基研研究会・iTHEMS研究会 2018
「非平衡系の物理学— 階層性と普遍性—」
2018年12月26-28日@京都大学基礎物理学研究所・パナソニック国際交流ホール

低エネルギー原子核反応における非平衡過程

関澤 一之

新潟大学 研究推進機構 超域学術院

今日の発表で伝えたいこと

➢ 原子核をぶつけたとき，何が起こるのか？

荷電平衡過程
Charge equilibration
N/Z

エネルギーの散逸
Energy dissipation
TKEL

超流動の位相の変化
Superfluid phase
$|\Delta(\boldsymbol{r})|e^{i\varphi(\boldsymbol{r})}$

質量平衡過程
Mass equilibration
A

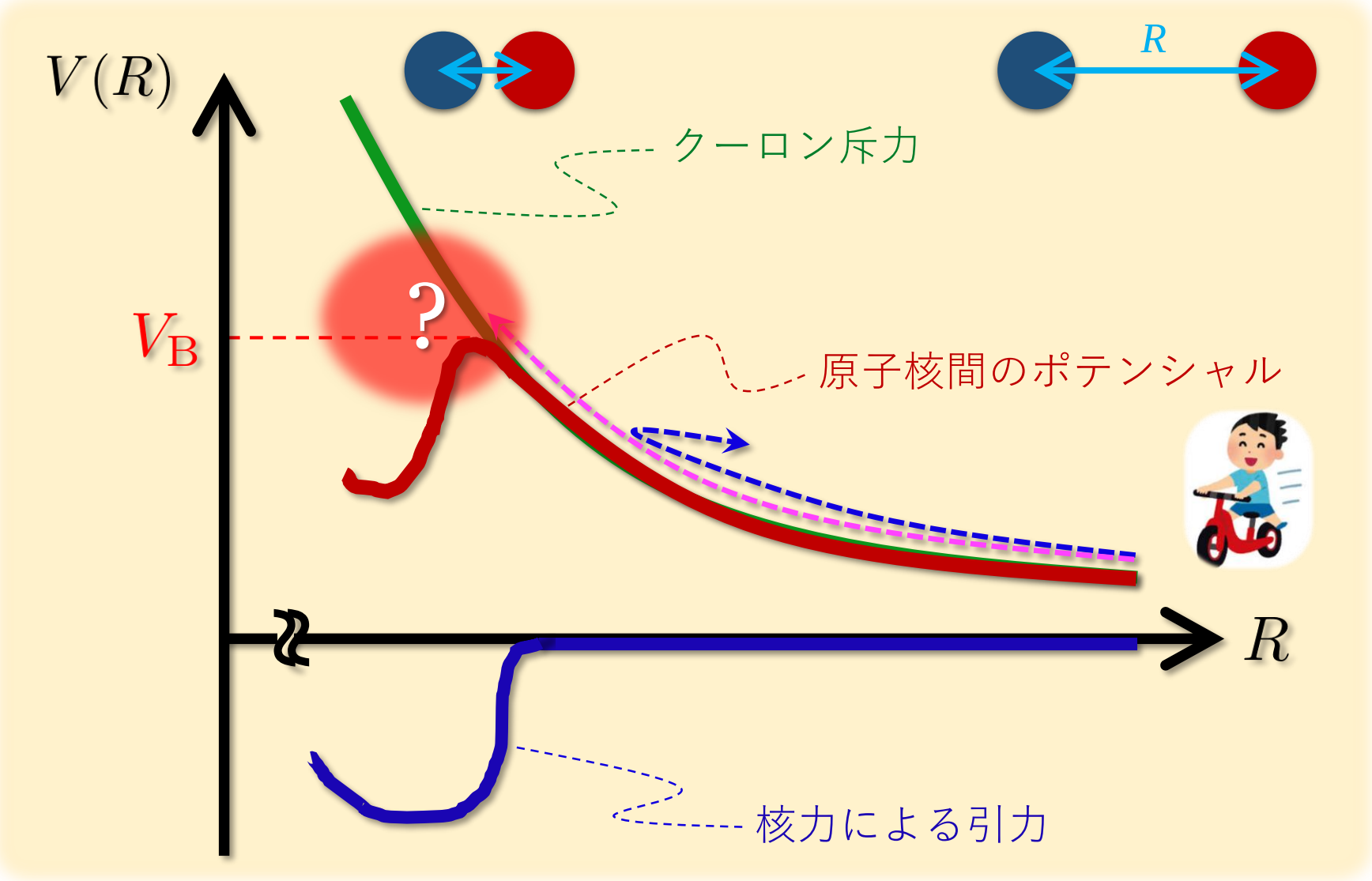
質量数分布の幅の増大
Mass distribution width
σ_A

“高エネルギー”ではない！！

Animation taken from: Brookhaven National Laboratory Website (http://www.bnl.gov/rhic/)

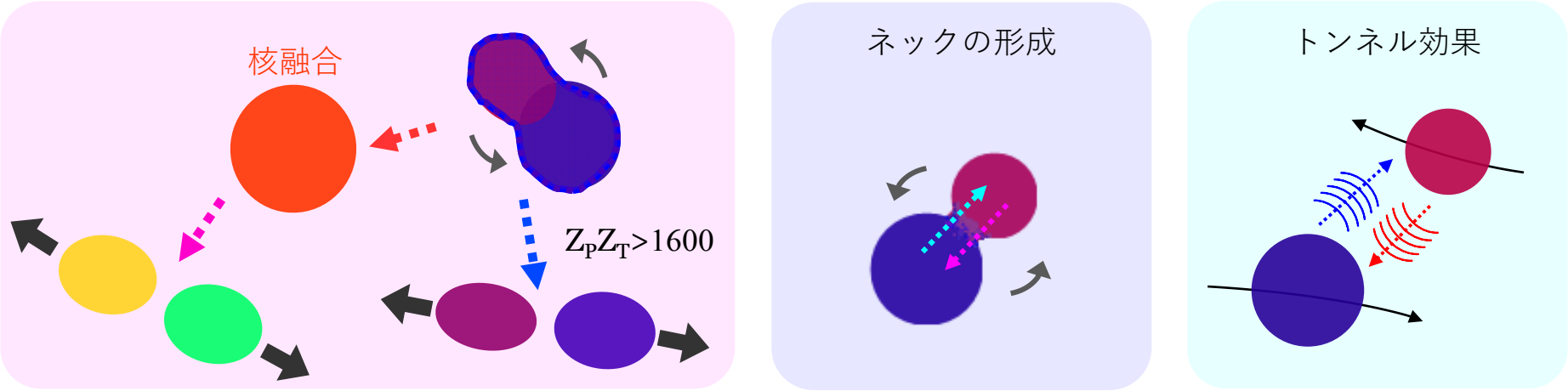
２つの原子核を“そっとぶつける”

フェルミ粒子多体系の非平衡ダイナミクス



➢ 私の行っている研究:
スパコンを用い，量子多体理論に基づく数値シミュレーションを実施

様々な量子多体ダイナミクスの記述が必要



核融合・核分裂　準核分裂　多核子移行・エネルギー散逸　核子移行

小さい ← 最近接距離 → 大きい

Remarks on TDHF (or TDDFT, TDEDF)

✓ There is no adjustable parameter on reaction dynamics

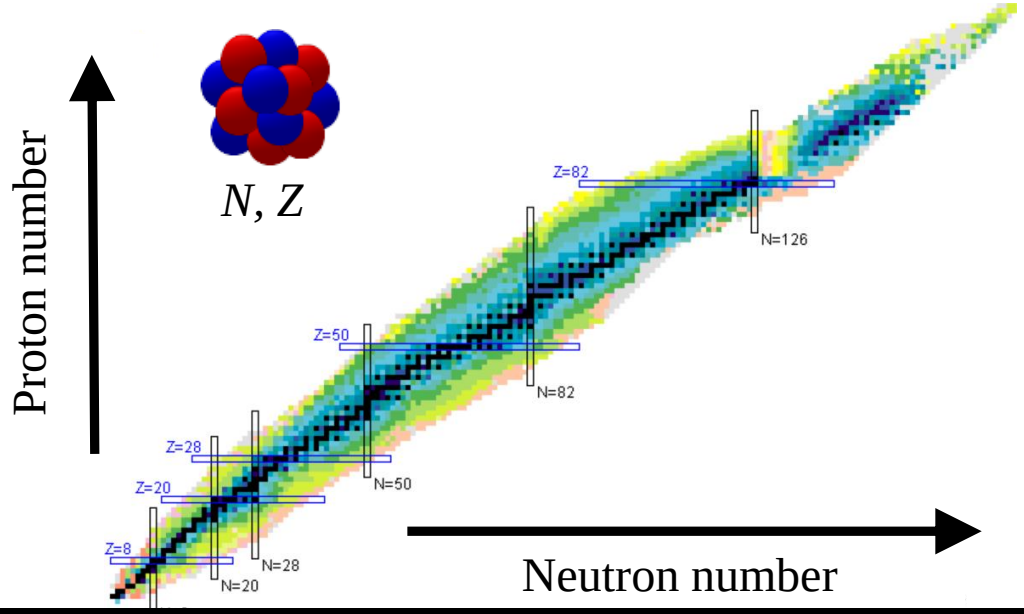
$$S = \int_{t_0}^{t_1} dt \left(i\hbar \sum_i \langle \phi_i(t) | \frac{\partial}{\partial t} | \phi_i(t) \rangle - E[\rho(t)] \right)$$

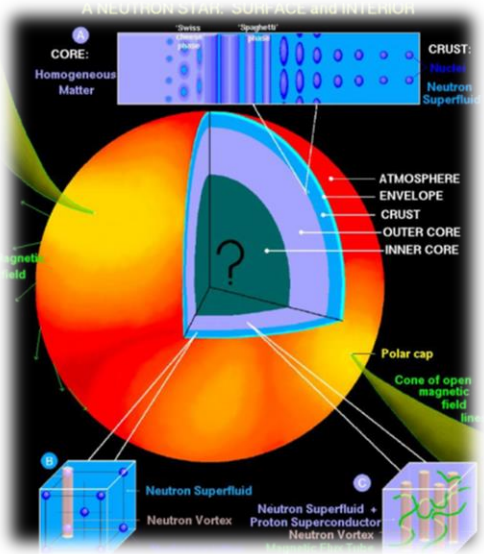
$$i\hbar \frac{\partial \phi_i(\boldsymbol{r}\sigma q, t)}{\partial t} = \hat{h}[\rho(t)]\phi_i(\boldsymbol{r}\sigma q, t) \quad : \text{TDHF eq.}$$

Effective interaction

$$E[\rho] = \langle \Phi | \hat{H} | \Phi \rangle$$

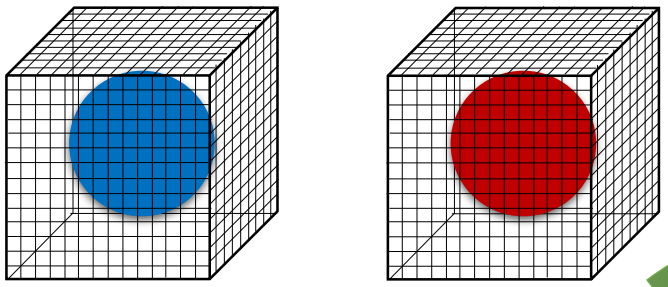
Energy Density Functional (EDF)





実時間・実空間で原子核反応を記述

1） 入射核・標的核の基底状態を計算



KS 方程式

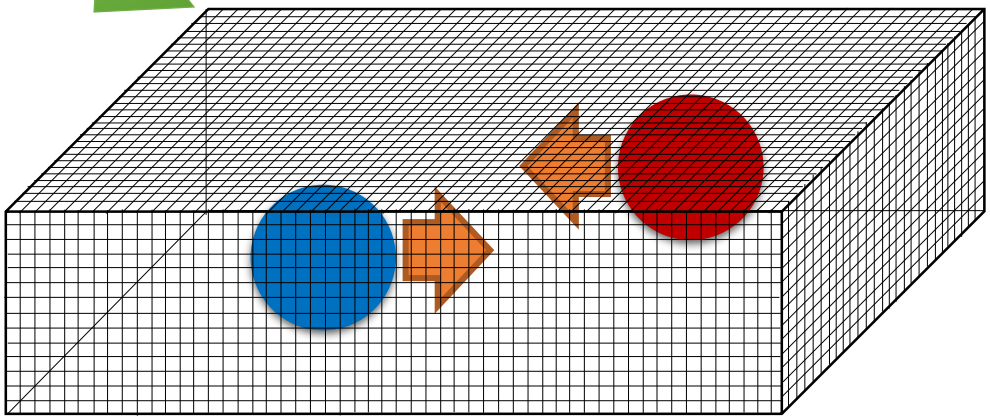
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{KS}}[\rho(\boldsymbol{r})]\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\,\phi_i(\boldsymbol{r})$$

2） 大きい計算格子に配置

3） 運動量を与え、実時間発展を計算

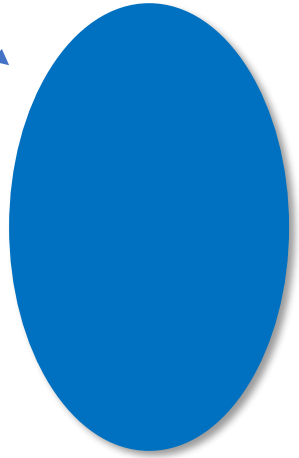
TDKS 方程式

$$i\hbar\frac{\partial\phi_i(\boldsymbol{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{KS}}[\rho(\boldsymbol{r},t)]\right]\phi_i(\boldsymbol{r},t)$$

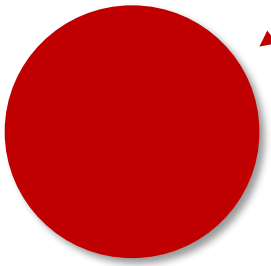


クーロン障壁近傍のエネルギーで
^{64}Niと^{238}Uが衝突したとき，何が起こるか？

ラグビーボール型に
大きく変形



ほぼ球形



標的核: ^{238}U

陽子数: Z=92

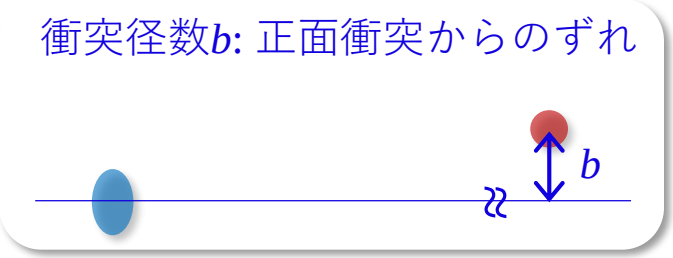
中性子数: N=146

入射核: ^{64}Ni

陽子数: Z=28

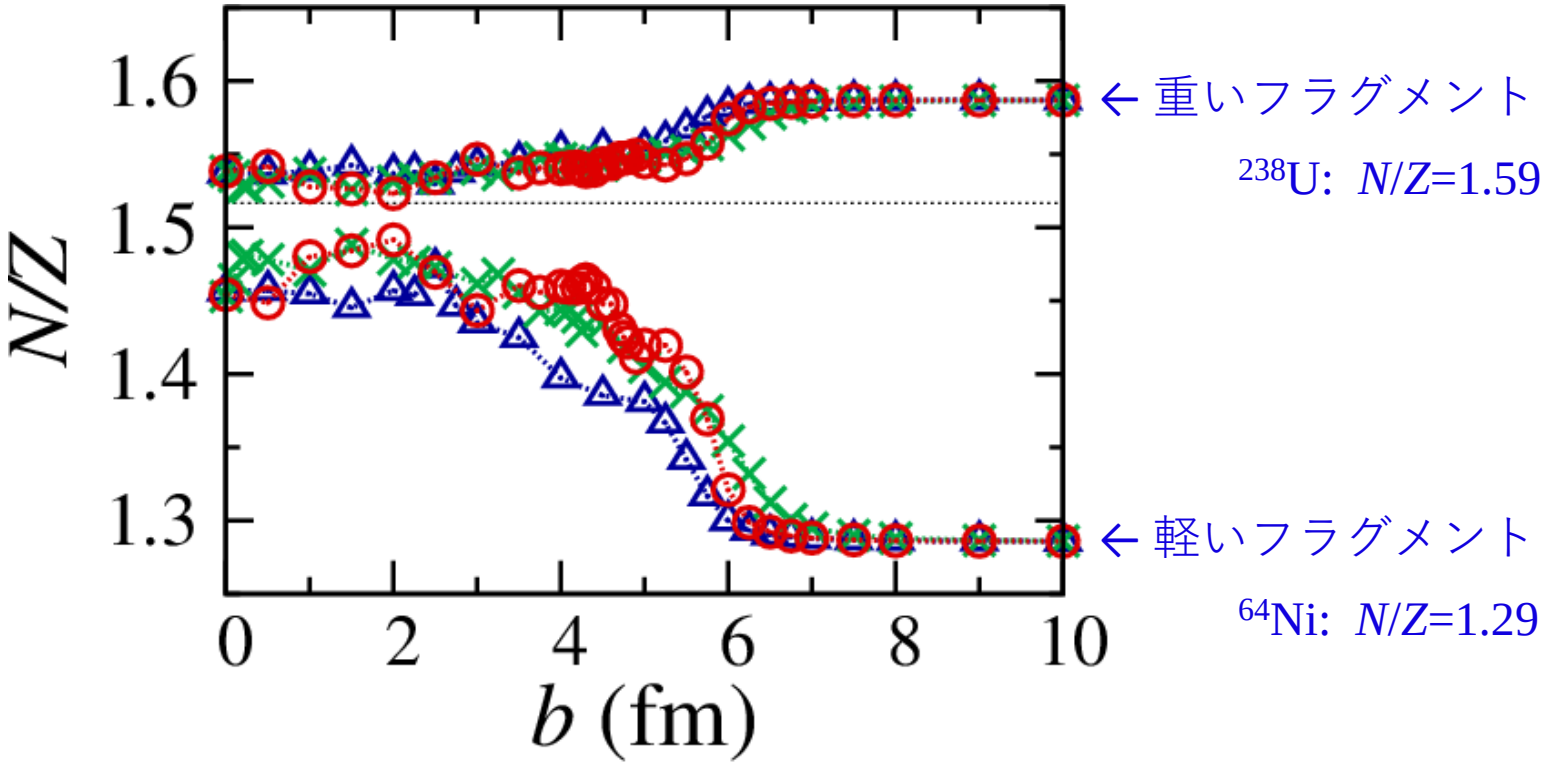
中性子数: N=36

^{64}Niと^{238}Uの衝突: 荷電平衡過程



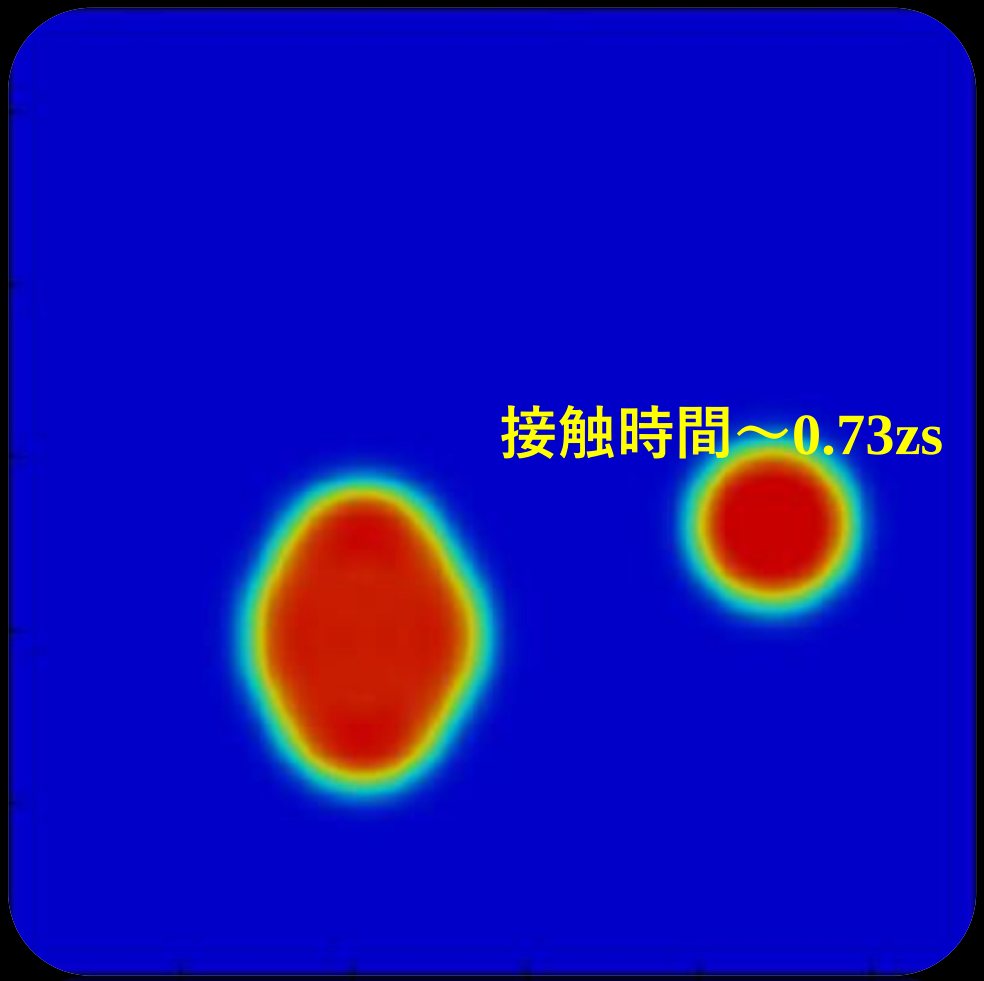
フラグメントのN/Z vs. 衝突径数b

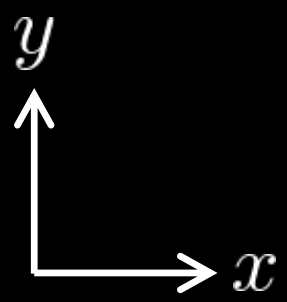
✓ 衝突径数(最近接距離)が小さくなると，系は荷電平衡に向かう



※色の違いは変形したウランの向き

例）^{238}Uの向きy方向，b=5.5 fmの場合



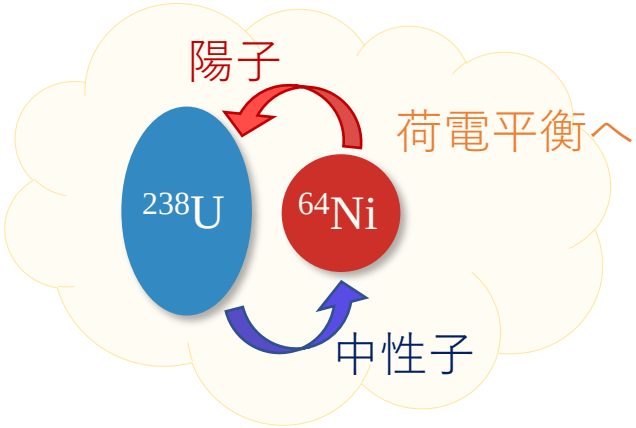


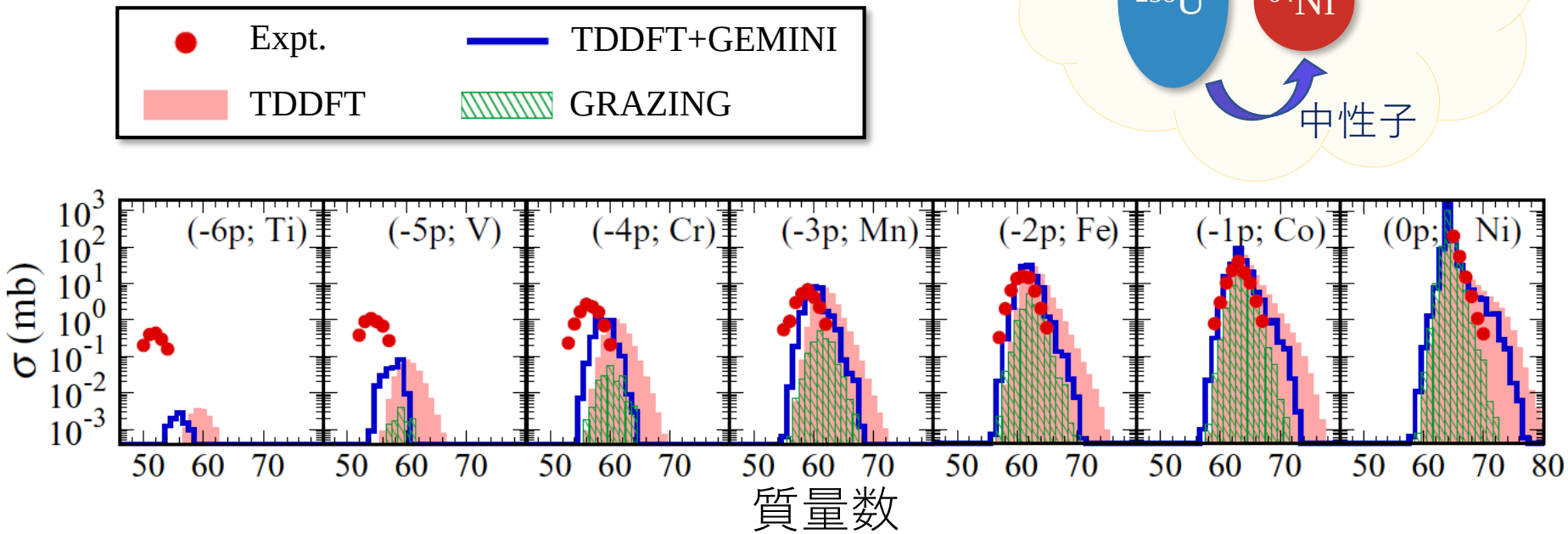
衝突平面

^{64}Niと^{238}Uの衝突でどの原子核が生成されるか（生成断面積）

KS and K. Yabana, PRC**88**(2013)014614; KS, PRC**96**(2017)014615

荷電平衡過程によって様々な原子核が生成される

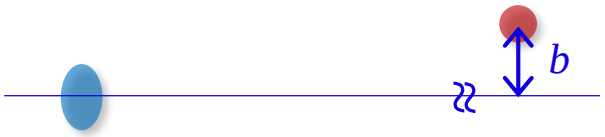


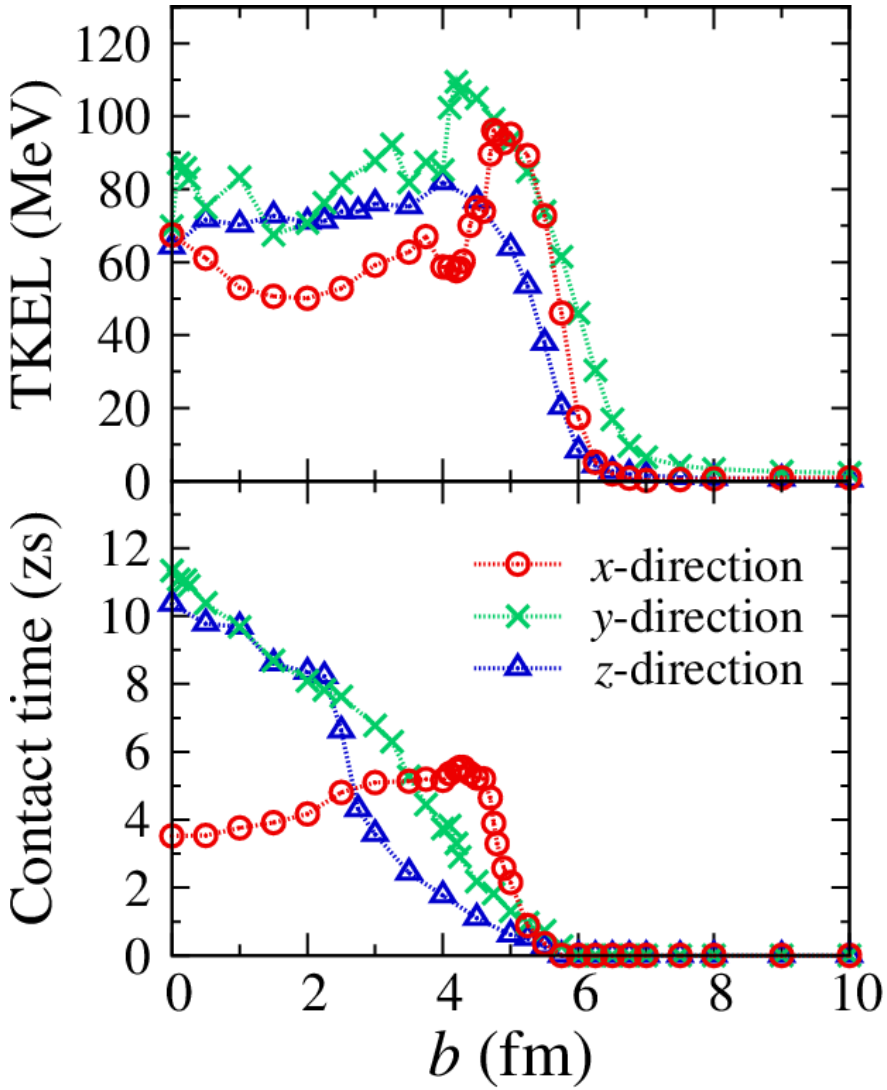


Expt.: L. Corradi et al., PRC**59**(1999)261

^{64}Niと^{238}Uの衝突: エネルギーの散逸

衝突径数b: 正面衝突からのずれ



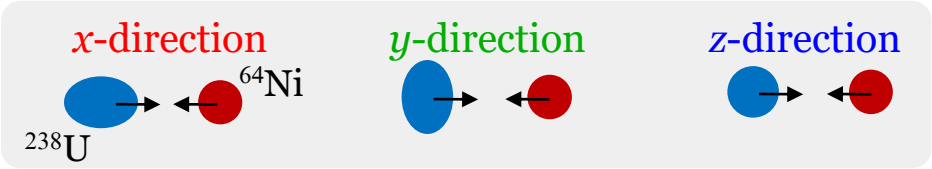


全運動エネルギー損失 (TKEL)

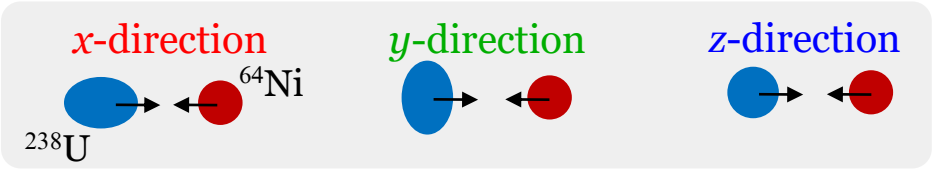
✓ 約2-3zsの接触時間で,
エネルギーが散逸

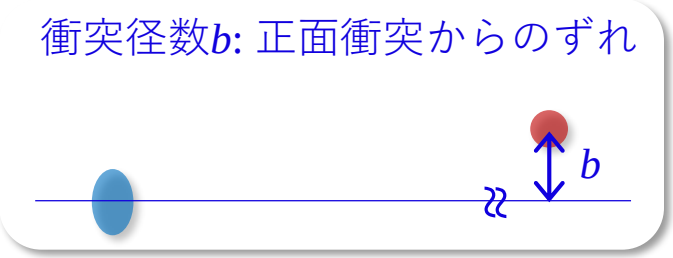
接触時間

✓ 顕著な方向依存性が見られる



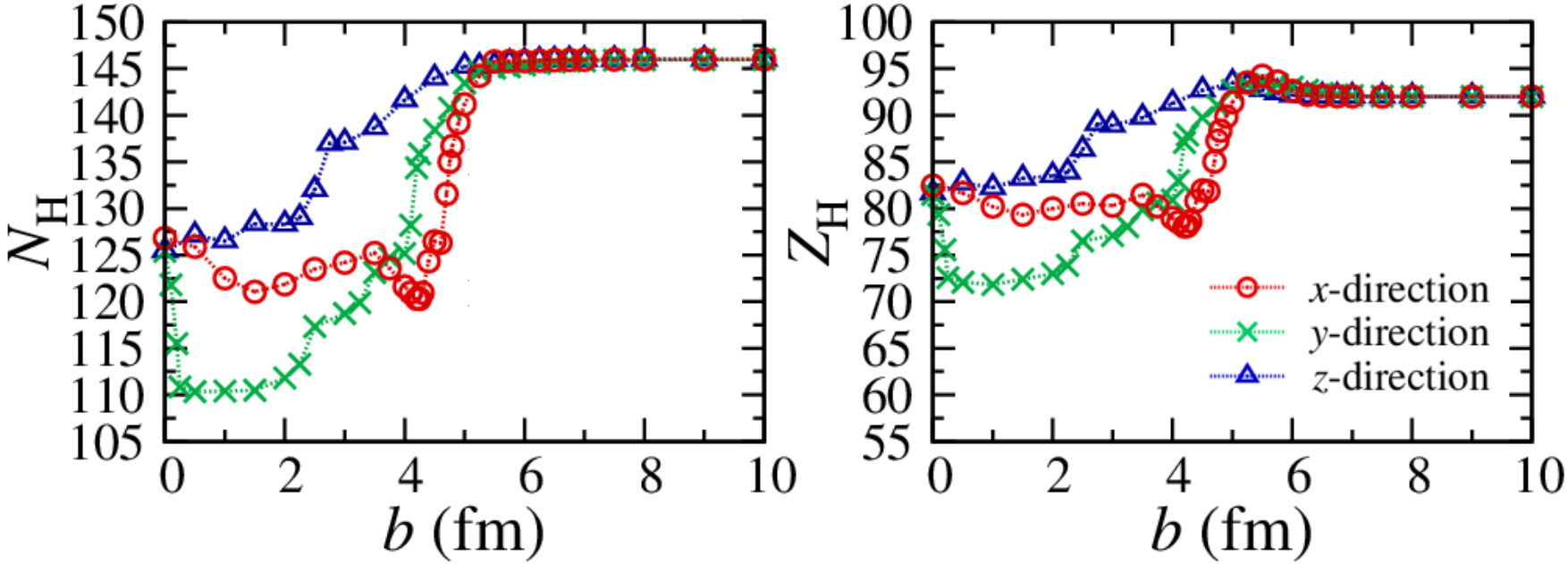
^{64}Niと^{238}Uの衝突: 質量平衡過程





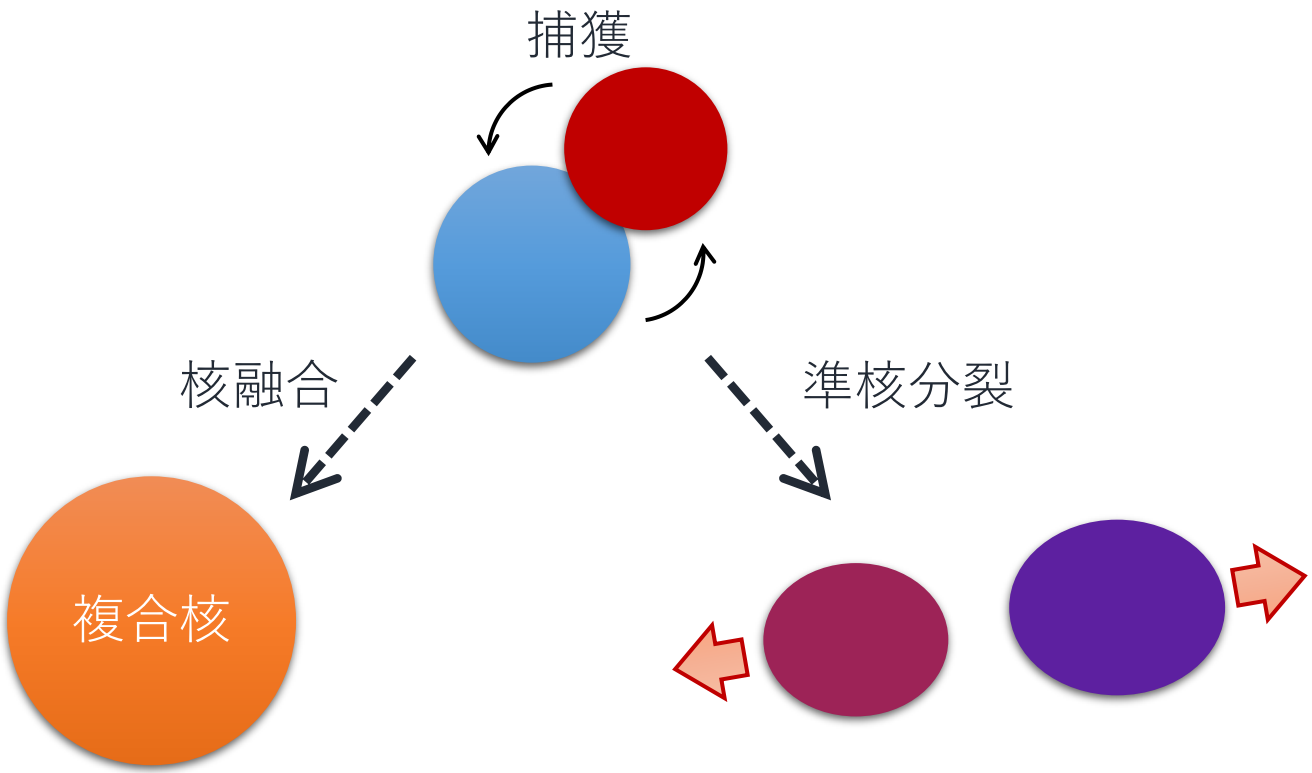
重いフラグメントの核子数 vs. 衝突径数b

✓ ^{238}Uから^{64}Niへ，多数の核子が移行している



準核分裂過程

重い核の核融合反応を妨げる主要な反応過程



$$\sigma_{\mathrm{ER}} \sim W_{\mathrm{surv}} * \sigma_{\mathrm{cap}} * P_{\mathrm{CN}}$$

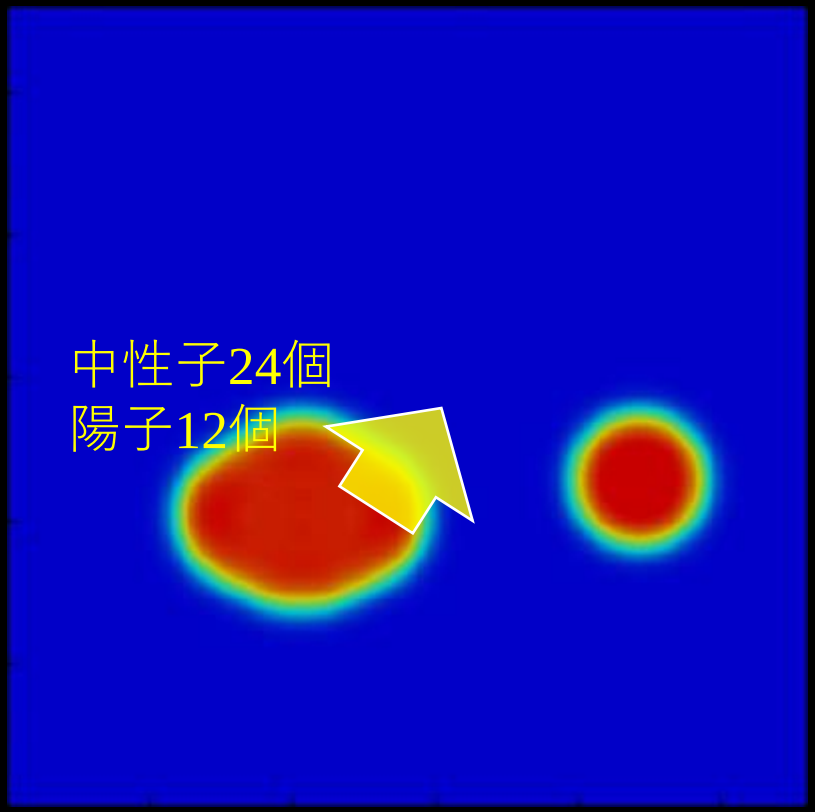
^{64}Ni+^{238}U at E_{lab}=390 MeV

KS and K. Yabana, PRC**93**(2016)054616

準核分裂過程の数値シミュレーション

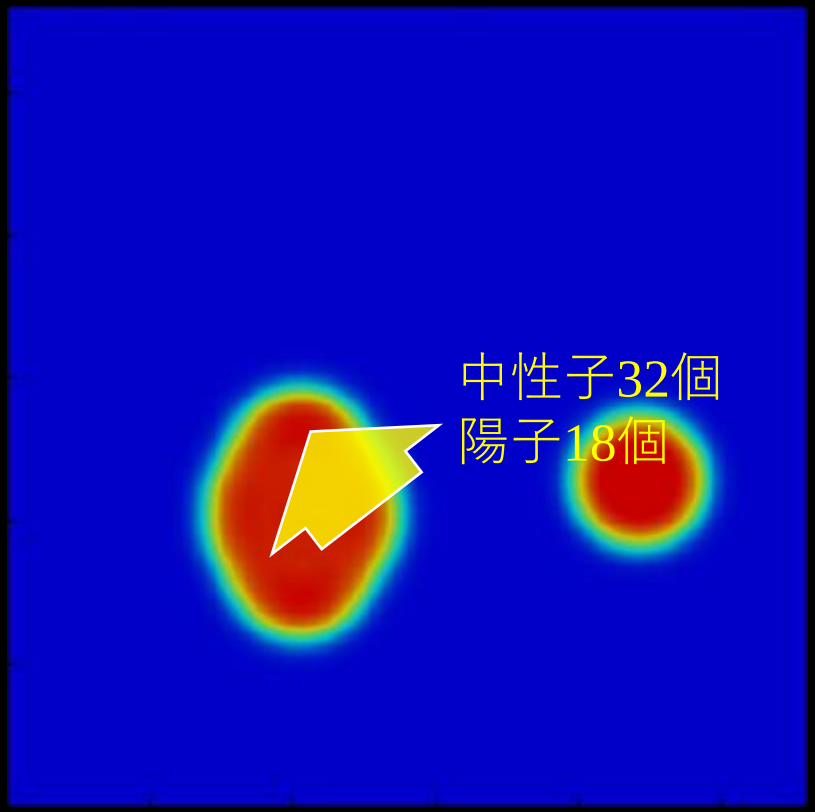
ウランの先端に衝突

^{208}Pbの殻効果



ウランの側面に衝突

より質量対称に分裂



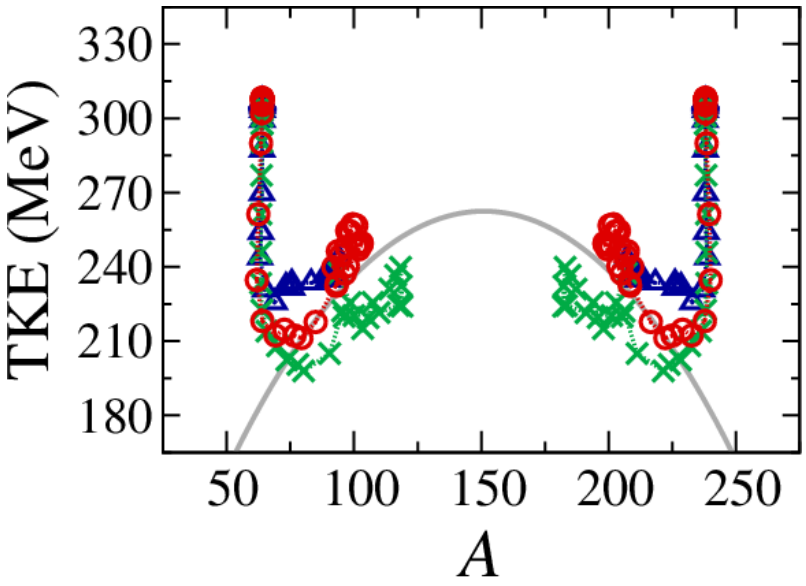
^{64}Ni+^{238}U at E_{lab}=390 MeV

KS and K. Yabana, PRC**93**(2016)054616

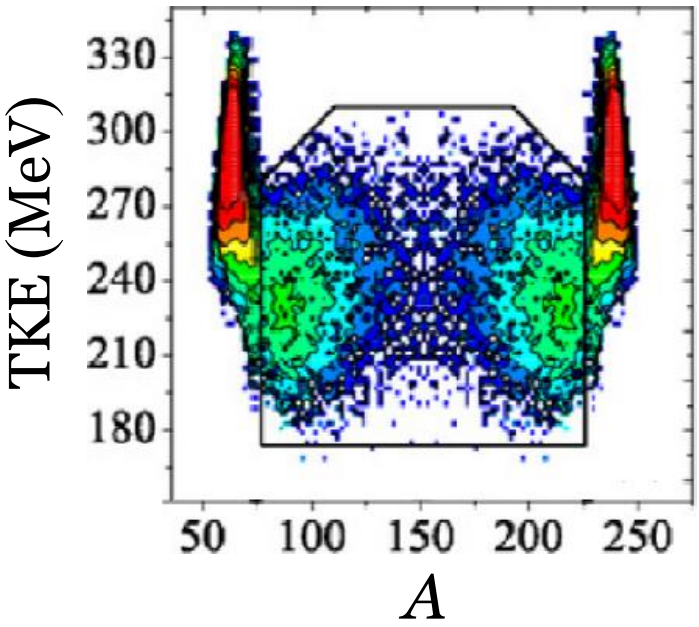
散逸したエネルギー・質量平衡化の傾向を定量的に再現

運動エネルギーとフラグメント質量の相関

理論計算

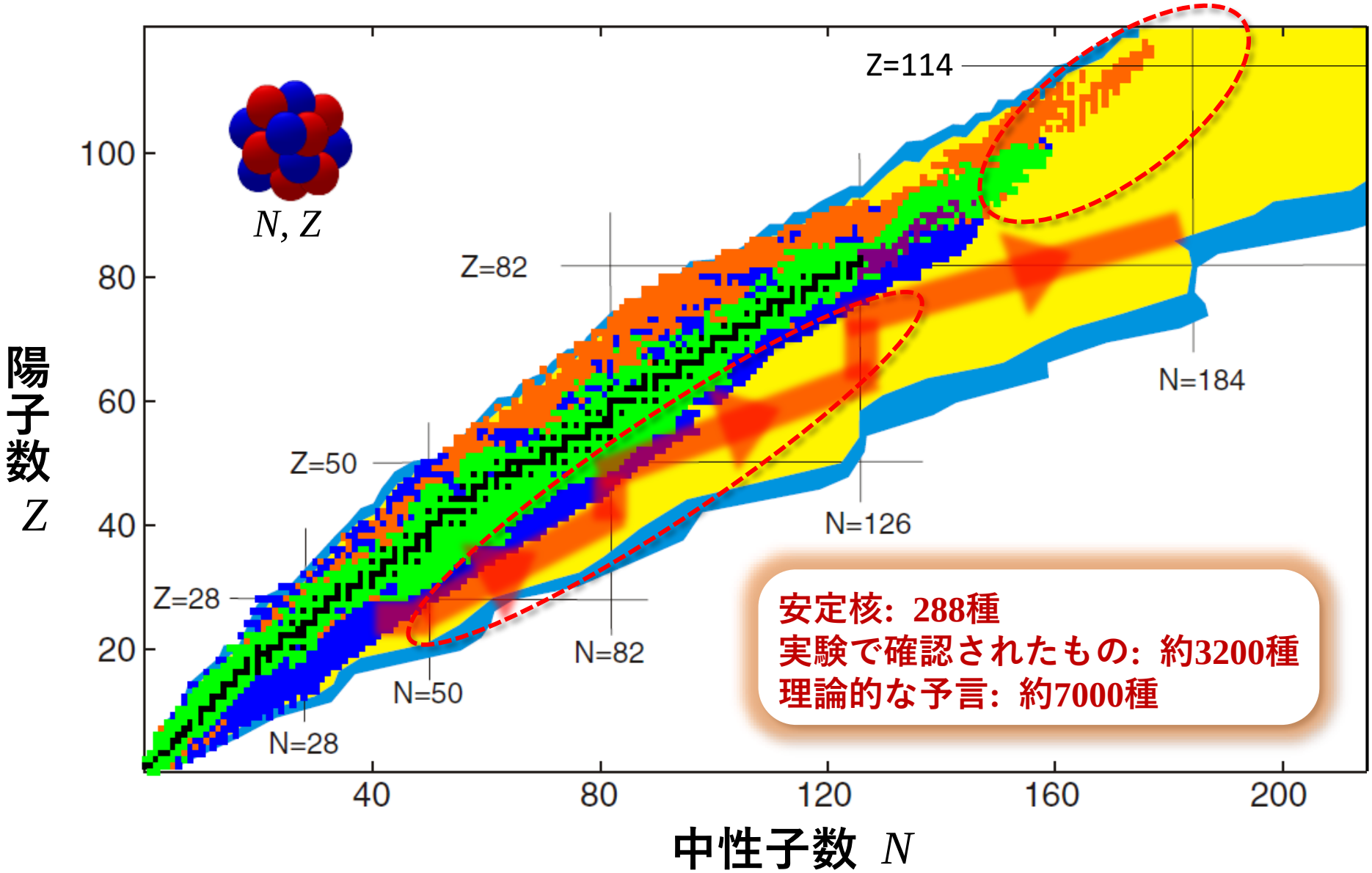


実験データ



Expt.: E.M. Kozulin *et al.*, PLB**686**(2010)227

反応の微視的理解 → 未知原子核の生成へ



安定核：288種
実験で確認されたもの：約3200種
理論的な予言：約7000種

M. Thoennessen, Rep. Prog. Phys. **76**, 056301 (2013)

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質量数分布の幅の増大
Mass distribution width
σ_A

最近の研究の１つは，2018年1月にPRLに掲載:

PHYSICAL REVIEW LETTERS **120,** 022501 (2018)

Exploring Zeptosecond Quantum Equilibration Dynamics: From Deep-Inelastic to Fusion-Fission Outcomes in ^{58}Ni + ^{60}Ni Reactions

E. Williams,[1,*] K. Sekizawa,[2] D. J. Hinde,[1] C. Simenel,[1] M. Dasgupta,[1] I. P. Carter,[1] K. J. Cook,[1] D. Y. Jeung,[1] S. D. McNeil,[1] C. S. Palshetkar,[1,†] D. C. Rafferty,[1] K. Ramachandran,[1,‡] and A. Wakhle[1]

[1]*Department of Nuclear Physics, Research School of Physical Sciences and Engineering, The Australian National University, Canberra, ACT 2601, Australia*

[2]*Faculty of Physics, Warsaw University of Technology, ulica Koszykowa 75, 00-662 Warsaw, Poland*

(Received 16 August 2017; revised manuscript received 27 October 2017; published 10 January 2018)

Australian National University (ANU) との共同研究

E. Williams

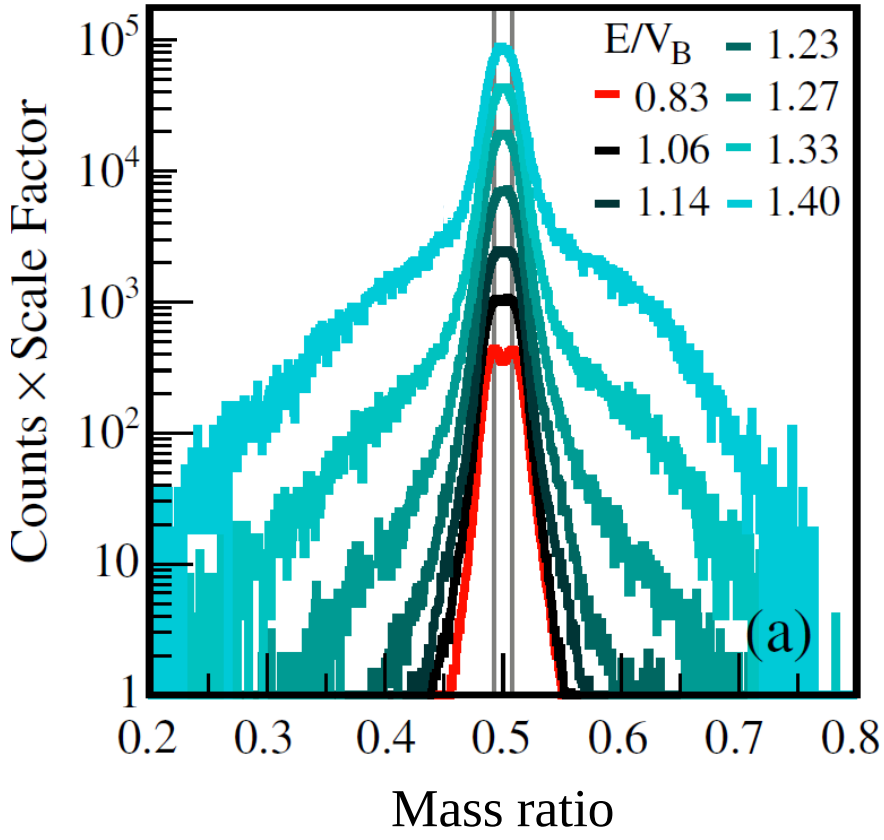
D.J. Hinde

M. Dasgupta

C. Simenel

反応によって生成された原子核の質量分布

- 従来の理論では，分布の幅を定量的に記述することができなかった



Mass ratio:

$$M_{\mathrm{R}} = \frac{M_i}{M_1 + M_2}$$

Method: Variational principle of Balian and Vénéroni

Variational space can be controlled by "state" and "observable"

- The action-like quantity defined by Balian and Vénéroni

$$J = \mathrm{Tr}\left[\hat{A}(t_1)\hat{D}(t_1)\right] - \int_{t_0}^{t_1} \mathrm{Tr}\left[\hat{A}(t)\left(\frac{d\hat{D}(t)}{dt} + i\left[\hat{H}(t), \hat{D}(t)\right]\right)\right] dt$$

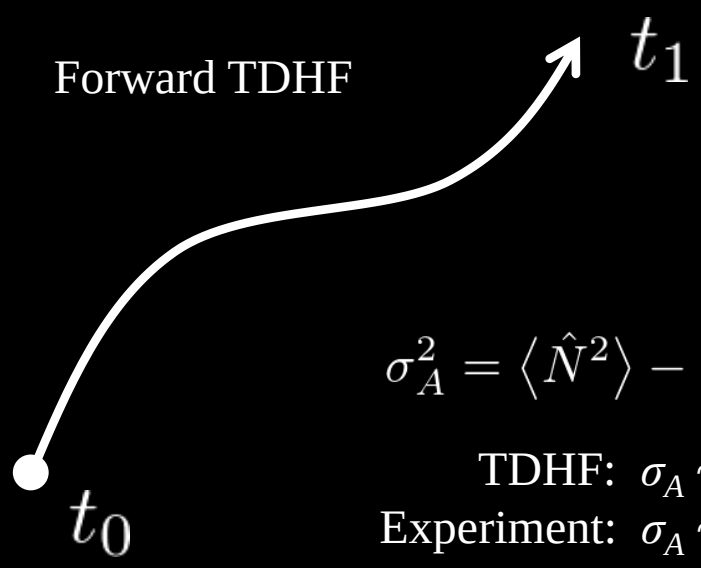
$\hat{D}(t)$: describes the state of the system

$\hat{A}(t)$: describes the evolution of the observable in the Heisenberg picture

R. Balian and M. Vénéroni, Phys. Rev. Lett. **47**, 1353 (1981); Ann. Phys. **216**, 351 (1992).
C. Simenel, Phys. Rev. Lett. **106**, 112501 (2011); Eur. Phys. J. A **48**, 152 (2012).

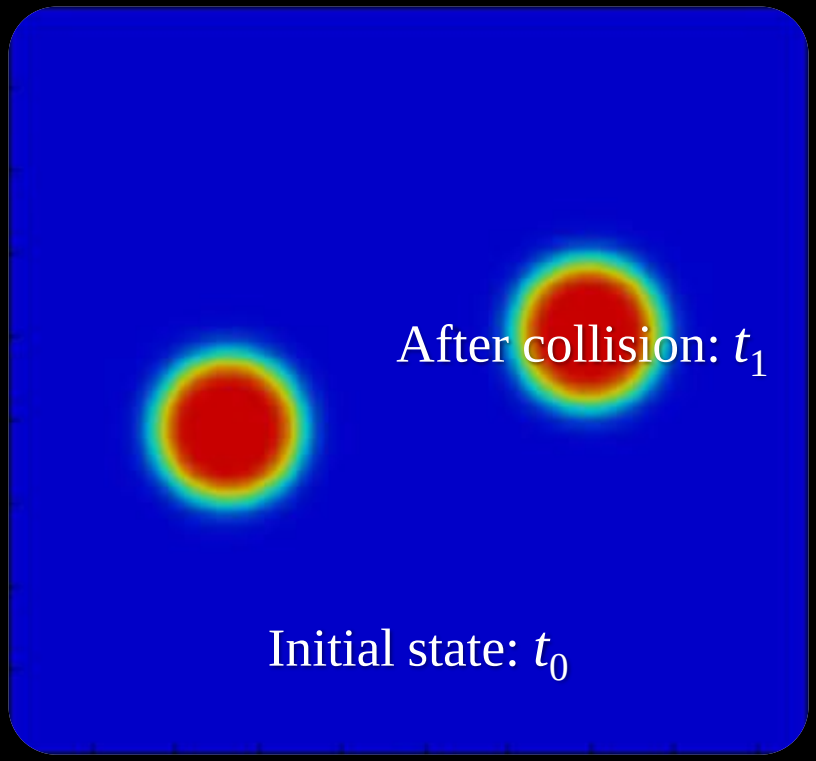
- **Unrestricted variation** (w.r.t. either *A* or *D*) → **TDSE**
- **Slater determinant** & <u>one-body observable</u> → **TDHF**
- **Slater determinant** & <u>fluctuations of one-body observable</u> → **TDRPA**

Numerical implementation of TDRPA for the mass width



$$\sigma_A^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$$

TDHF: $\sigma_A \sim 1.5$
Experiment: $\sigma_A \sim 7.1$



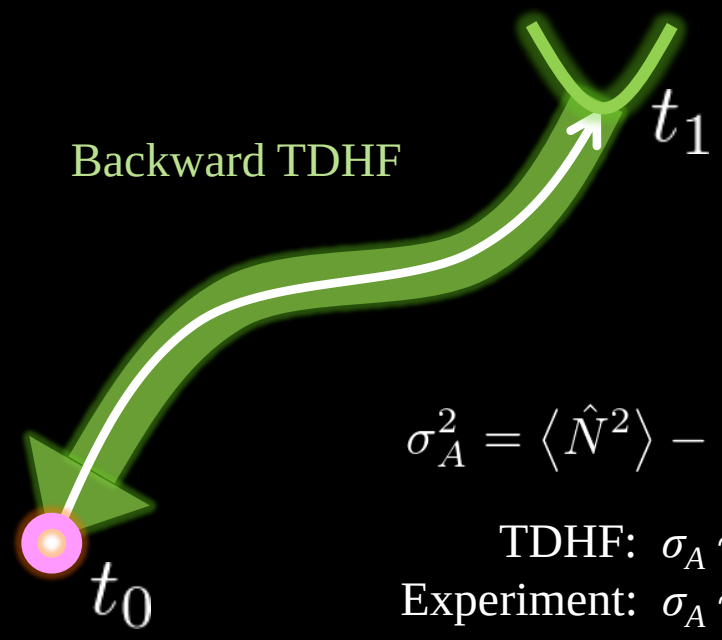
R. Balian and M. Vénéroni, Phys. Rev. Lett. **47**, 1353 (1981); Ann. Phys. **216**, 351 (1992).
C. Simenel, Phys. Rev. Lett. **106**, 112502 (2011); Eur. Phys. J. A **48**, 152 (2012).

Numerical implementation of TDRPA for the mass width

The Balian-Vénéroni prescription (TDRPA):

$$\sigma_X^2(t_1) = \lim_{\varepsilon \to 0} \frac{\mathrm{Tr}\{[\rho(t_0) - \rho_X(t_0, \varepsilon)]^2\}}{2\varepsilon^2}$$

$$\rho_X(t_1, \varepsilon) = e^{i\varepsilon \hat{X}} \rho(t_1) e^{-i\varepsilon \hat{X}}$$



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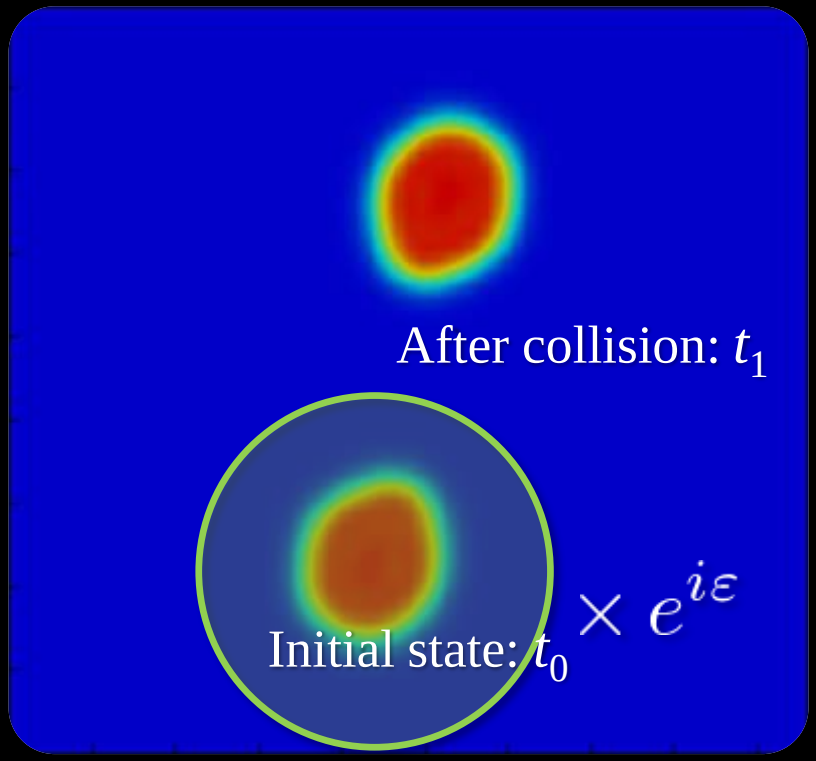


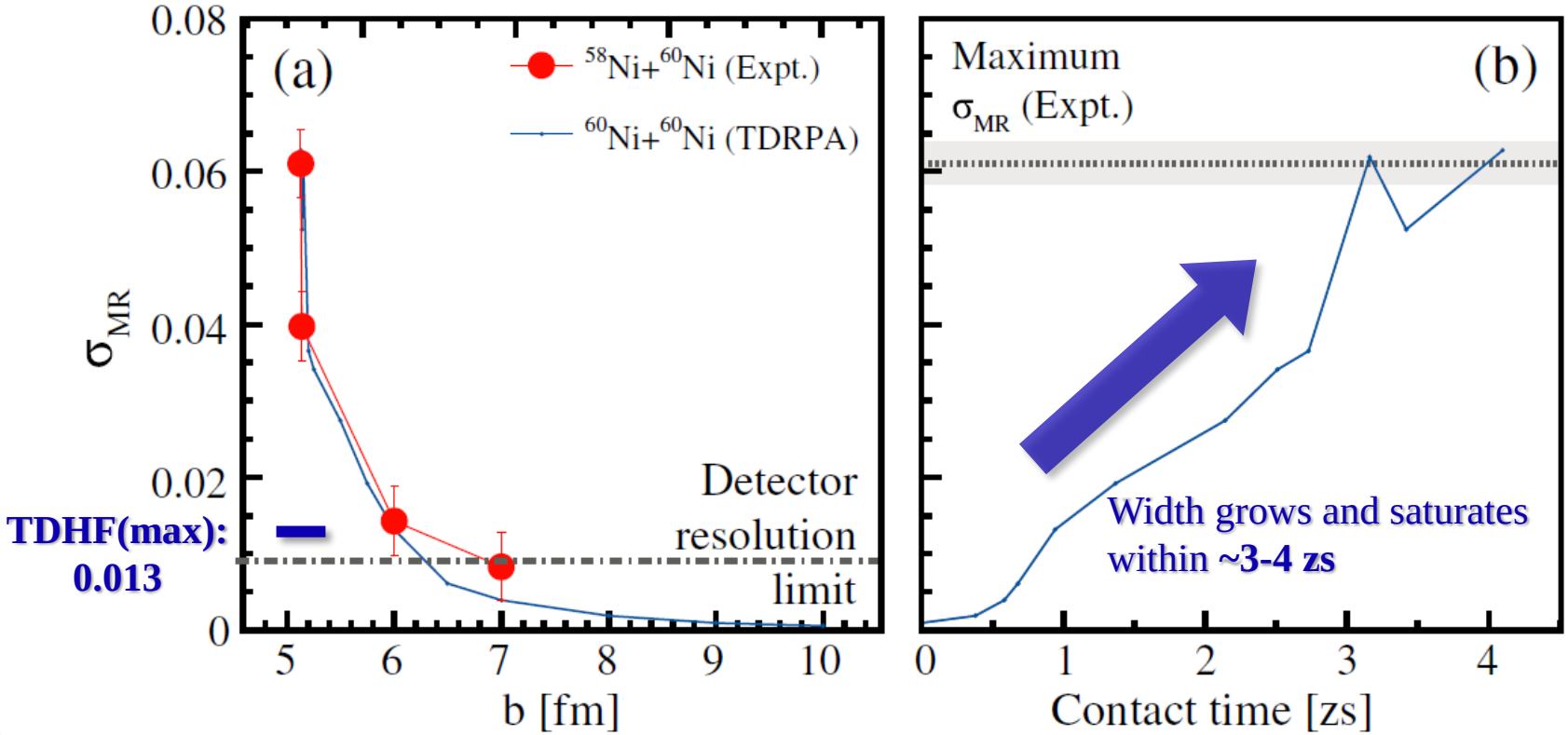
R. Balian and M. Vénéroni, Phys. Rev. Lett. **47**, 1353 (1981); Ann. Phys. **216**, 351 (1992).
C. Simenel, Phys. Rev. Lett. **106**, 112502 (2011); Eur. Phys. J. A **48**, 152 (2012).

^{58,60}Ni+^{60}Ni at E/V_B=1.4

E. Williams, KS, D. Hinde *et al.*, Phys. Rev. Lett. **120**, 022501 (2018)

拡張理論によって，分布の幅の増大を定量的に記述

Width of the mass ratio distribution, σ_{MR}: Expt. vs Theory



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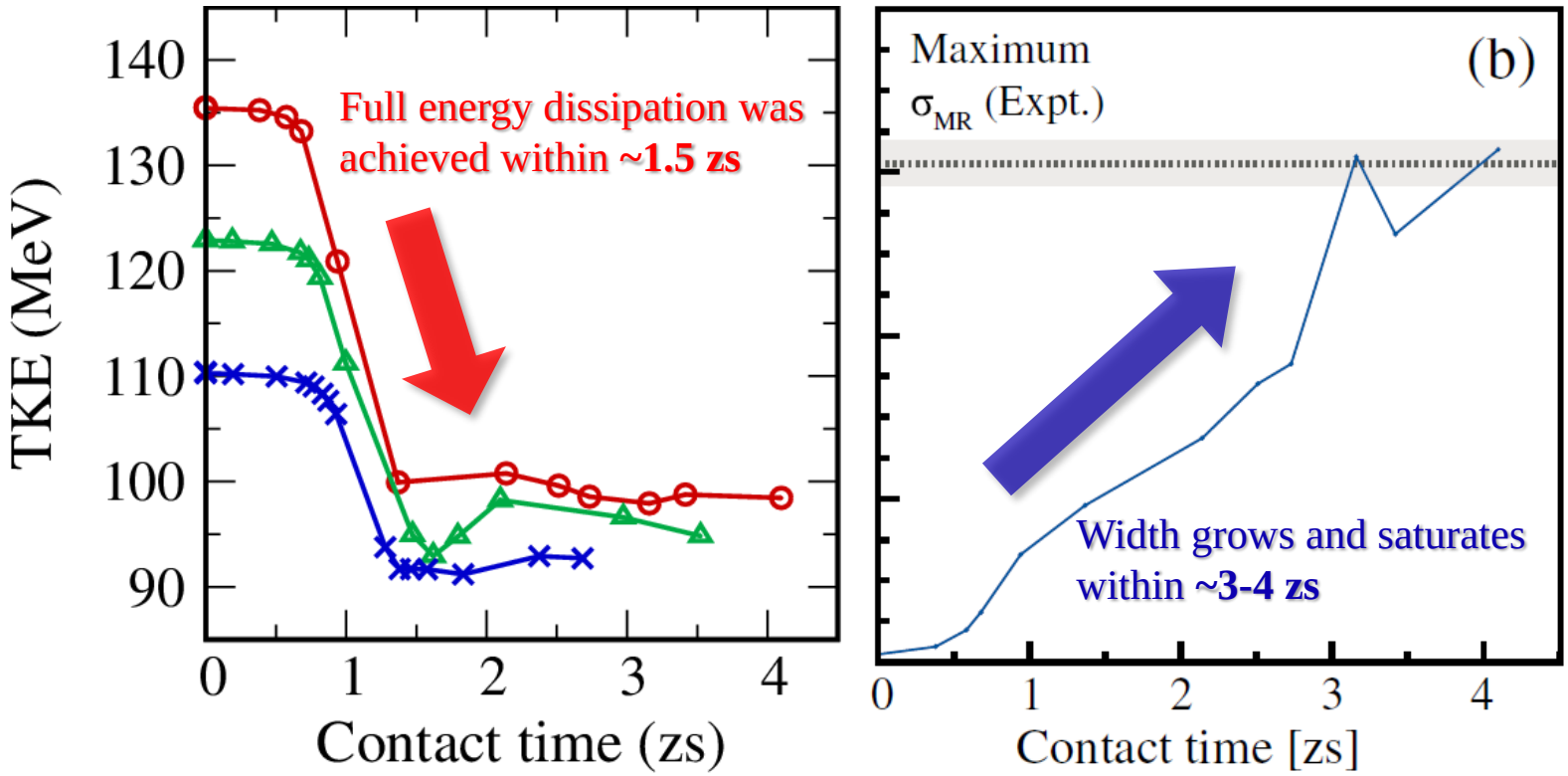

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質量平衡過程
Mass equilibration
A

質量数分布の幅の増大
Mass distribution width
σ_A

TDSLDA: TDDFT with local treatment of pairing

Kohn-Sham scheme is extended for non-interacting quasiparticles

➢ TDSLDA equations (formally equivalent to TDHFB or TD-BdG equations)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow\uparrow}(\boldsymbol{r},t) & h_{\uparrow\downarrow}(\boldsymbol{r},t) & 0 & \Delta(\boldsymbol{r},t) \\ h_{\downarrow\uparrow}(\boldsymbol{r},t) & h_{\downarrow\downarrow}(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h^*_{\uparrow\uparrow}(\boldsymbol{r},t) & -h^*_{\uparrow\downarrow}(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & 0 & -h^*_{\downarrow\uparrow}(\boldsymbol{r},t) & -h^*_{\downarrow\downarrow}(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix}$$

$$h_\sigma = \frac{\delta E}{\delta n_\sigma} \quad : \text{ s.p. Hamiltonian}$$

$$\Delta = -\frac{\delta E}{\delta \nu^*} \quad : \text{ pairing field}$$

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_k<E_c} |v_{k,\sigma}(\boldsymbol{r},t)|^2 \quad : \text{ number density}$$

$$\nu(\boldsymbol{r},t) = \sum_{E_k<E_c} u_{k,\uparrow}(\boldsymbol{r},t)v^*_{k,\downarrow}(\boldsymbol{r},t) \quad : \text{ anomalous density}$$

$$\boldsymbol{j}_\sigma(\boldsymbol{r},t) = \hbar\sum_{E_k<E_c} \mathrm{Im}[v^*_{k,\sigma}(\boldsymbol{r},t)\boldsymbol{\nabla} v_{k,\sigma}(\boldsymbol{r},t)] \quad : \text{ current}$$

A large number (10^4-10^6) of 3D coupled non-linear PDEs have to be solved!!

# of qp orbitals ~ # of grid points

TDSLDA: TDDFT with local treatment of pairing

Kohn-Sham scheme is extended for non-interacting quasiparticles

➢ TDSLDA equations (formally equivalent to TDHFB or TD-BdG equations)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h_{\uparrow\uparrow}(\boldsymbol{r},t) & h_{\uparrow\downarrow}(\boldsymbol{r},t) & 0 & \Delta(\boldsymbol{r},t) \\ h_{\downarrow\uparrow}(\boldsymbol{r},t) & h_{\downarrow\downarrow}(\boldsymbol{r},t) & -\Delta(\boldsymbol{r},t) & 0 \\ 0 & -\Delta^*(\boldsymbol{r},t) & -h^*_{\uparrow\uparrow}(\boldsymbol{r},t) & -h^*_{\uparrow\downarrow}(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & 0 & -h^*_{\downarrow\uparrow}(\boldsymbol{r},t) & -h^*_{\downarrow\downarrow}(\boldsymbol{r},t) \end{pmatrix} \begin{pmatrix} u_{k,\uparrow}(\boldsymbol{r},t) \\ u_{k,\downarrow}(\boldsymbol{r},t) \\ v_{k,\uparrow}(\boldsymbol{r},t) \\ v_{k,\downarrow}(\boldsymbol{r},t) \end{pmatrix}$$

Supercomputing!!

$$h_\sigma = \frac{\delta E}{\delta n_\sigma} \quad : \text{ s.p. Hamiltonian}$$

$$\Delta = -\frac{\delta E}{\delta \nu^*} \quad : \text{ pairing field}$$

$$n_\sigma(\boldsymbol{r},t) = \sum_{E_k<E_c} |v_{k,\sigma}(\boldsymbol{r},t)|^2 \quad : \text{ number density}$$

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A large number (10^4-10^6) of 3D coupled non-linear PDEs have to be solved!!

# of qp orbitals ~ # of grid points

*The number indicates the rank according to the TOP500 list (June 2018)

Piz Daint, CSCS, Switzerland (No. 6)

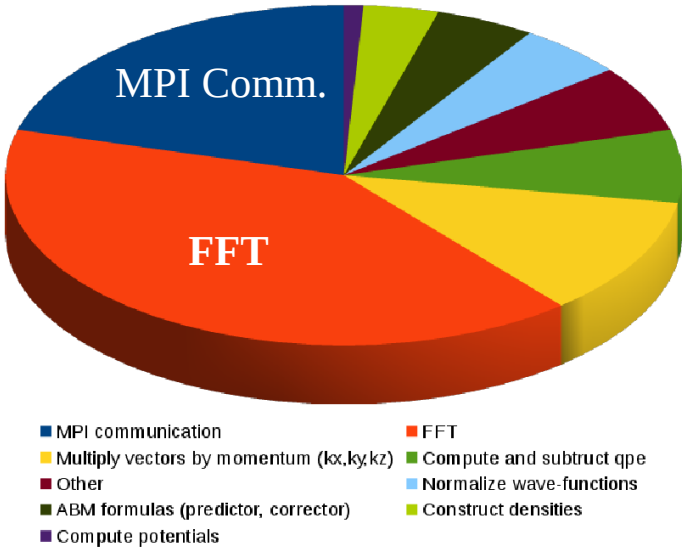
TITAN, ORNL, USA (No. 7)

TSUBAME3.0, Japan (No. 19)

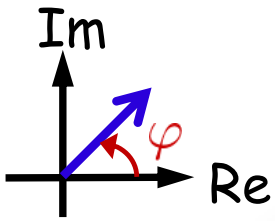
The fastest machine:
Summit, ORNL, USA
GPU, 188 PFlops/s

Present computing capabilities:

- ✓ Full 3D (w/o symmetry restrictions)
- ✓ Volume as large as 100^3 lattice points
- ✓ Evolution up to 10^6 time steps (as long as 10^{-19} sec)



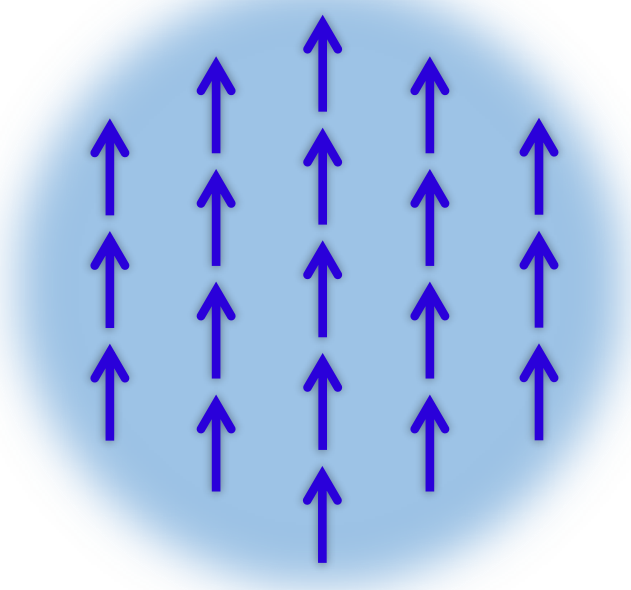
The **Pairing field** provides a variety of **dynamic** excitation modes



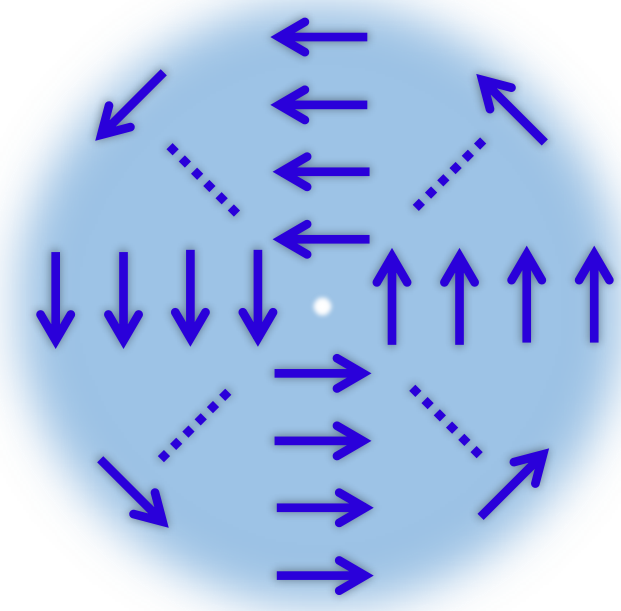
$$|\Delta(\boldsymbol{r},t)|e^{\mathrm{i}\varphi(\boldsymbol{r},t)}$$

**Superfluid velocity*

$$\boldsymbol{v}_s(\boldsymbol{r},t) \propto \boldsymbol{\nabla}\varphi(\boldsymbol{r},t)$$



Collective rotation
(of the phase)



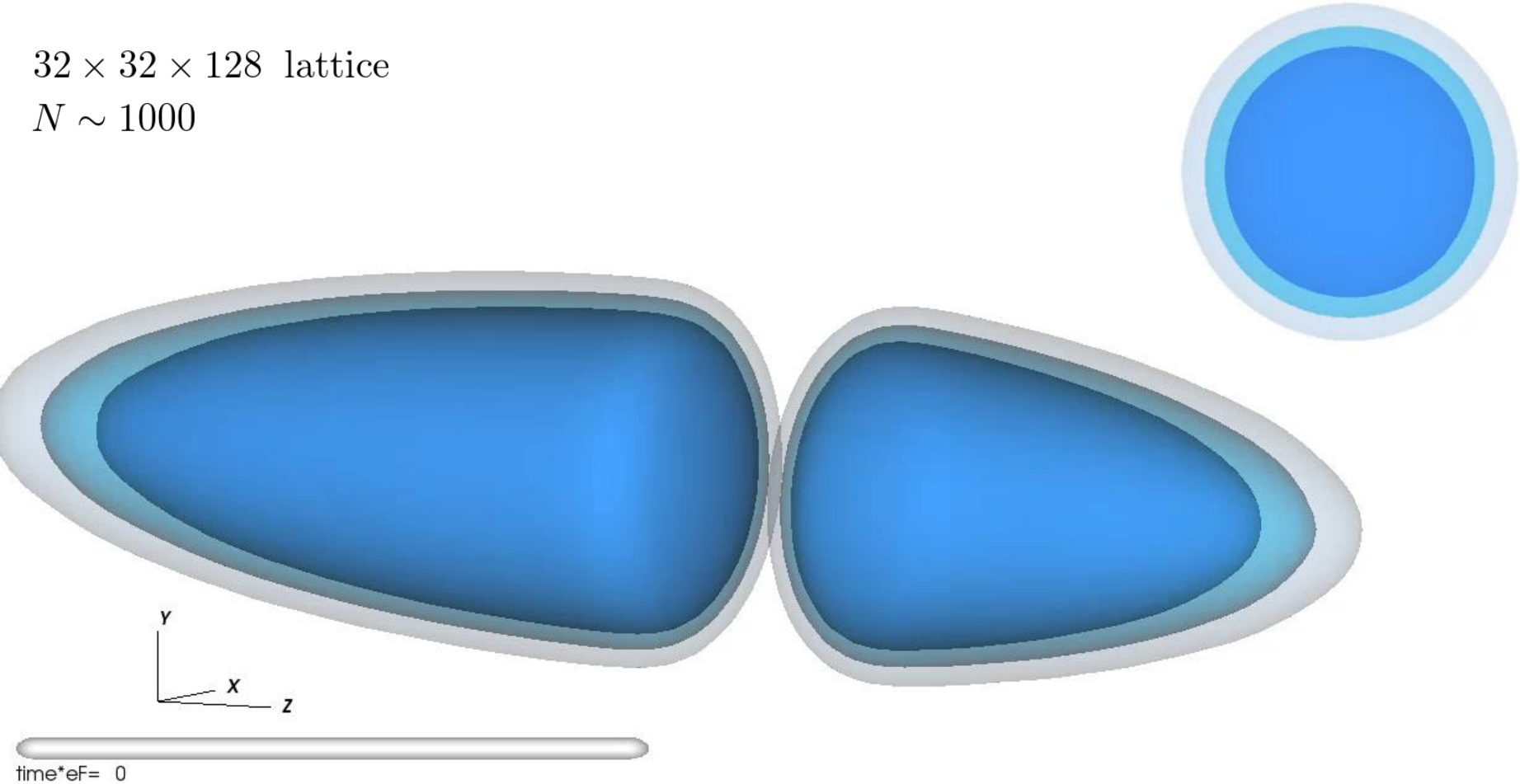
Quantum vortex

Result of TDSLDA simulation:

Phase discontinuity creates a vortex ring which decays into a vortex line

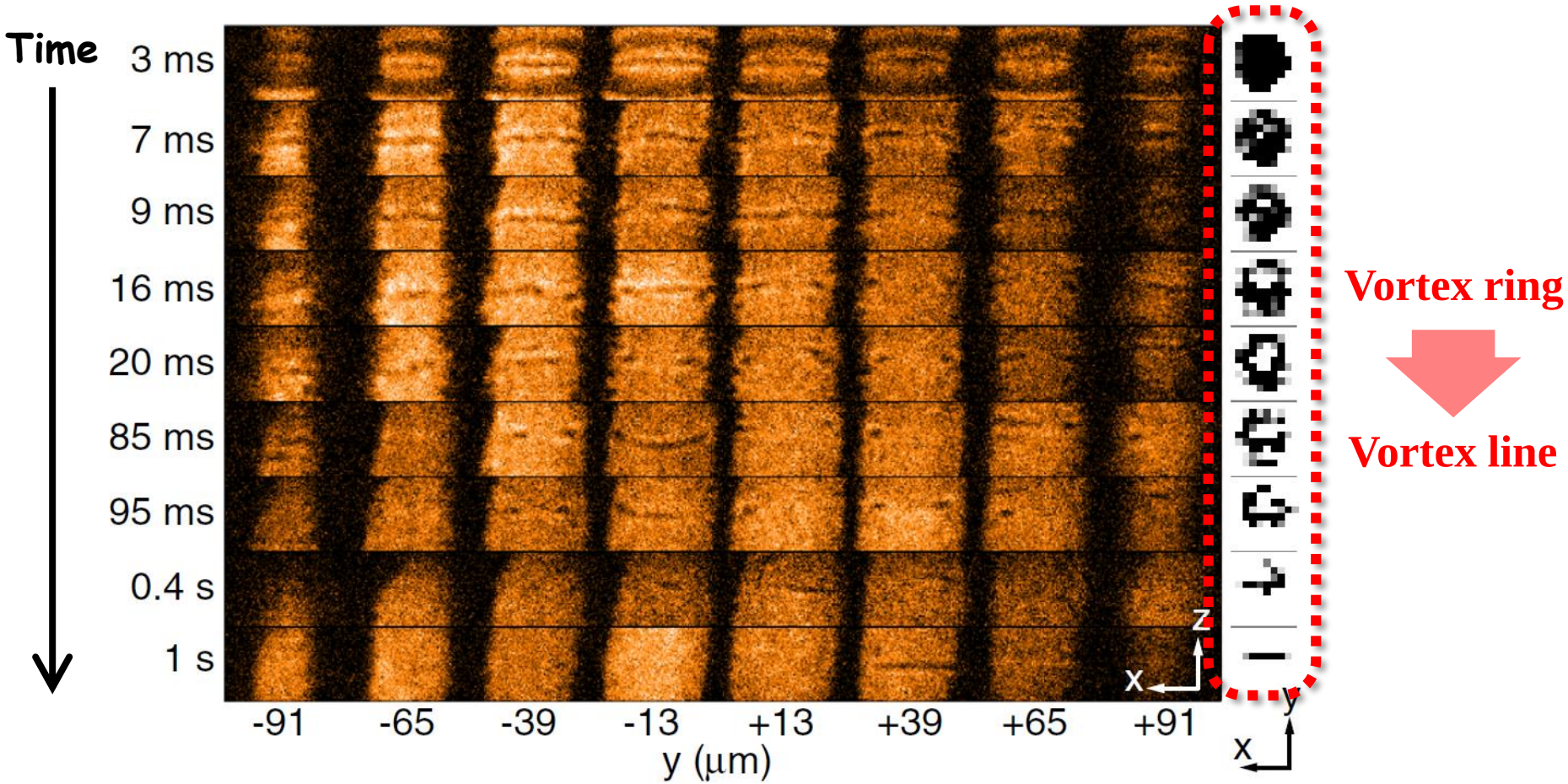
$32 \times 32 \times 128$ lattice

$N \sim 1000$



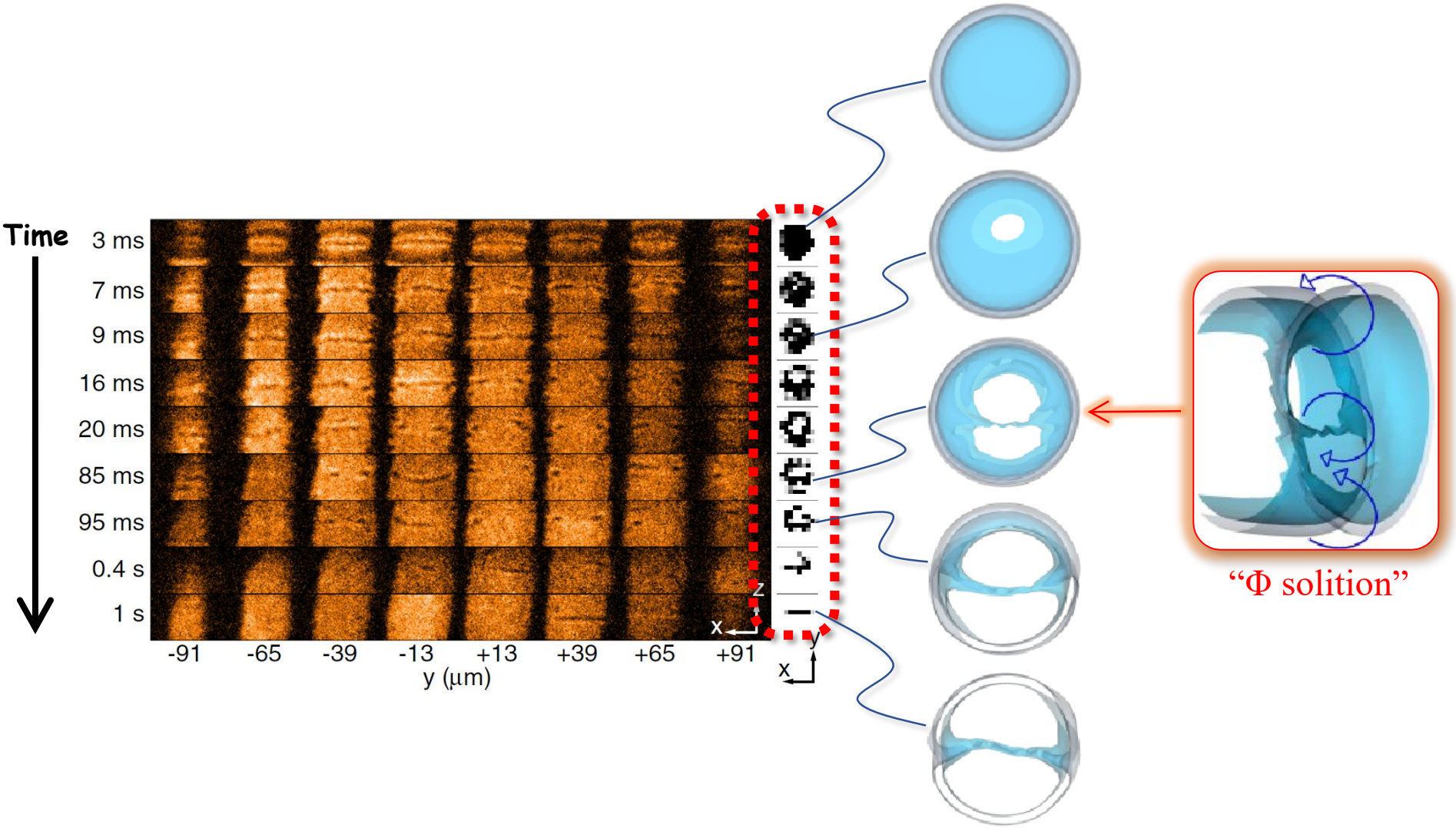
G. Wlazłowski, A. Bulgac, M.M. Forbes, and K.J. Roche, Phys. Rev. A **91**, 031602 (2015)

The cascades of solitonic excitations have been identified experimentally



M.J.H. Ku, B. Mukherjee, T. Yefsah, and M.W. Zwierlein, Phys. Rev. Lett. **116**, 045304 (2016)

Each stage of solitonic cascade could be reproduced with TDSLDA!



Having a validated tool at hand
we explore new physics particular to fermionic systems

Spin-imbalance (polarization)!!

Fermionic superfluidity is due to the Cooper pairing mechanism

Then, what happens if the numbers of men/women are imbalanced??

But, what about dynamics??

Answer:
phase separation

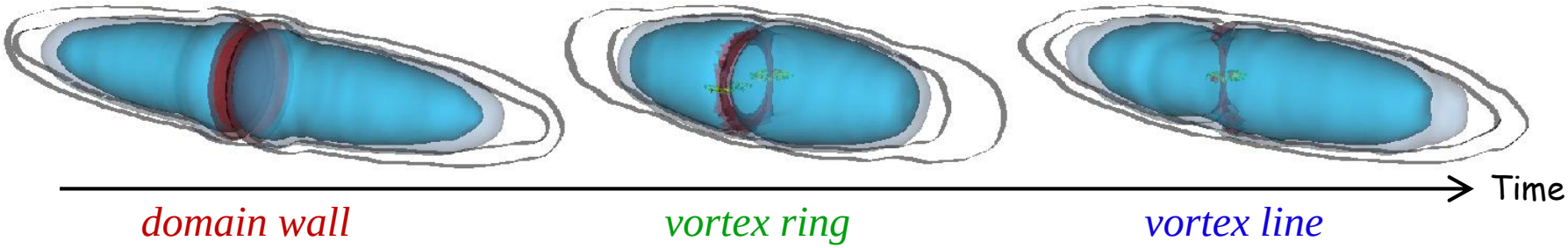
M.W. Zwierlein et al., Science **311**, 492 (2006)

Spin polarization affects the stability of topological defects

P = 20%

P = 40%

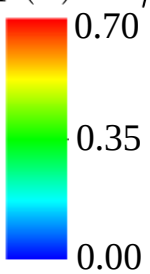
$P \geqq$ 50%

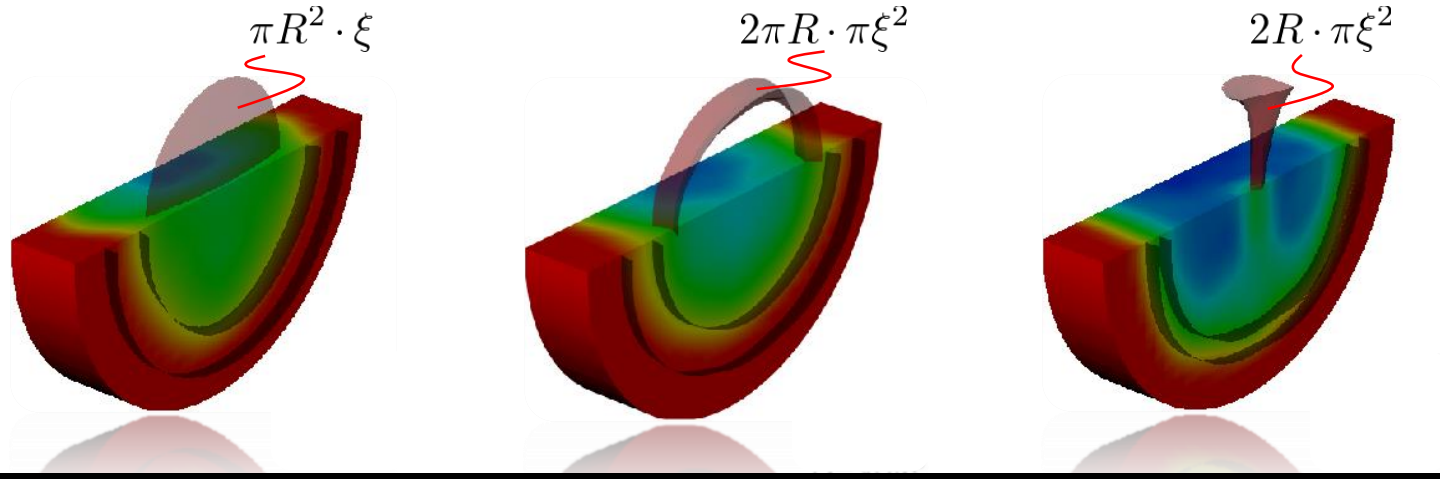


R: radius of the cloud
ξ: coherence length

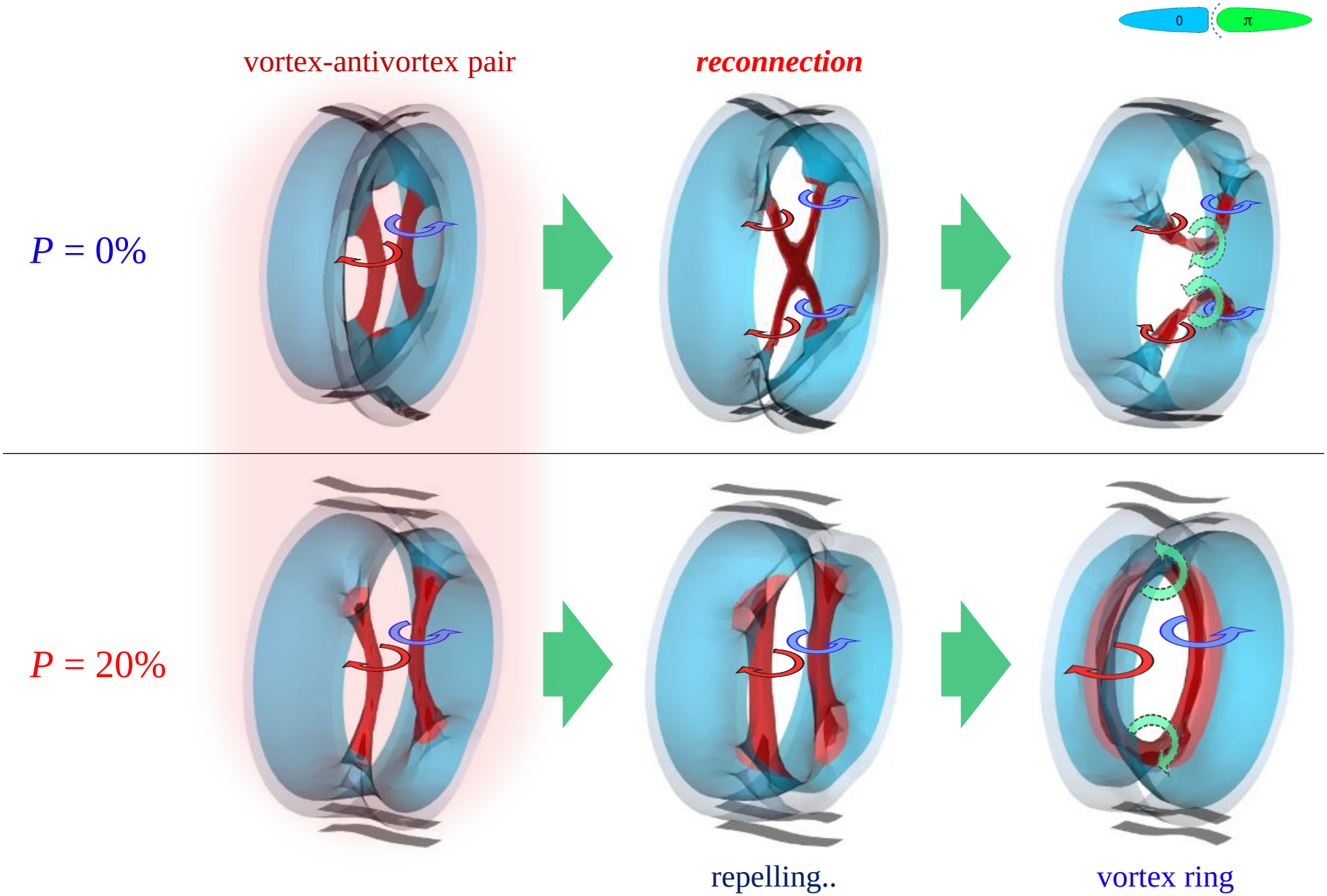
✓ Unpaired particles prefer to stay inside the defects

Local polarization
$p(\boldsymbol{r}) = \frac{n_a(\boldsymbol{r}) - n_b(\boldsymbol{r})}{n_a(\boldsymbol{r}) + n_b(\boldsymbol{r})}$



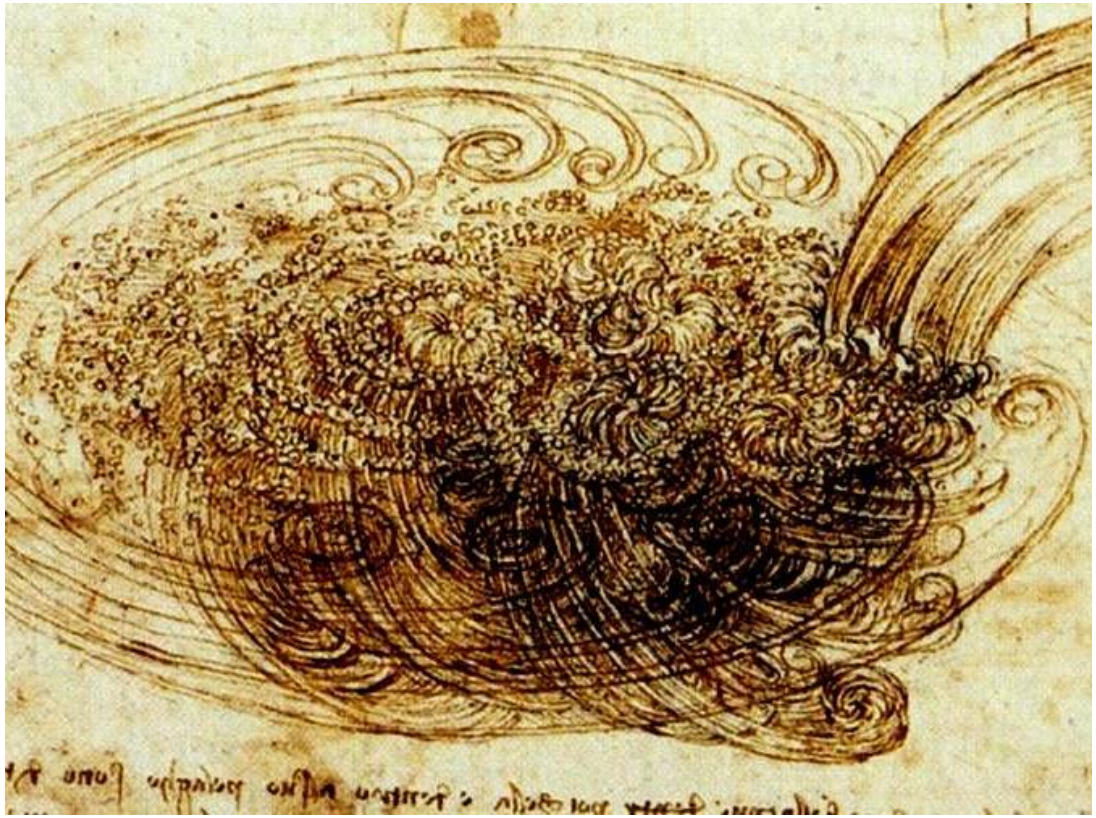


Spin polarization may hinder vortex crossings/reconnections

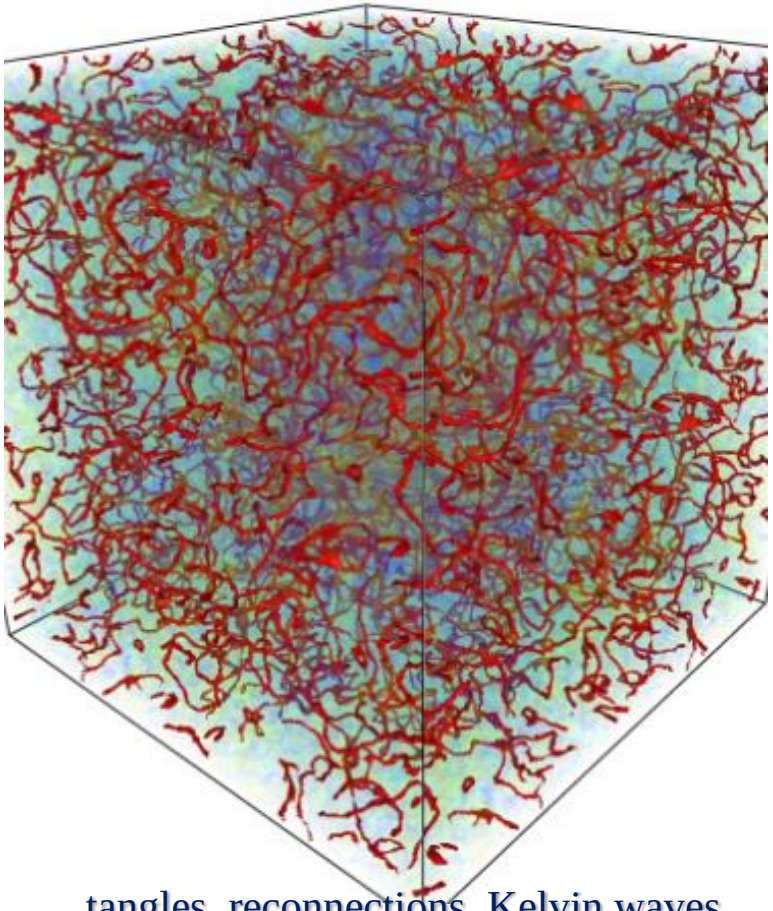


G. Wlazłowski, K.S., M. Marchwiany, and P. Magierski, Phys. Rev. Lett. **120**, 253002 (2018)

What's more? - Implication to *quantum turbulence*



chaotic, dissipation to smaller scales



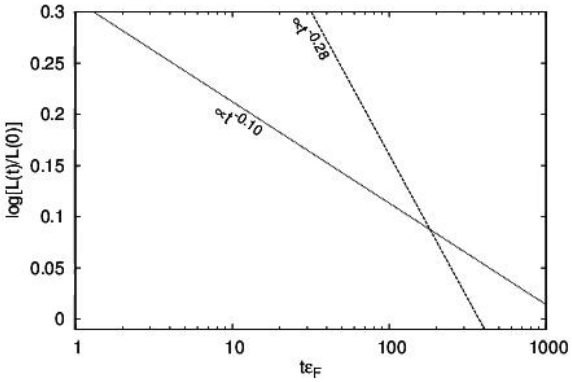
tangles, reconnections, Kelvin waves

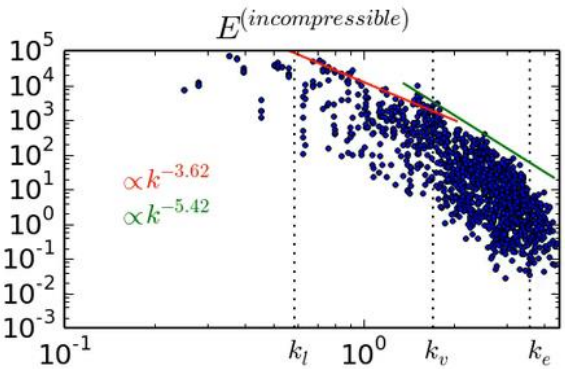
Left: Work by Leonardo da Vinci

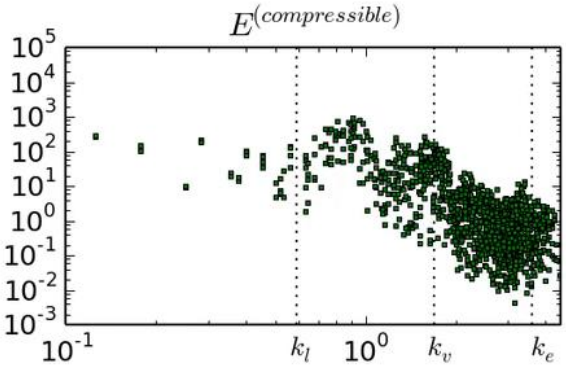
Right: Fig. 1 taken from
A. Villois et al., Phys. Rev. E **93**, 061103(R) (2016)

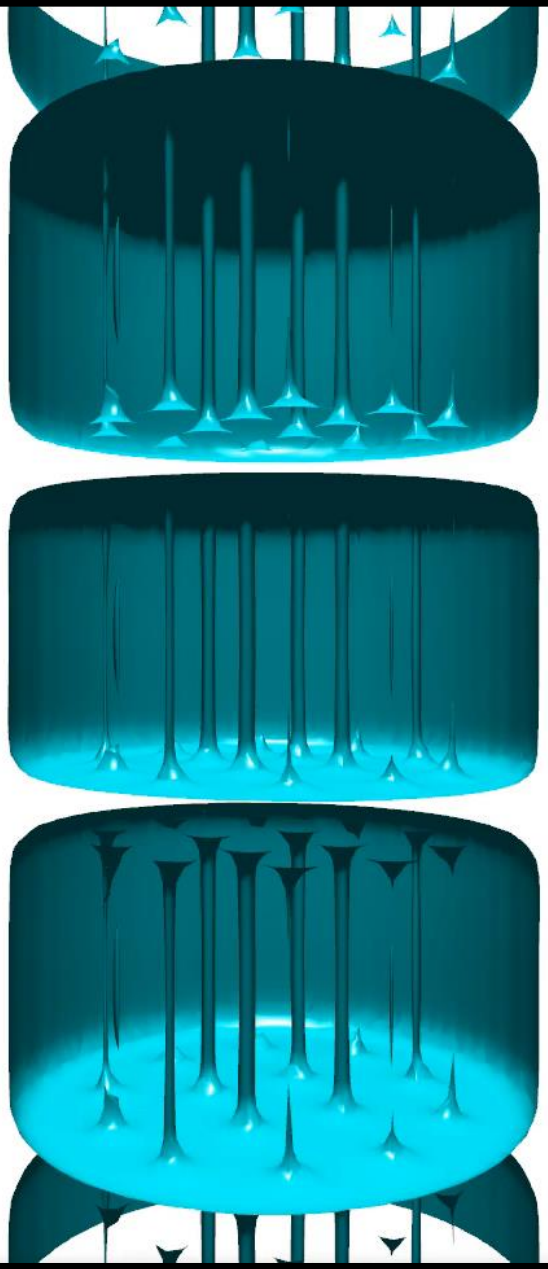
Computational/theoretical challenge

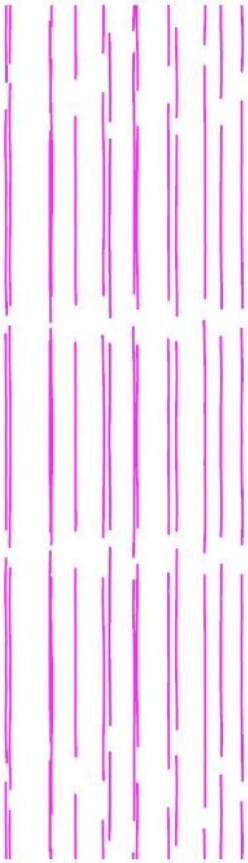
Microscopic simulation of quantum turbulence in superfluid fermi gas











time = 0 $[\varepsilon_F^{-1}]$

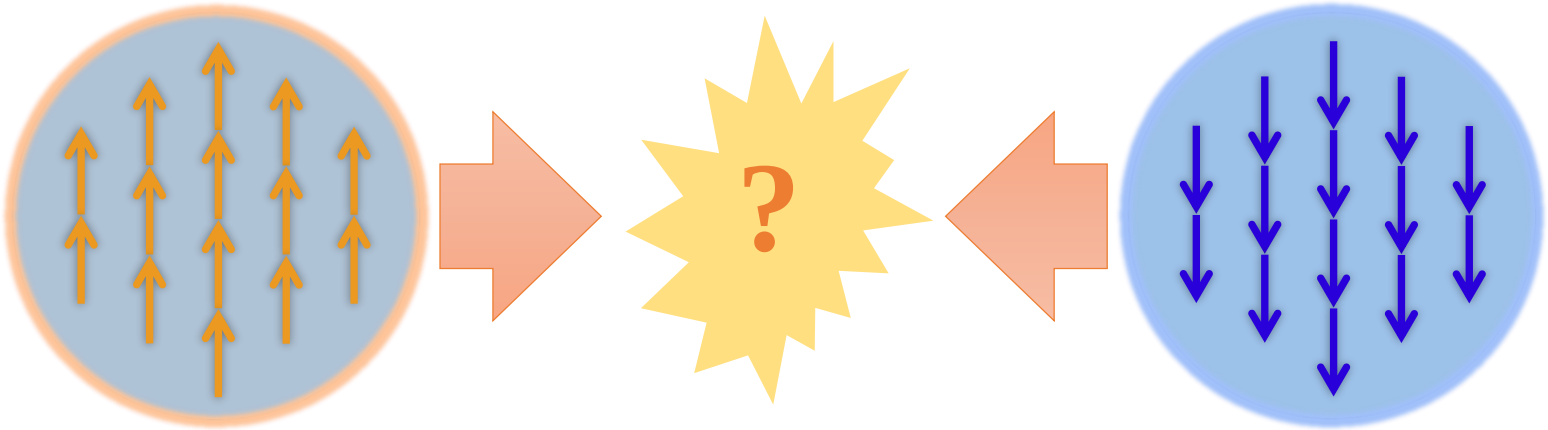
Very preliminary

3D, TDSLDA calculations (Fayans w/o LS) predicts novel phenomena associated with solitonic excitations!!

Q. What happens when two **superfluid** nuclei with different **phases** collide??

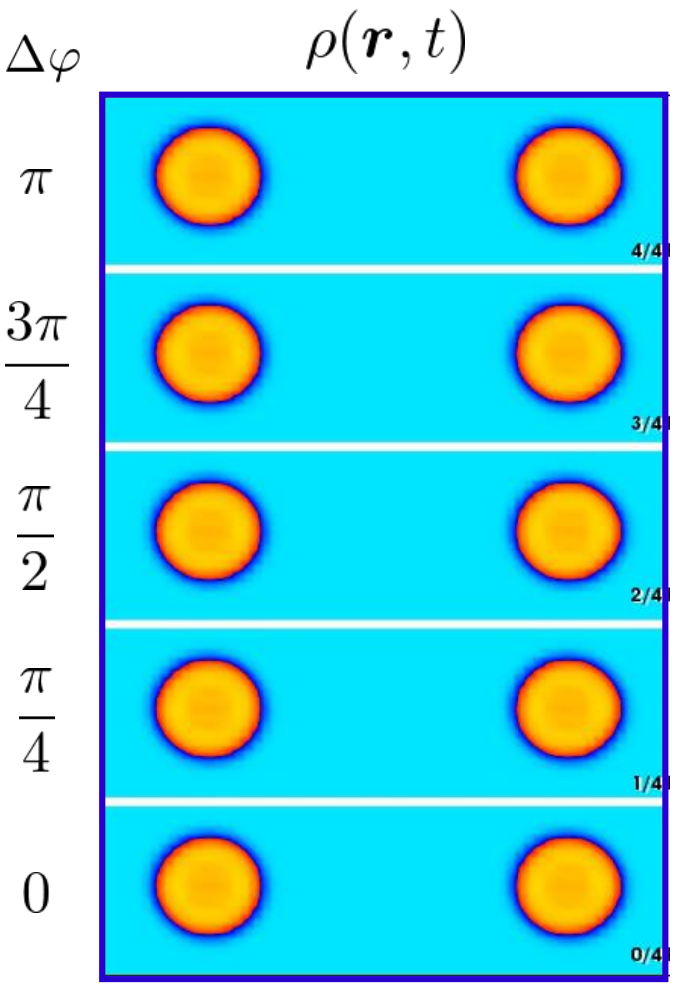
$$\Delta\varphi \ (\equiv \varphi_1 - \varphi_2)$$

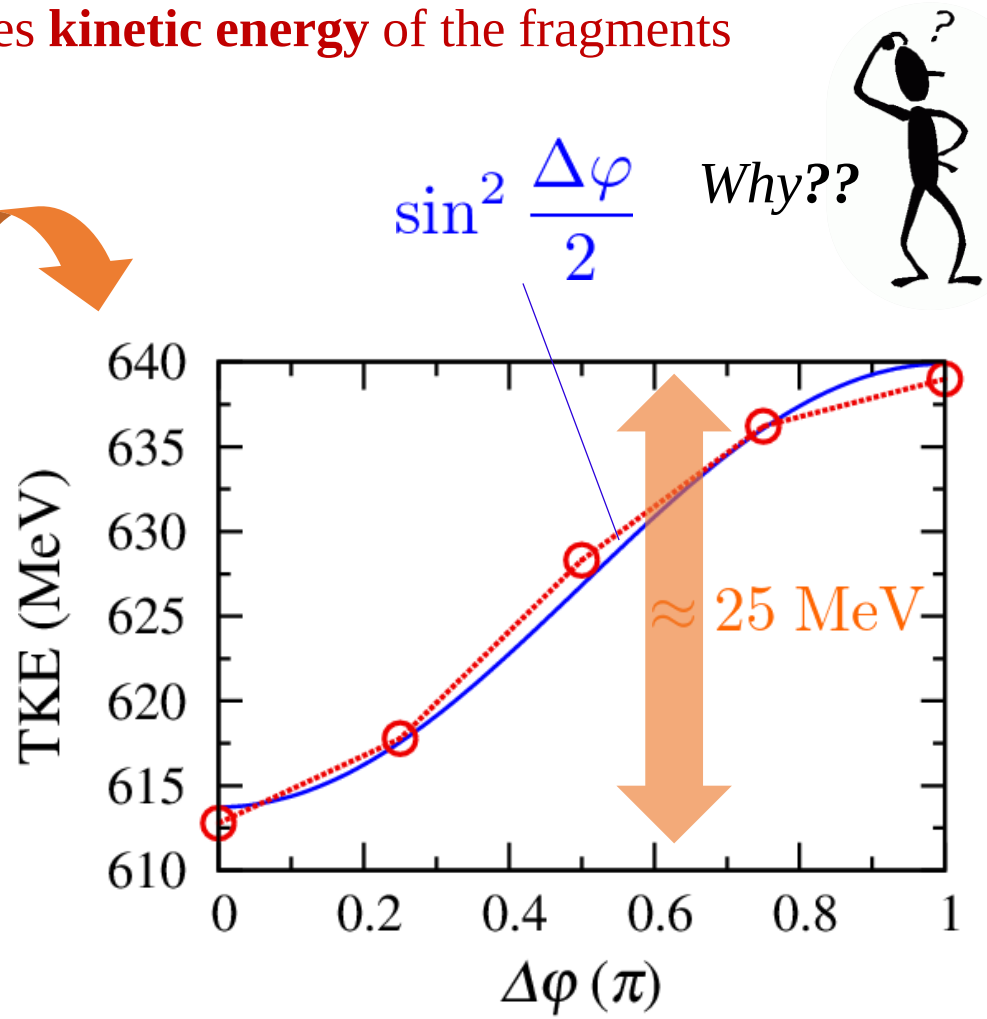
$$|\Delta_1(\boldsymbol{r},t)|e^{\mathrm{i}\varphi_1(\boldsymbol{r},t)} \qquad |\Delta_2(\boldsymbol{r},t)|e^{\mathrm{i}\varphi_2(\boldsymbol{r},t)}$$



TDSLDA results: $^{240}Pu+^{240}Pu$ head-on collisions ($E/V_{Bass}=1.1$)

The phase difference changes **kinetic energy** of the fragments



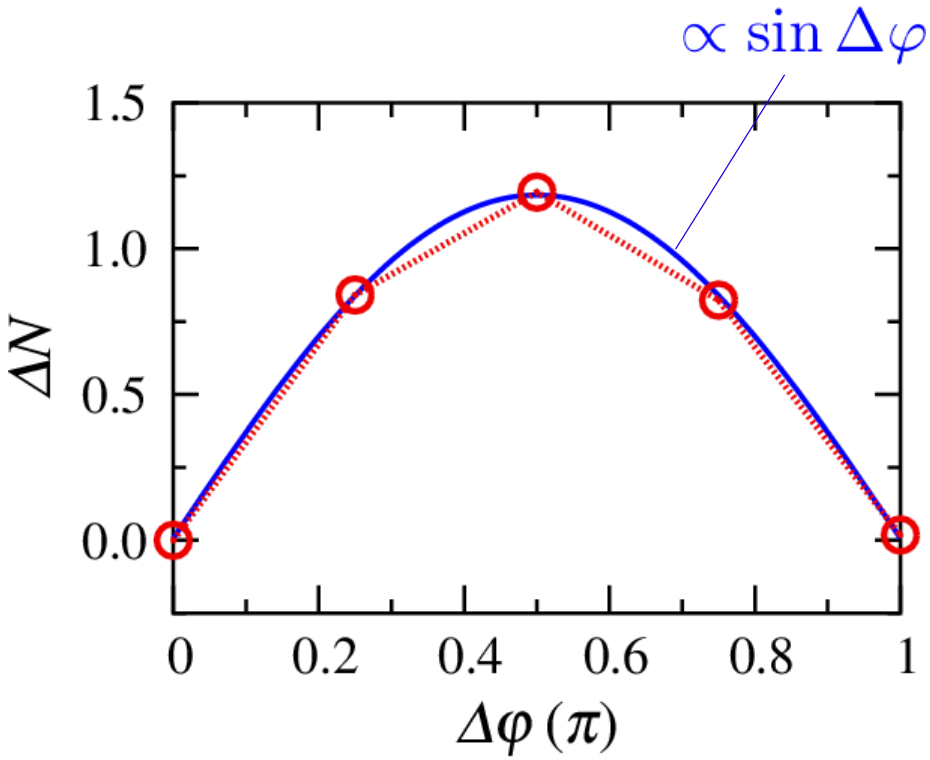


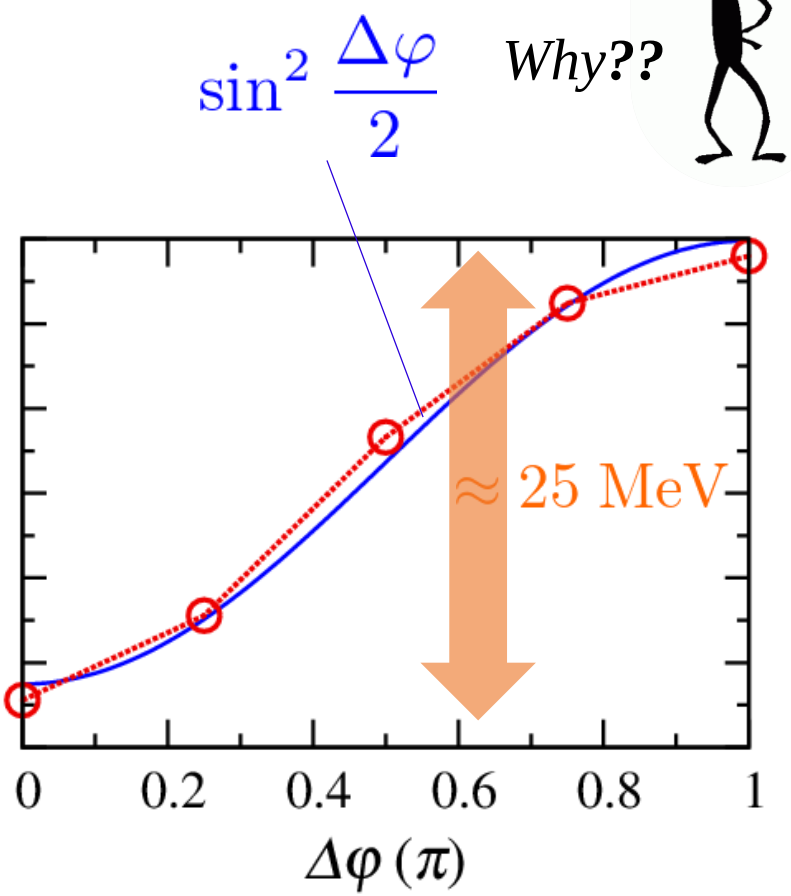
P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

TDSLDA results: $^{240}Pu+^{240}Pu$ head-on collisions ($E/V_{Bass}=1.1$)

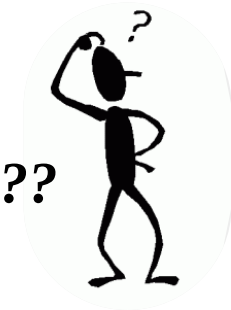
The phase difference changes **kinetic energy** of the fragments

Note:
It cannot be explained by Josephson effect!





Why??

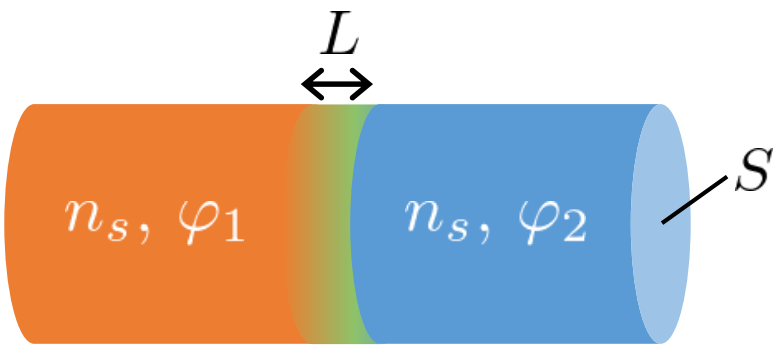


P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

Additional energy is required to attach two superfluids with different phases

➢ The additional energy (derived from Ginzburg-Landau theory)

$$E = \frac{S}{L}\frac{\hbar^2}{2m} n_s \sin^2\frac{\Delta\varphi}{2}$$



$\Delta\varphi\ (\equiv \varphi_1 - \varphi_2)$

*It does not depend on the absolute value of the pairing!

e.g.) $S=\pi R^2$, $L\sim R=6$ fm, $n_s=0.08$ fm^{-3} → $E\sim 30$ MeV

S: Attaching area

L: Length scale over which the phase varies

n_s: Superfluid density

P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

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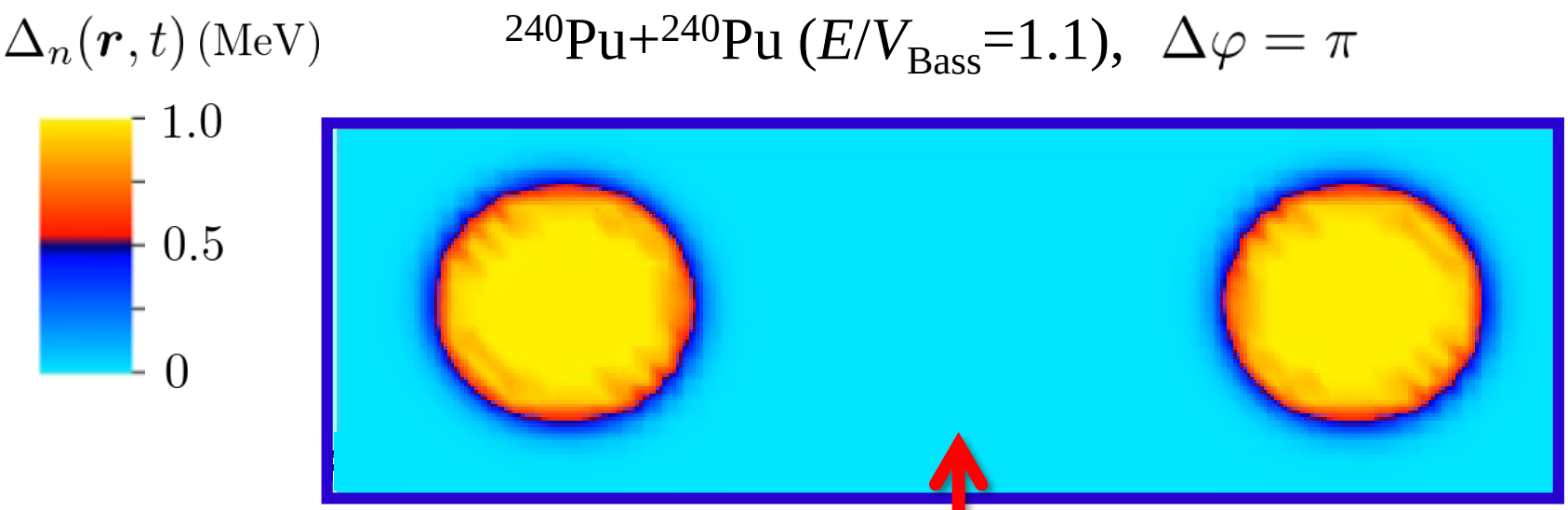
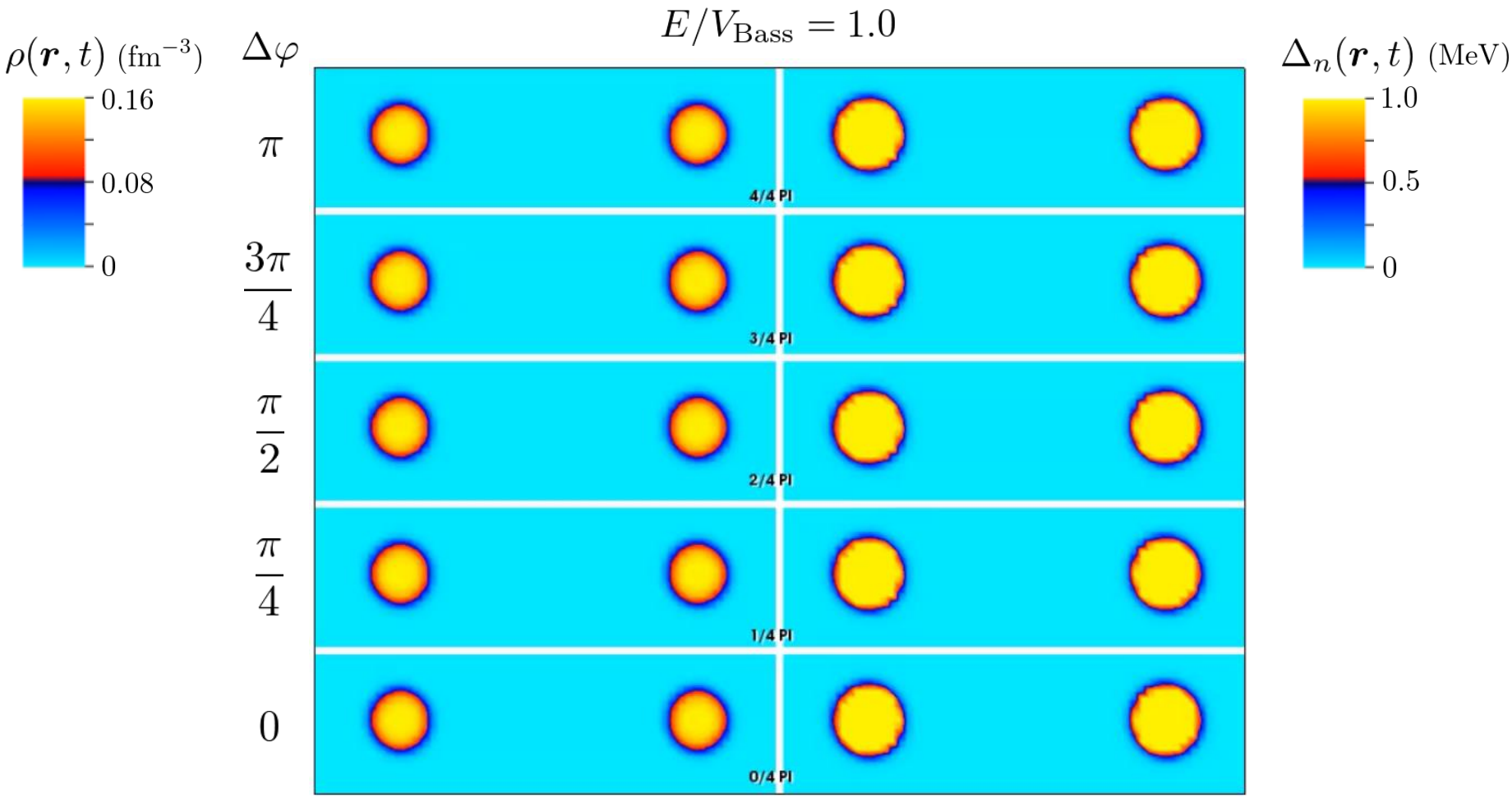


Pairing field is vanishing!
(due to phase discontinuity)

P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

TDSLDA results: ^{90}Zr+^{90}Zr head-on collisions

Fusion reaction is suppressed by the phase difference



P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

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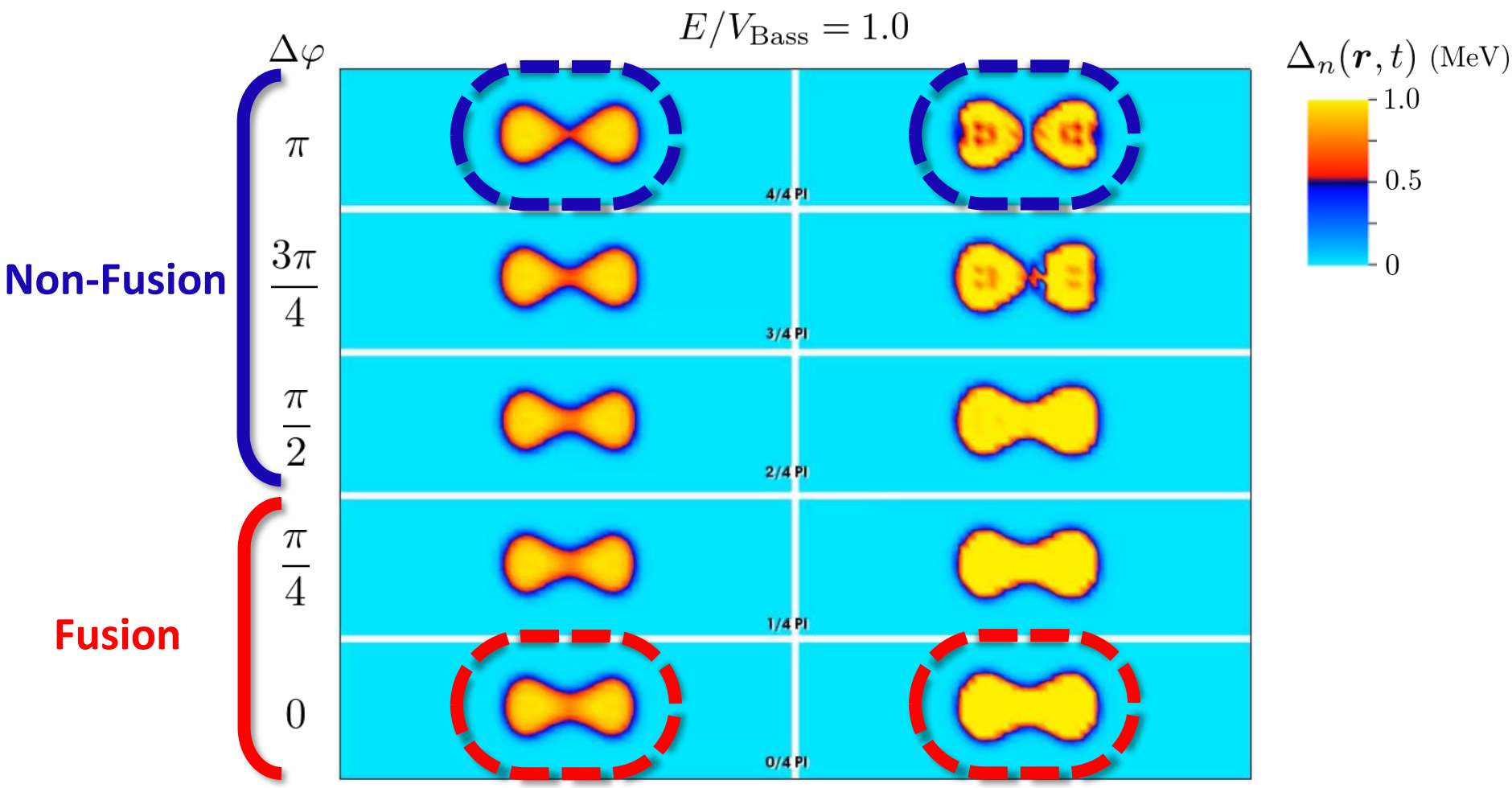
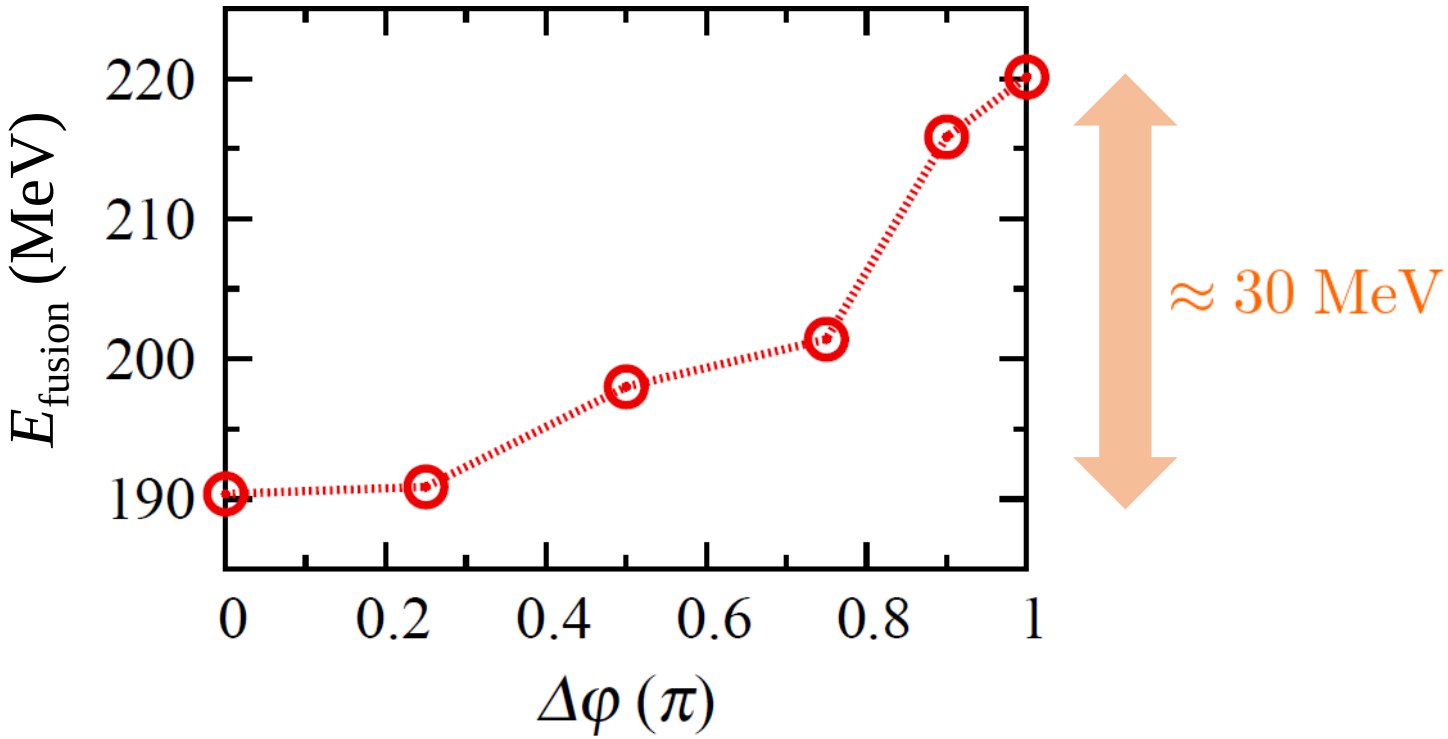


P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

Fusion reaction is suppressed by the phase difference

*$E_{\mathbf{fusion}}$: the lowest energy at which fusion reaction is observed



P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

When two superfluid nuclei with different phases collide
solitonic excitations might be induced

$$\Delta\varphi \ (\equiv \varphi_1 - \varphi_2)$$

$$|\Delta_1(\boldsymbol{r},t)|e^{\mathrm{i}\varphi_1(\boldsymbol{r},t)}$$

$$|\Delta_2(\boldsymbol{r},t)|e^{\mathrm{i}\varphi_2(\boldsymbol{r},t)}$$

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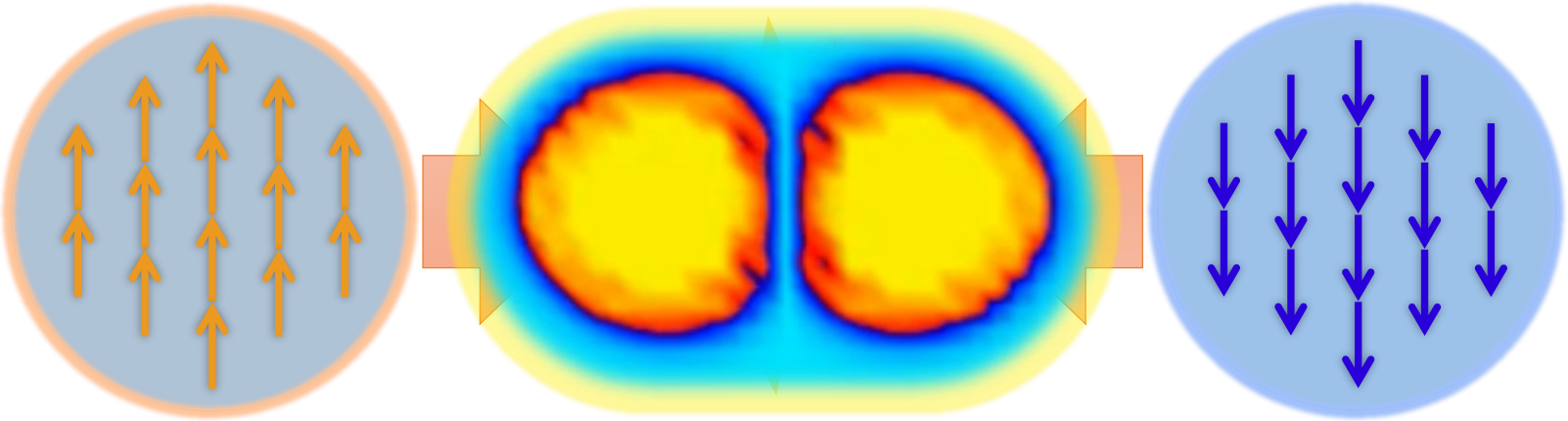

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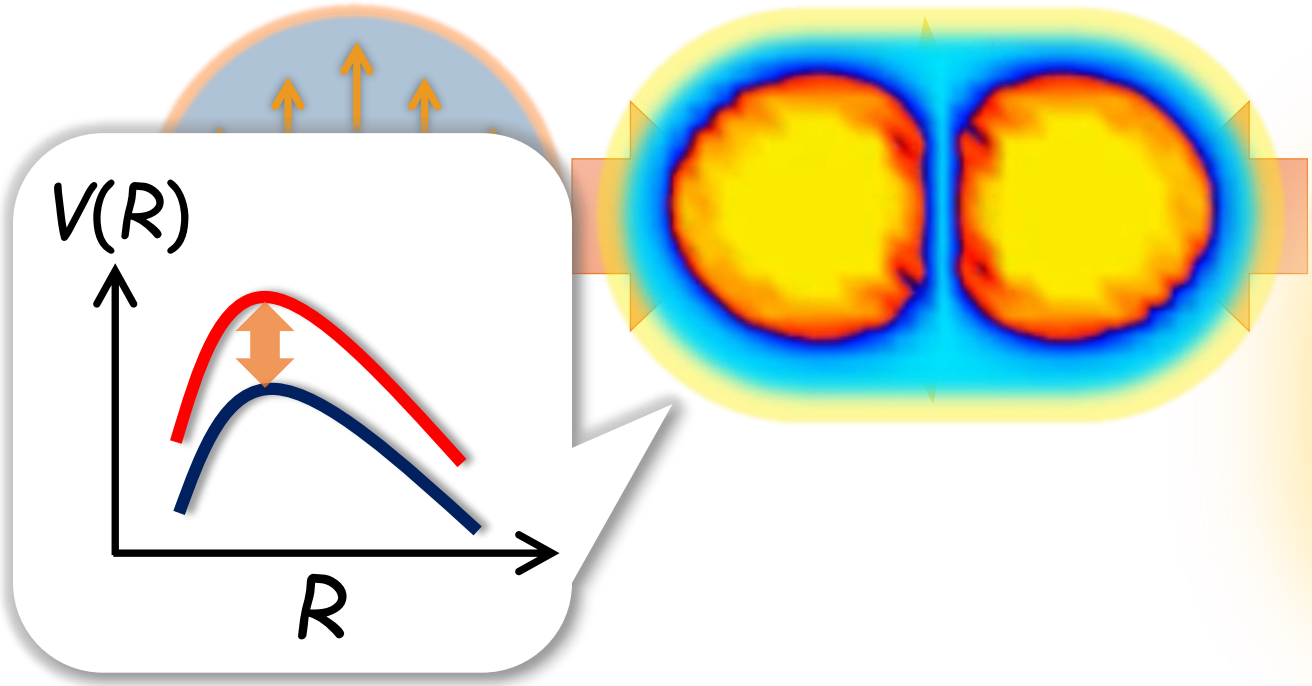
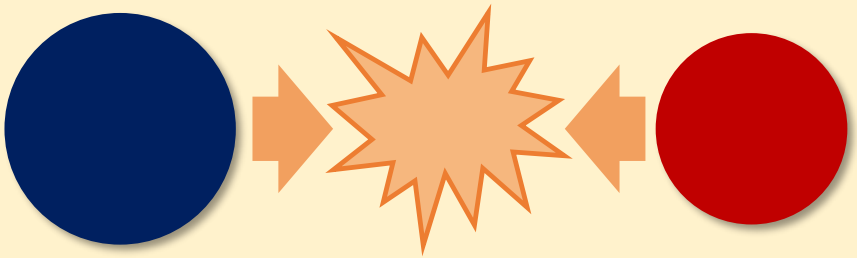


It may affect:

- TKE (~10-30 MeV)
- Fusion dynamics
- Neck formation
- Contact time
- Scattering angle

まとめ

- 原子核をぶつけると，様々な非平衡過程が起こる



荷電平衡過程
Charge equilibration
N/Z

エネルギーの散逸
Energy dissipation
TKEL

超流動の位相の変化
Superfluid phase
$|\Delta(\boldsymbol{r})|e^{i\varphi(\boldsymbol{r})}$

質量平衡過程
Mass equilibration
A

質量数分布の幅の増大
Mass distribution width
σ_A

Kazuyuki Sekizawa
Specially Appointed Assistant Professor
Center for Transdisciplinary Research
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sekizawa@phys.sc.niigata-u.ac.jp
http://sekizawa.fizyka.pw.edu.pl/english/