Fission Dynamics of Superheavy Compound Nuclei

Yoritaka Iwata School of Science, The University of Tokyo

<u>Collaborations:</u> S. Heinz (GSI) T. Otsuka (U. Tokyo)



Introduction to TDDFT calculations

Motivation: Study fission using the TDDFT

Present status

Difficulty in front of us

• TDDFT for collision dynamics

TDDFT for superheavy synthesis & more

Iwata-Otsuka-Maruhn-Itagaki PRL (2010) Iwata-Otsuka-Maruhn-Itagaki EPJA (2010) Iwata-Otsuka-Maruhn-Itagaki NPA (2010) Iwata JMP (2012); arXiv:1204.3723 Iwata-Heinz J. Phys Conf. Ser. (2012); arXiv:1208.6215 Iwata-Heinz CERN Rep. (2012); arXiv:1209.6142 Iwata-Heinz IJMPE (2012); arXiv:1212.0161 Iwata J. Phys Conf. Ser. (2013); arXiv:1303.4698 EDF = energy density functional

Skyrme EDF

"Energy Density Functional in Nuclear Physics" Nova publishers, New York in press; arXiv:1211.2355

Intro, TDHF



Skyrme, 1950s

$$\begin{split} v_{i,j}(\boldsymbol{k}, \boldsymbol{k}') &= t_0(1 + x_0 P_{\sigma})\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)) + \frac{t_1}{2}(1 + x_1 P_{\sigma})\{\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\boldsymbol{k}^2 + \boldsymbol{k}'^2\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\} + t_2(1 + x_2 P_{\sigma})\boldsymbol{k}'\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\boldsymbol{k} \\ &+ \frac{t_e}{2}[\{3(\boldsymbol{\sigma}_i \cdot \boldsymbol{k}')(\boldsymbol{\sigma}_j \cdot \boldsymbol{k}') - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\boldsymbol{k}'^2\}\delta(\boldsymbol{r}_i - \boldsymbol{r}_j) + \delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\{3(\boldsymbol{\sigma}_i \cdot \boldsymbol{k})(\boldsymbol{\sigma}_j \cdot \boldsymbol{k}) - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\boldsymbol{k}^2\}] \\ &+ \frac{t_e}{2}[3(\boldsymbol{\sigma}_i \cdot \boldsymbol{k}')\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)(\boldsymbol{\sigma}_j \cdot \boldsymbol{k}) - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\boldsymbol{k}'\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\boldsymbol{k}], \end{split}$$

- 1st order of *k* is absent; time reversal invariance.
- Interaction is described by the delta function; zero-range formalism

$$\begin{aligned} v_{i,j}(\boldsymbol{k}, \boldsymbol{k}') &= t_0 (1 + x_0 P_{\sigma}) \delta(\boldsymbol{r}_i - \boldsymbol{r}_j)) + \frac{t_1}{2} (1 + x_1 P_{\sigma}) \{ \delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \boldsymbol{k}^2 + \boldsymbol{k}'^2 \delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \} + t_2 (1 + x_2 P_{\sigma}) \boldsymbol{k}' \delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \boldsymbol{k} \\ &+ \frac{t_e}{2} [\{ 3(\boldsymbol{\sigma}_i \cdot \boldsymbol{k}')(\boldsymbol{\sigma}_j \cdot \boldsymbol{k}') - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \boldsymbol{k}'^2 \} \delta(\boldsymbol{r}_i - \boldsymbol{r}_j) + \delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \{ 3(\boldsymbol{\sigma}_i \cdot \boldsymbol{k})(\boldsymbol{\sigma}_j \cdot \boldsymbol{k}) - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \boldsymbol{k}^2 \}] \\ &+ \frac{t_e}{2} [3(\boldsymbol{\sigma}_i \cdot \boldsymbol{k}') \delta(\boldsymbol{r}_i - \boldsymbol{r}_j)(\boldsymbol{\sigma}_j \cdot \boldsymbol{k}) - (\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \boldsymbol{k}' \delta(\boldsymbol{r}_i - \boldsymbol{r}_j) \boldsymbol{k}], \end{aligned}$$

After adding some terms, which cannot be derived from invariance argument e.g., spin-orbit interaction, three-body type medium effect

$$v_{i,j}^{LS}(\mathbf{k}, \mathbf{k}') = iW_0 \mathbf{k}' \, \delta(\mathbf{r}_i - \mathbf{r}_j) \, (\sigma_i + \sigma_j) \times \mathbf{k}$$

$$v_{i,j}^{DD}(\mathbf{k}, \mathbf{k}') = \frac{t_3}{6} (1 + x_3 P_\sigma) \rho(\frac{\mathbf{r}_i + \mathbf{r}_j}{2})^\alpha \delta(\mathbf{r}_i - \mathbf{r}_j)$$

$$V_{i,j}(\mathbf{k}, \mathbf{k}') = v_{i,j}(\mathbf{k}, \mathbf{k}') + v_{i,j}^{LS}(\mathbf{k}, \mathbf{k}') + v_{i,j}^{DD}(\mathbf{k}, \mathbf{k}')$$

$$\mathsf{Total Energy:}_{E_{V_K}} = \int V_K \mathbf{k} \, \mathbf{k}' \, dr^3 = \int H_{V_K}(\mathbf{r}) \, dr^3$$
Obtain the condition for the total energy to have the minimum with respect to the functional form
$$V_{\text{eff}} \, \begin{array}{c} \mathsf{Variational Principle} \\ \mathsf{Vonlinear problem} \end{array}$$
but in Banach spaces as well
$$\mathsf{Nonlinear problem}$$

Actual calculation is in the form of

 $= \frac{1}{2} \sum_{l,m} \int \bar{\psi}_l(\boldsymbol{r}'_i) \bar{\psi}_m(\boldsymbol{r}'_j) V_{i,j}(\boldsymbol{k}, \boldsymbol{k}') (1 - P_r P_\sigma P_\tau) \psi_l(\boldsymbol{r}_i) \psi_m(\boldsymbol{r}_j) d\boldsymbol{r}_i d\boldsymbol{r}_j d\boldsymbol{r}'_i d\boldsymbol{r}'_j$

Interaction term

Intro. TDHF



This framework is expected to reproduce collective dynamics.

Lesinski *et al.*, PRC (2007)

Nice description in low-energy HIC

"(roughly) the radius of a nucleus < 10 fm ($R = 1.2 * A^{(1/3)}$)" **Collision times** for a nucleon passing through 20 fm is the problem:

Mean free path of a nucleus



Let us assume the situation with colliding ground state nuclei with boost:

If the energy is set to the Fermi energy (25 \sim 30% of the speed of light) +10MeV/A, the mean-free path is less than 20fm.

If the incident energy is less than that, the expected collision time becomes less than 1.

→ Collisionless framework such as TDDFT gives a sufficient framework to study low-energy heavy-ion collision

Fig. 2. The calculated nucleon mean free path, λ , in a nuclear Fermi gas of temperature T and Fermi energy, $E_{\rm F} = 38$ MeV. The nucleon mean free path is given as a function of its energy above the Fermi energy, $(E_1 - E_{\rm F})$, for various values of T. The curves are obtained by calculating the expression (9), which assumes isotropic differential cross sections. The four circled points are computed from (8) using more realistic anisotropic cross sections and a temperature of T = 1. They show that the error involved in the isotropic assumption is not important in the present discussion.

Collins-Griffin, NPA (1980)

Remarks on Skyrme EDF

The Skyrme energy density functional is zero-range interaction.

The zero-range formalism in nuclear physics revives (compared to the finite-range force necessity) in the context of making the ultimate density function formalism, which is well developed in condensed matter physics.

Towards finding the ultimate energy density functional

- Today there are so many Skyrme parameter sets; the predictability of Skyrme EDF calculations is limited.
- We do not know whether such an ultimate functional exists or not; nuclear force is not so simple as the Coulomb force.
- We have already stopped sticking to the interaction obtained by the <u>mean-field</u> approx.; all the possible terms described by the densities are the candidate for the interaction terms nowadays.
- Skyrme type functional form can be derived without assuming the single Slater formalism (shown by Iwata-Maruhn).

Towards including more than the time-dependent mean-field description

Iwata JPCS, to appear

Time-scaled scenario of low-energy HICs

Momentum Eq. Internal Thermal Eq. Excitation Charge. Eq. We have found what happens here 3rd 1st 2nd fast moderate slow Time[s] 1×10⁻²⁴ 1×10^{-22} 1×10-20 1×10^{-18} 1×10^{-16} 1×10⁻¹⁴ Giant resonances are located around here Contact Detector 0 [s] Fission ~ 10^{-15} s: Collectivity Localization (single particle degrees of freedom) **Described by TDDFT** * Thermal effect (beyond the eq. of motion) ~ 10000 steps (a few 1000 fm/c ~ 10^{-20} s)

Universal wave propagation property

⁵²Ca + ³⁶Ca → (⁸⁸Zr)

hand sides, respectively. The colored parts correspond to the parts



TABLE I: Comparison of speeds, where $|v_F|$ is fixed to 1/3 of the speed of light (corresponding to the nuclear standard value). The propagation speed of charge-equilibrating flow is calculated by the propagation speed of the wave front of N/Z = 1.10. The relative velocity of collision at the contact is slower than that at the initial time, because of the deceleration due to the Coulomb repulsion.

Motion	Speed	Description
Propagation of charge-equilibrating flow	$0.90 v_F $	$\sim 6.5/(0.75 \times 10^{-22}) \text{ fm/s}$
Relative velocity for $E/A=2.0$ MeV	$0.36 v_F $	Speed given at the initial time
Relative velocity for $E/A=1.0$ MeV	$0.23 v_F $	Speed given at the initial time



FIG. 1: (Color online) Propagation of neutro, ³⁶Ca correspond to the ions coming from the left

This type of fast wave propagation (reaction dynamics), which <u>contributes to</u> achieve fusion (not necessarily successful), is <u>universal</u> to any low-energy heavy-ion reactions independent of "energies", impact parameters, reaction type (whether fusion or fragmentation).



FIG. 1: (Color online) Propagation of neutron-rich flow is depicted for the collision between ⁵²Ca and ³⁶Ca, where ⁵²Ca and ³⁶Ca, where ⁵²Ca and ³⁶Ca, where ⁵²Ca and ³⁶Ca, where ⁵²Ca and ³⁶Ca correspond to the ions coming from the left and right hand sides, respectively. The colored parts correspond to the parts with N/Z > 1 (each frame is 40×30 fm²), and the density contour equal to 0.02 fm⁻³ is shown by a thick black curve. Three-dimensional time-dependent Hartree-Fock calculations with a Skyrme interaction (SLy4d) is carried out; the single-particle wave functions are represented on a Cartesian grid with the spacing of 0.8 fm, and the time unit of calculation is set to 1.5 $\times 10^{-24}$ s. The initial distance between the two colliding ions are set to 20 fm, then the relative velocity of collision is given.

Upper energy limit formula (Iwata-Otsuka-Maruhn-Itagaki)

Nucleons with the fermi velocity are decisive to the (all the) equilibration :

- \rightarrow rapid process (0.3c)
- \rightarrow independent of relative velocity of collision
- \rightarrow dependence of the sort of colliding nuclei

Calculations and Experiments are well explained.

$$\frac{E_{\text{CE,lab}}}{A} = \frac{\hbar^2 (3\pi^2 \rho_{\min})^{2/3}}{2m} + \frac{e^2 Z_1 Z_2}{4\pi\epsilon_0 r_0} \frac{A_1 + A_2}{A_1 A_2 (A_1^{1/3} + A_2^{1/3})},$$
(1)

$$\rho_{\min} = \min_{i} \left(\frac{N_{i} (\frac{4\pi r_{0}}{3} A_{i}^{1/3})^{-1}}{(1 - 3\bar{\epsilon})(1 + \bar{\delta})}, \frac{Z_{i} (\frac{4\pi r_{0}}{3} A_{i}^{1/3})^{-1}}{(1 - 3\bar{\epsilon})(1 - \bar{\delta})} \right), \quad (2)$$

where m, e, ϵ_0 , and r_0 are the nucleon mass, the charge unit, the vacuum permittivity, and the usual nuclear radius parameter (1.2 fm), respectively.

			, .		
	Collision	TDHF (SLy4d)	TDHF (SkM*)	Equation (1)	Fermi gas
(i) (ii) (iii) (iv) (v) (v) (vi) (vii) (viii)	208 Pb + 238 U $208 Pb + 132 Xe$ $208 Pb + 132 Sn$ $208 Pb + 40 Ca$ $208 Pb + 24 Mg$ $208 Pb + 24 O$ $208 Pb + 16 O$ $208 Pb + 4 He$ $244 fc + 24 O$	$\begin{array}{c} 6.5 \pm 0.5 \\ 6.5 \pm 0.5 \\ 6.5 \pm 0.5 \\ 3.5 \pm 0.5 \\ 2.5 \pm 0.5 \\ 2.5 \pm 0.5 \\ 1.5 \pm 0.5 \\ 1.5 \pm 0.5 \\ < 1.0 \end{array}$	$\begin{array}{c} 6.5 \pm 0.5 \\ 6.5 \pm 0.5 \\ 6.5 \pm 0.5 \\ 3.5 \pm 0.5 \\ 2.5 \pm 0.5 \\ 2.5 \pm 0.5 \\ 1.5 \pm 0.5 \\ <1.0 \\ < 1.0 \end{array}$	6.91 6.50 6.36 2.36 2.18 1.75 0.48 5.99	9.46 9.03 9.03 5.14 3.52 3.52 2.50 0.70
	mg + 0	5.5 ± 1.0	5.5 ± 1.0	 5.39	9.50
					<u> </u>

TABLE I. $E_{CE,cm}/A$ values [MeV] obtained by TDHF calculations compared to those obtained by transforming the results of Eq. (1) into the center-of-mass frame. For reference, the values obtained by the Fermi gas model with the standard parameter are also shown.

Charge equilibration is <u>dominant</u> at the early stage of low-energy heavy-ion reactions

- dynamical mixture between neutrons and protons averaging local N/Z ratio (arising from "the symmetry energy")
- very fast mechanism taking only $\sim 10^{-22}$ s

governing the early stage of heavy-ion collision

prevents to produce exotic nuclei

decisive to exotic nuclear synthesis

- There exists an <u>upper-limit energy</u> for fast charge equilibration, which is represented by the upper energy-limit formula (Iwata-Otsuka-Maruhn-Itagaki)
- The mechanism of fast charge equilibration is ultimately reduced to the propagation of nucleon wave at the speed almost equal to the (amplitude of) Fermi velocity.
 - = zero sound propagation (collective dynamics ~ mean-field effect)

lwata, JMP (2012); ArXiv:1204.3723

Iwata-Otsuka et al., PRL (2010)

Charge equilibration is <u>dominant</u> at the early stage of low-energy heavy-ion reactions

Appearance of charge equilibration SUPPRESS the production of exotic nuclei



As the most probable quantum dynamics, the TDDFT results predict that it is difficult/impossible to produce exotic and very heavy nuclei.

Indeed, energy should be higher than the upper-limit energy for exotic production, but final fragments become smaller for higher energies.

Superheay reactions including fission

²⁴⁸Cm + ⁴⁸Ca -> ²⁹⁶116* is calculated;



Motivation:

Superheavy

Theoretical prediction of possibility

Producing neutron-rich and heavy nuclei



Superheavy

Superheavy synthesis reaction

Recent Progress of computer technology makes us possible to treat heavy system in a systematic way.

Iwata-Heinz, JPCS (2012)



superheavy experiments ~~> **pico barn**

Quite different from the experiments

In order to have better predictability (to compensate for shortcomings of the TDDFT), The additional thermal treatment is necessary. Before going into the additional treatment, the reason is simply summarized here

Iwata JPCS, to appear





Iwata JPCS, to appear

Correct treatment of the thermal instability of the compound nuclei al treatment.

the reason is simply summarized here

F = 268 MeV



1) obtain TDDFT fragments (A_i and Z_i) with excitation (E_i^*) and kinetic (K_i) energies;

Cooling due to alpha and neutron emission

2) for each fragment calculate evaporation energy:

$$\begin{cases} E_{i,\alpha,evap} = E_{i,1\alpha,evap} + E_{i,\alpha,kin}, \\ E_{i,n,evap} = E_{i,1n,evap} + E_{i,n,kin}, \end{cases}$$

where $E_{i,\alpha,evap}$ and $E_{i,n,evap}$ are the cooling energies due to one alpha-particle and one neutron emissions, respectively, and $E_{i,\alpha,kin}$ and $E_{i,n,kin}$ denotes the kinetic energy of alpha-particle and neutron, respectively (cf. Boltzmann distribution);



Evaporation prescription (3/3)

Cooling due to alpha and neutron emission

For *n* neutron emission channel, calculate the remaining energy



we can obtain the alpha-decay chain

Result of SHE reaction (example)

Based on the prescriptions, for example, we have obtained the following alpha-decay chain depending on the impact parameter

Calculation for the cross section is not yet !

as well as the possible (incl. possibility) fission dynamics of each fragment

 $E = 268 \mathrm{MeV},$ 248 Cm $+^{48}$ Ca $\rightarrow ^{292}$ Lv + 4nWe want to know the fission property (fission dynamics) of obtained product after alpha and neutron emission $\bigcirc \Pi \pm 2\alpha \pm 4\pi$ \rightarrow (280 Ds) \rightarrow 3 α + 4n, ($b \leq 4$ fm) 248 Cm + 48 Ca \rightarrow 246 Cf + 47 Ar + 3n $\rightarrow {}^{242}\text{Cm} + {}^{47}\text{Ar} + \alpha + 3n$ \rightarrow (²³⁸Pu)+⁴⁷ Ar + 2 α + 3n, (b = 6 fm) 248 Cm + 48 Ca $\rightarrow ^{245}$ Bk + 48 K + 3n $\rightarrow {}^{241}\text{Am} + {}^{48}\text{K} + 1\alpha + 3n$ $\rightarrow (^{237}\text{Np})^{-48}\text{K} + 2\alpha + 3n, \quad (b = 8 \text{ fm})$ $^{248}\text{Cm} + ^{48}\text{Ca} \rightarrow ^{248}\text{Cm} + ^{48}\text{Ca}, (b > 10 \text{ fm});$

Fission dynamics

After the alpha and neutron emissions,

The compound nucleus is still hot ...; we prepare a new initial state

 $(^{296}116)* = (^{296}Lv)*$



E* [MeV]

Compound nucleus; Going into a stable fused system in TDDFT



Note that, **including us**, all TDDFT trials for calculating fission dynamics failed. It is due to the difficulty of preparing good initial condition.



Following the TDDFT property, the total energy is conserved



The distance between two nuclei is "uniquely" determined by the excitation energy

The relation between these two states are understood by calculating the overlap between the two states (now ongoing), which corresponds also to the calculation of the probability:



the symmetric fission of $^{296}Lv^*$ (compound) E_{cm} = 268 MeV (the energy is strictly conserved)



Before going into the additional treatment, the reason is simply summarized here



These two calculations can be connected by the additional treatment; i.e., the relation between the final state of TDDFT1 and the initial state of TDDFT2 can be quantitatively obtained by calculating <u>the correlation function</u>.

Superheavy

Note: more terms in modern EDF

What does TDDFT fission dynamics tell us ?



1) The fission dynamics actually appears purely by the TDDFT dynamics (after preforming):

single particle degree of freedom might be important to the preforming stage pairing (level crossing) plays a role in the preforming stage (but other effects is also necessary) thermal equilibration effect might be important; adiabatic approach should not be ultimate.

2) The duration time of fission dynamics is rather short than we have expected; which is actually about 10⁻²¹ s:

once an ideal state is formed, fission is completed quickly (by collective motion) Preforming (clustering) stage might consume incomparably long time (10⁻¹⁸ to 10⁻¹⁵s at least)

Summary

- The present status of the TDDFT is shown.
- Now TDDFT confront difficulties with respect to treatment of heavy system treatment of fission, fragmentation (late processes)
 = reduced to the treatment of thermal property !

Evaporation residue cross section:~1 (light systems)
$$\sigma_{ER}(E_{cm}) = \sum_{J} \sigma_{CP}(E_{cm}, J) \times P_{CN}(E_{cm}, J) \times P_{SV}(E_{cm}, J)$$
CaptureCompound form. prob.Survival prob.

Summary

As a way of overcoming some difficulties, we have proposed a sequence of method

evaporation prescription to calculate (Iwata-Heinz)

fission dynamics by preparing <u>a new initial state</u> (Iwata-Heinz)

by calculating the correlation function, the physical meaning of the new initial state is clarified (Iwata-Otsuka)

where difficulties mostly arise from the difference of the time scales.