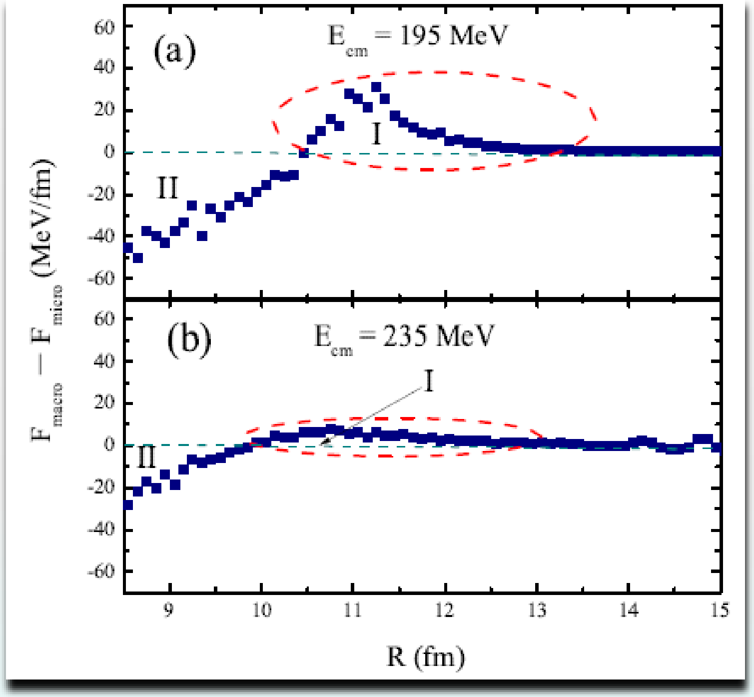
Microscopic reason of Energy Dissipation (II)

In the ImQMD simulations, we define:

$$F_{\rm macro}(R) \equiv \sum_{j=1}^{A} f^j(t)\big|_{\{t|R(t)=R\}},$$

$$F_{\rm micro}(R) = -\frac{dU(R)}{dR}.$$

The difference between F_{macro} and F_{micro}



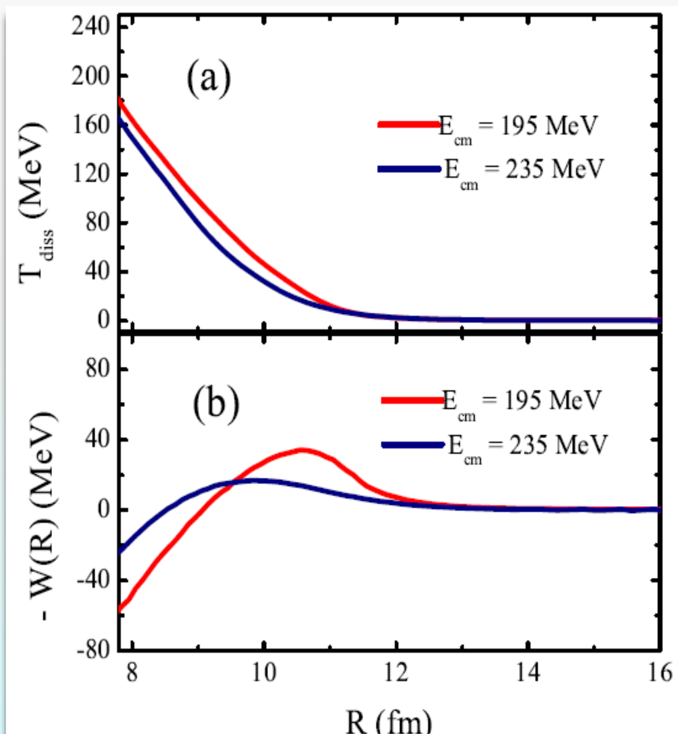
The work done by the intrinsic system to the collective system :

$$W(R) \equiv \int_{\infty}^{R} dR' \left[F_{\rm macro}(R') - F_{\rm micro}(R')\right],$$

Wen, et. al., in preparation.

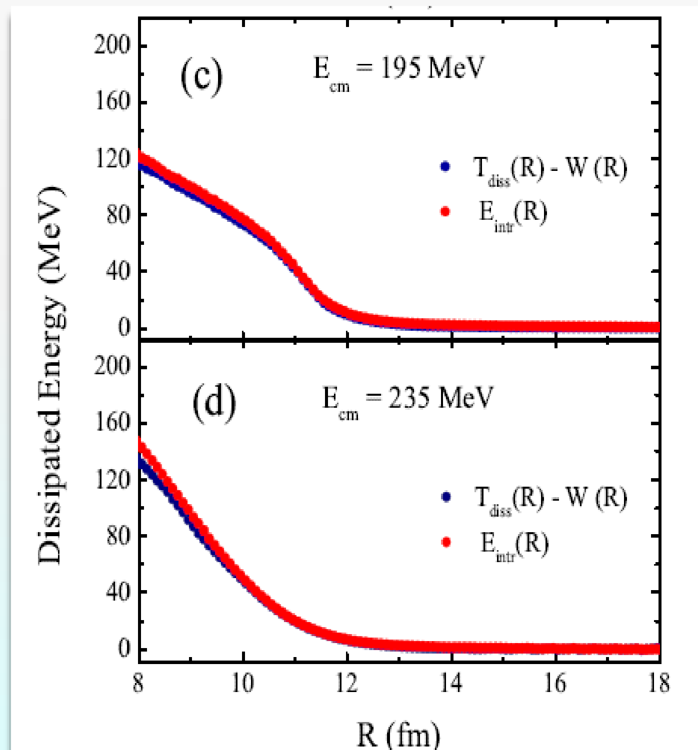
Reproducing Dissipated Energy

- The two sources of dissipation discussed above :
  - Nucleon exchange — $T_{\mathbf{diss}}$.
  - Rearrangement of intrinsic degree of freedom — $-W$.



When we sum up $T_{\mathbf{diss}}$ and $-W$:

$$E_{\rm diss}(R) \equiv T_{\rm diss}(R) - W(R)$$
$$= T_{\rm diss}(R) + \int_R^\infty dR' \left[F_{\rm macro}(R') - F_{\rm micro}(R')\right].$$



Wen, et. al., in preparation.

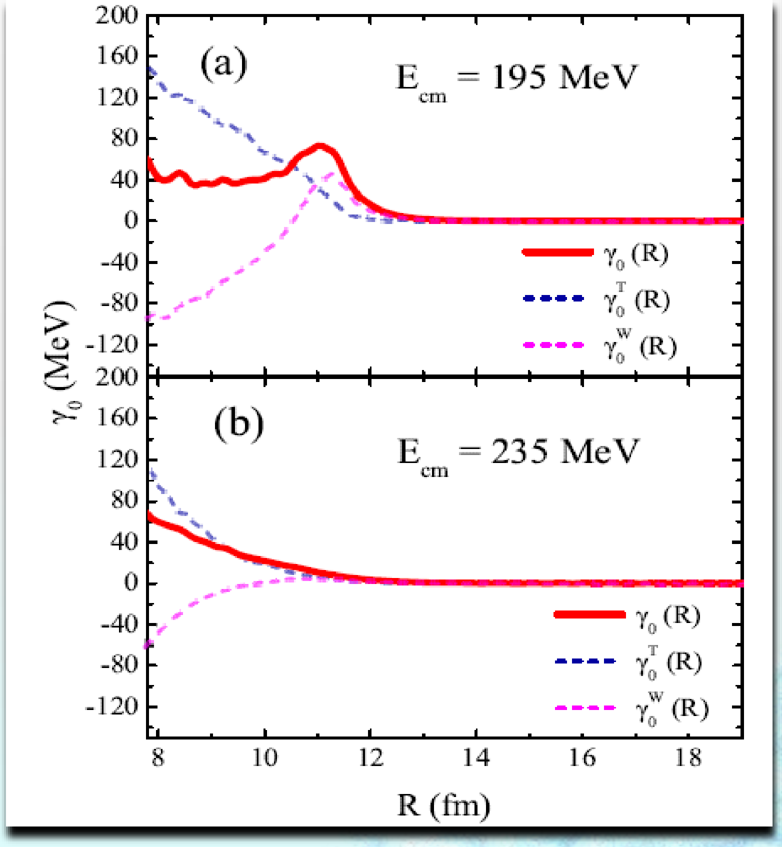
Discussion about Friction Parameter

Since $$E_{\text{intr}}(R) \simeq E_{\text{diss}}(R),$$

We may express the friction parameter as

$$\gamma_0(R) = \frac{1}{\langle P \rangle_R} \left\langle \left(\frac{dT_{\text{diss}}(R)}{dR} - \frac{\partial W(R)}{\partial R} \right) \right\rangle.$$

- The friction parameter is determined by two microscopic competitive processes.
- The peak structure of the friction parameter at E_{cm} = *195* MeV comes from the inflection point in –*W(R)*.



Wen, et. al., in preparation.

Conclusions

- Macroscopic parameters as well as precise information on the random force characterizing the Langevin type description of the nuclear fusion are extracted from ImQMD simulations.

- The dissipation dynamics of the relative motion between two fusing nuclei is associated with non-Gaussian distributions of the random force.

- A proper treatment of the non-Markovian (memory) effect in the Langevin dynamics are decisive for the dynamics of emergence in the nuclear dissipative fusion motion.

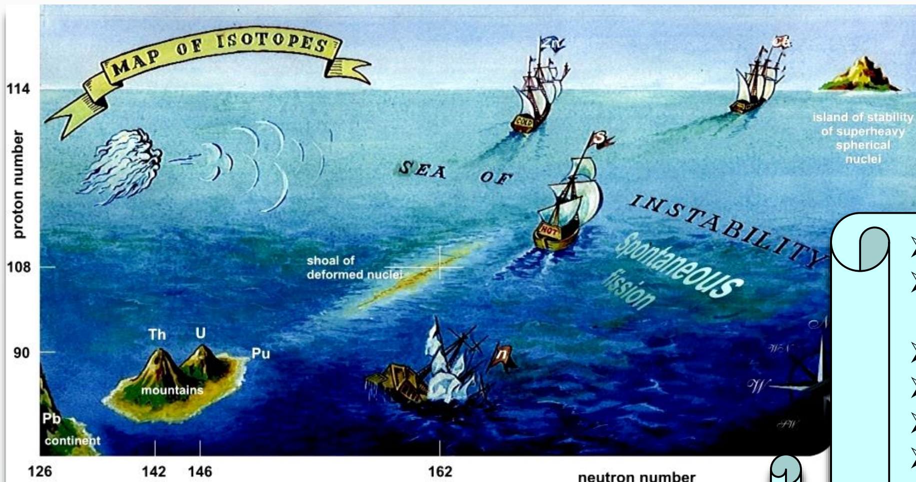
- Energy dependence of the nucleus-nucleus potential, friction parameter as well as random force are studied..

- Microscopic dynamics of energy dissipation are analyzed in the ImQMD model. Nucleon exchanging and rearrangement of intrinsic degrees of freedom play competitive role in the dissipation process.

Thank you !

Nuclear Fusion Reaction

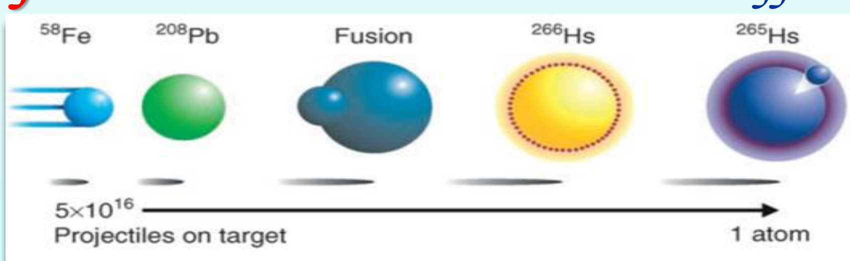
- *Nuclear theorists predicts the existence of the* ***super-heavy island.***



W. Myers, W. Swiatecki, *Nucl. Phys.*, 81, 1-60 (1966);
A. Sobiczewski, et. al. *Phys. Lett.*, 22, 50 (1966);
H. Meldner, et. al., *Nucl. Phys. A, 131, 1* (1969);
G. Nilsson et al., *Nucl. Phys. A, 131, 1–66,* (1969).
...

- S. Hofmann et. al., *Rev. Mod. Phys., 72(3):733–767 (2000);*
- K. Morita et. al., *Journal of the Physical Society of Japan,* 76:045001 (2007);
- Y. Oganessian. *J. Phys. G: Nucl. Part. Phys., 34(4):R165 (2007);*
- Y. Oganessian et. al., *Phys. Rev. C, 74(4):044602* (2006);
- Y. Oganessian et. al., *Phys. Rev. Lett., 104:142502 (2010);*
- D. Rudolph et. al., *Phys. Rev. Lett., 111:112502* (2013);
- J. Khuyagbaatar et. al., *Phys. Rev. Lett., 112:172501 (2014)*

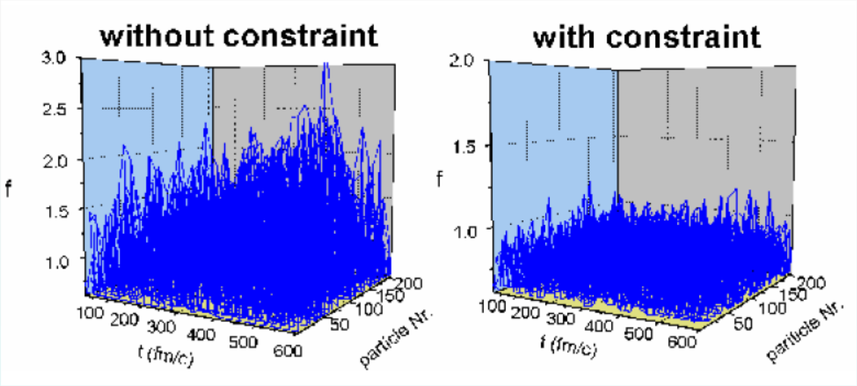
- *Mechanism of* ***fusion reaction*** *deserves more research effort.*



Improved quantum molecular dynamics model

A series of improvements

- **The Hamiltonian is calculated using the Skyrme energy density functional method.**
- The fermionic properties of nucleons are remedied by using the phase space occupation constraint method, which is important for low-energy collisions



- *A*-dependent width of the Gaussian packet.
- … …

Good properties

A true n-body theory

- Keep track of all correlations among the particles.
- Be able to treat nonequilibrium situations which appear at the early stage of heavy ion collision.
- Collective fluctuations included and collective variables develops into distribution.
- Extended to low energy heavy-ion collisions near barrier.

N. Wang, Z. Li, and X. Wu, Phys. Rev. C 65, 064608(2002).
N. Wang, Z. Li, X. Wu, J. Tian, Y. Zhang, and M. Liu, Phys. Rev. C 69, 034608 (2004).

Next

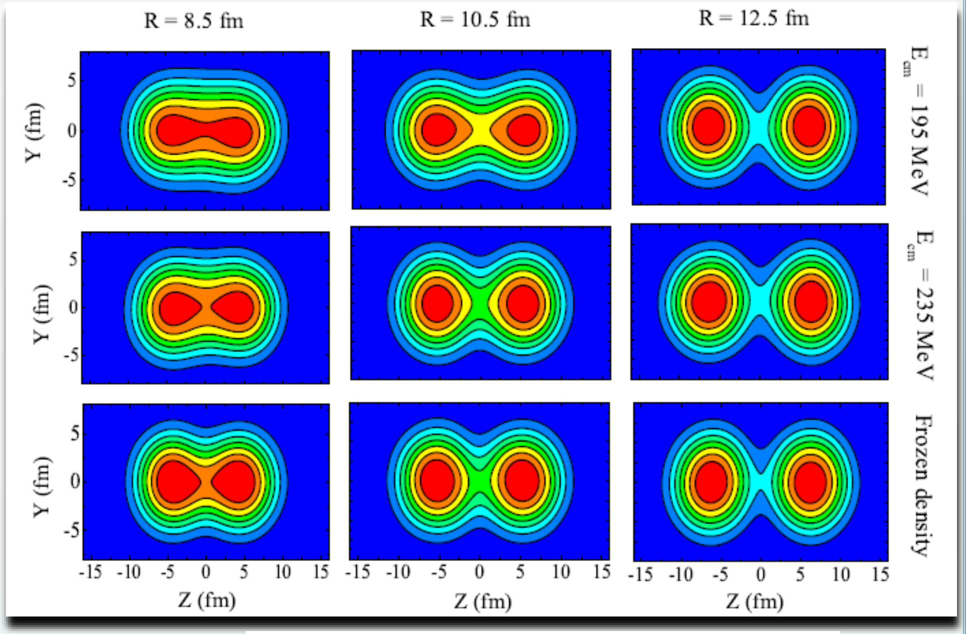
How about

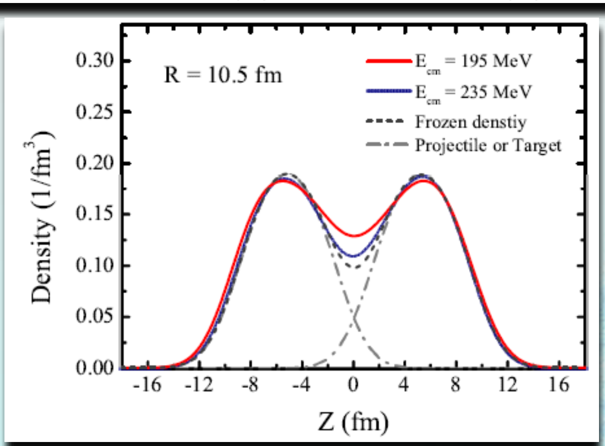
- At higher incident energy above the Coulomb barrier;
- What is the microscopic dissipation mechanism in fusion reactions;
- For asymmetric reaction systems;
- For heavier and lighter reaction systems;
- For the reaction with impact parameter not equal to zero; the dissipation of angular momentum.

Incident Energy Dependence in Density Profile

Adiabatic vs. Diabatic Processes

- The density at E_{cm} = *195* MeV in the neck region is obviously higher .
- At E_{cm} = *235* MeV the nucleus *keeps* its original shape into a small relative distance *R, remaining* nearly the same as the one with frozen density.





This bulk aspects of *diabatic nature of fusion reaction has been discussed by means of* density profile in TDHF calculation.

K. Washiyama et. al., Phys. Rev. C, 78:024610 (2008).

Microscopic reason of Energy Dissipation (II)

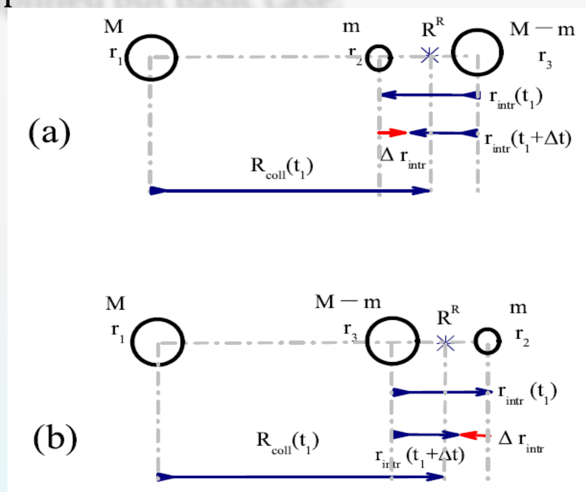
Theoretical analysis

In the ImQMD simulations, we define:

$$F_{\mathrm{macro}}(R) \equiv \sum_{j=1}^{A} f^{j}(t)\big|_{\{t|R(t)=R\}},$$

$$F_{\mathrm{micro}}(R) = -\frac{dU(R)}{dR}.$$

In a simplified but basic case:

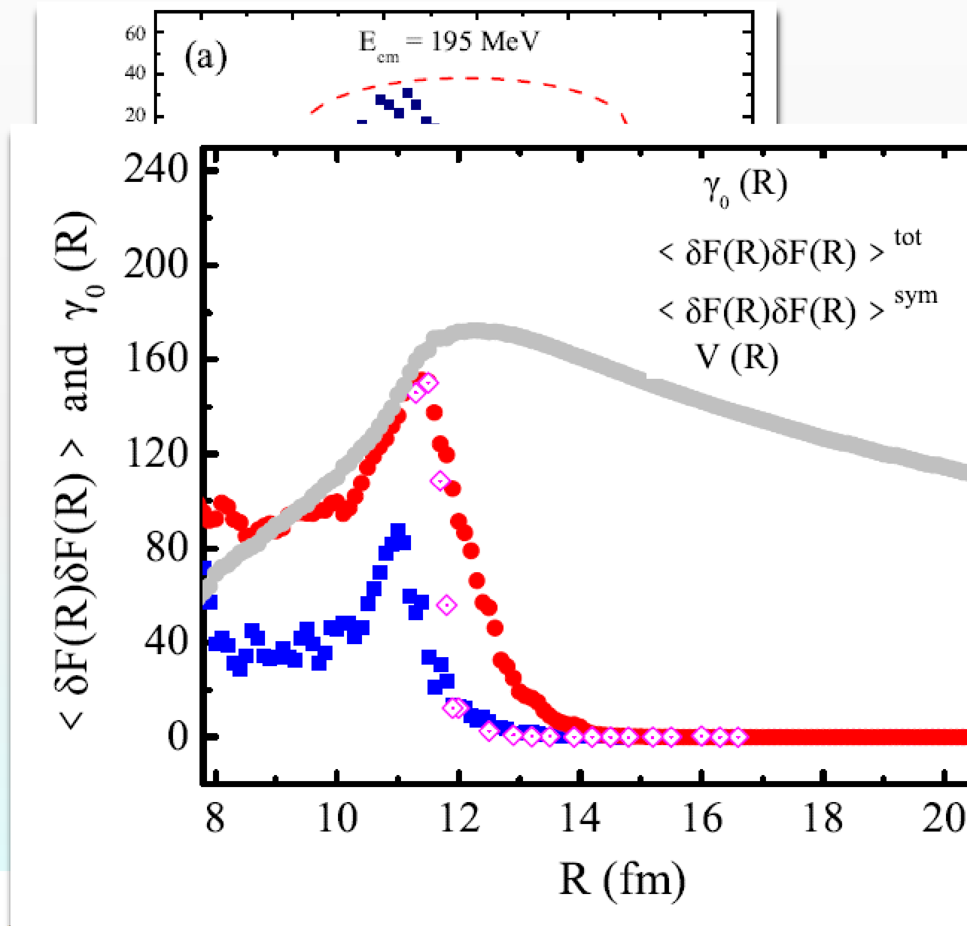


We may get

$$F_{\mathrm{macro}}(R) - F_{\mathrm{micro}}(R) = -\alpha_{\mathrm{sup}}(R)\beta_{\mathrm{adia}}(R),$$

$$\beta_{\mathrm{adia}}(R) \equiv \frac{v(R)}{V(R)},$$

The difference between F_{macro} and F_{micro}



$$W(R) = \int_{\infty} dR' \left[F_{\mathrm{macro}}(R') - F_{\mathrm{micro}}(R')\right],$$

Wen, et. al., in preparation.