Tsukuba-CCS workshop on "microscopic theories of nuclear structure and dynamics"
December 11th, 2018, CCS, University of Tsukuba

Recent progress of nuclear dynamics studies with TDDFT

Kazuyuki Sekizawa

Center for Interdisciplinary Research
Institute for Research Promotion, Niigata University, Japan

My recent studies: TDDFT for Nuclear Many-Body Problem

Multinucleon transfer and quasifission processes in heavy-ion reactions

Tsukuba, Tohoku, Kyushu

PRC**96**(2017)041601(R),
PRC**96**(2017)014615,
PRC**93**(2016)054616,
PRC**90**(2014)064614,
PRC**88**(2013)014614


K. Yabana


K. Hagino


K. Washiyama

BARC, Mumbai, India

B.J. Roy and his coworkers

B.J. Roy *et al.*,
PRC**97**(2018)034603,
PRC**92**(2015)024603

Dissipation and fluctuation mechanism in deep-inelastic collisions

ANU, Canberra, Australia
Texas A&M, USA

E. Williams, K. Sekizawa, D. Hinde *et al.*,
PRL**120**(2018)022501


E. Williams


D.J. Hinde


M. Dasgupta


C. Simenel


A. Wakhle

Superfluid dynamics in fermionic systems

WUT, Warsaw, Poland

PRL**120**(2018)253002
PRL**119**(2017)042501
PRL**117**(2016)232701


G. Wlazłowski


P. Magierski

UW, Seattle, USA


A. Bulgac


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PRC**96**(2017)041601(R),
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E. Williams, K. Sekizawa, D. Hinde *et al.*,
PRL**120**(2018)022501

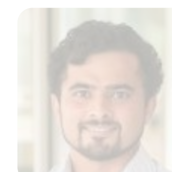
Today's talk


E. Williams


D.J. Hinde


M. Dasgupta


C. Simenel


A. Wakhle

Superfluid dynamics in fermionic systems

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The most remarkable progress

Inclusion of pairing - TDSLDA

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)

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

$h_\sigma = \dfrac{\delta E}{\delta n_\sigma}$: s.p. Hamiltonian

$\Delta = -\dfrac{\delta E}{\delta \nu^*}$: pairing field

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

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

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

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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!!

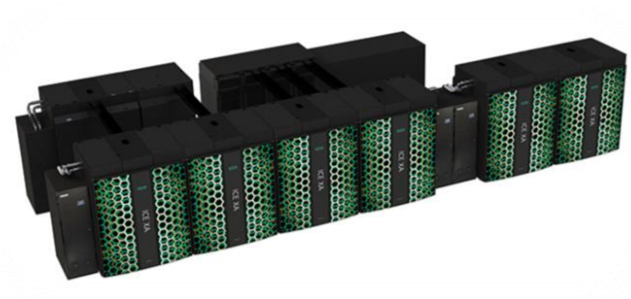
# of qp orbitals ~ # of grid points

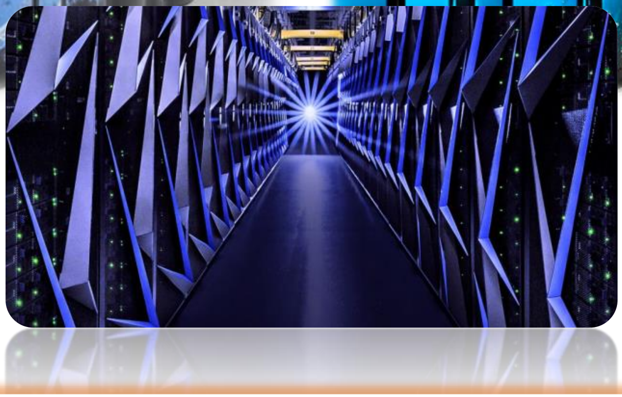
*The number indicates the rank according to the TOP500 list (June 2018)

Piz Daint, CSCS, Switzerland (No. 6)

TITAN, ORNL, USA (No. 7)

TSUBAME3.0, Japan (No. 19)

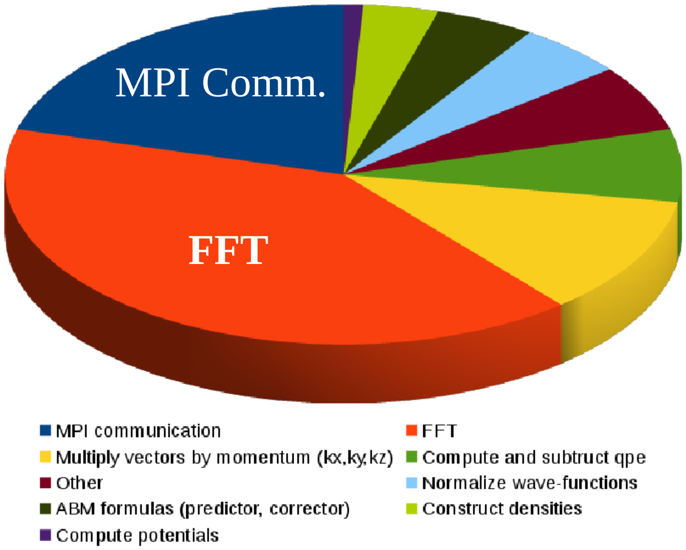




The fastest machine:
Summit, ORNL, USA
GPU, 188 PFlops/s

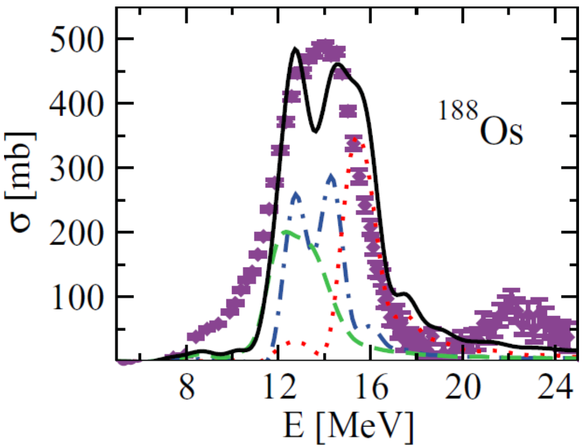
Present computing capabilities:

- ✓ 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)



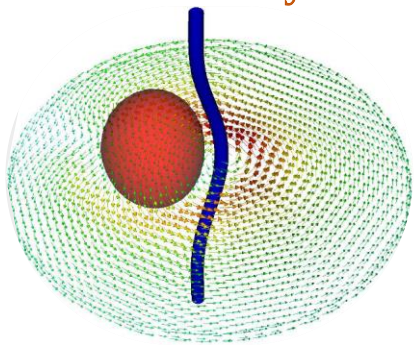
TDSLDA is a versatile tool!!

IVGDR



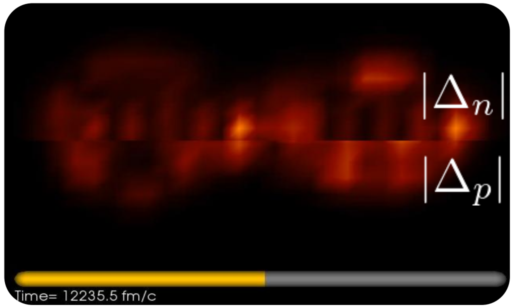
Phys. Rev. C **84**, 051309(R) (2011)
I. Stetcu, A. Bulgac, P. Magierski, and K.J. Roche

Vortex-nucleus dynamics



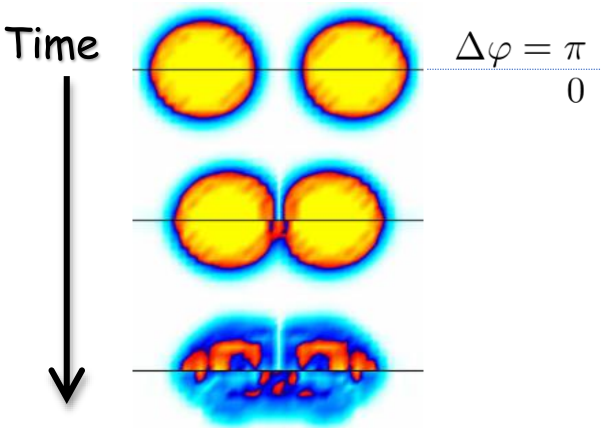
Phys. Rev. Lett. **117**, 232701 (2016)
G. Wlazłowski, K.S., P. Magierski, A. Bulgac, and M.M. Forbes

Induced fission of ^{240}Pu



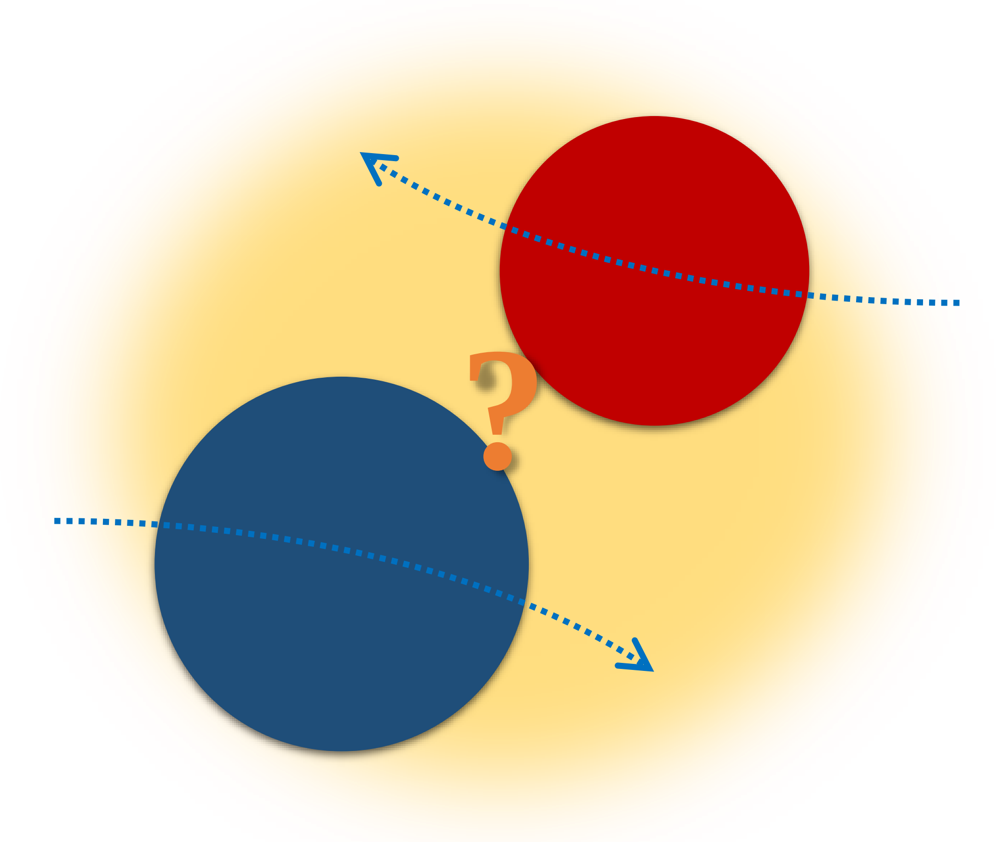
Phys. Rev. Lett. **116**, 122504 (2016)
A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu

Low-energy heavy ion reactions



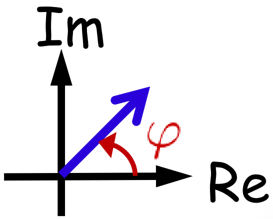
Phys. Rev. Lett. **119**, 042501 (2017)
P. Magierski, K.S., and G. Wlazłowski

What are the effects of pairing on reaction dynamics?



- More adiabatic dynamics
- Neck formation
- Contact time
- Scattering angle
- Total kinetic energy
- Transfer processes
- ...

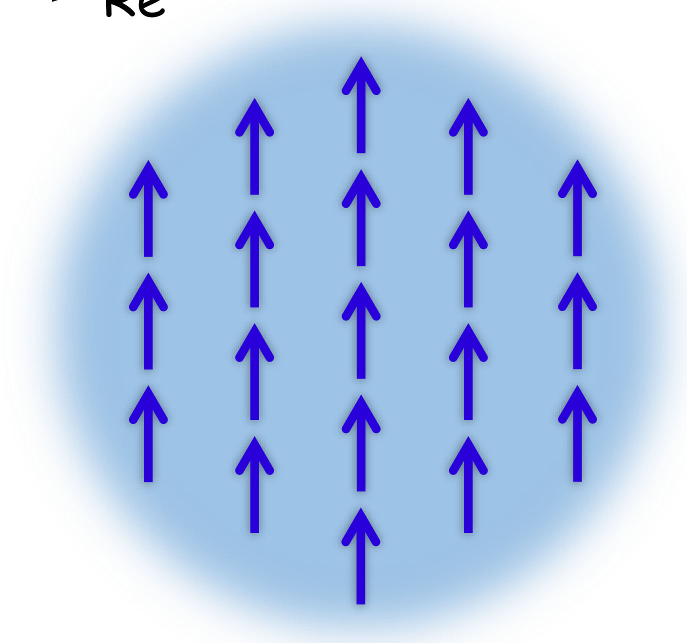
The **Pairing field** provides a variety of **dynamic** excitation modes



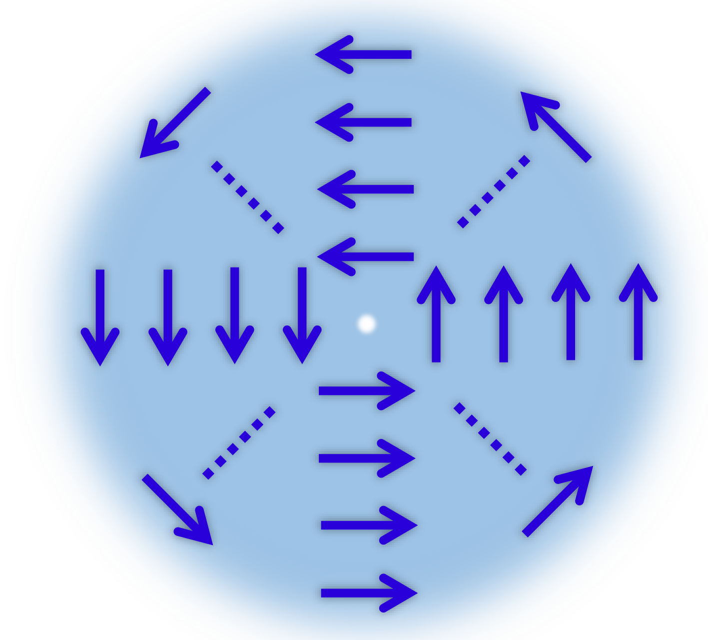
$$|\Delta(\boldsymbol{r},t)|e^{\mathrm{i}\varphi(\boldsymbol{r},t)}$$

**Superfluid velocity*

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



Collective rotation
(of the phase)



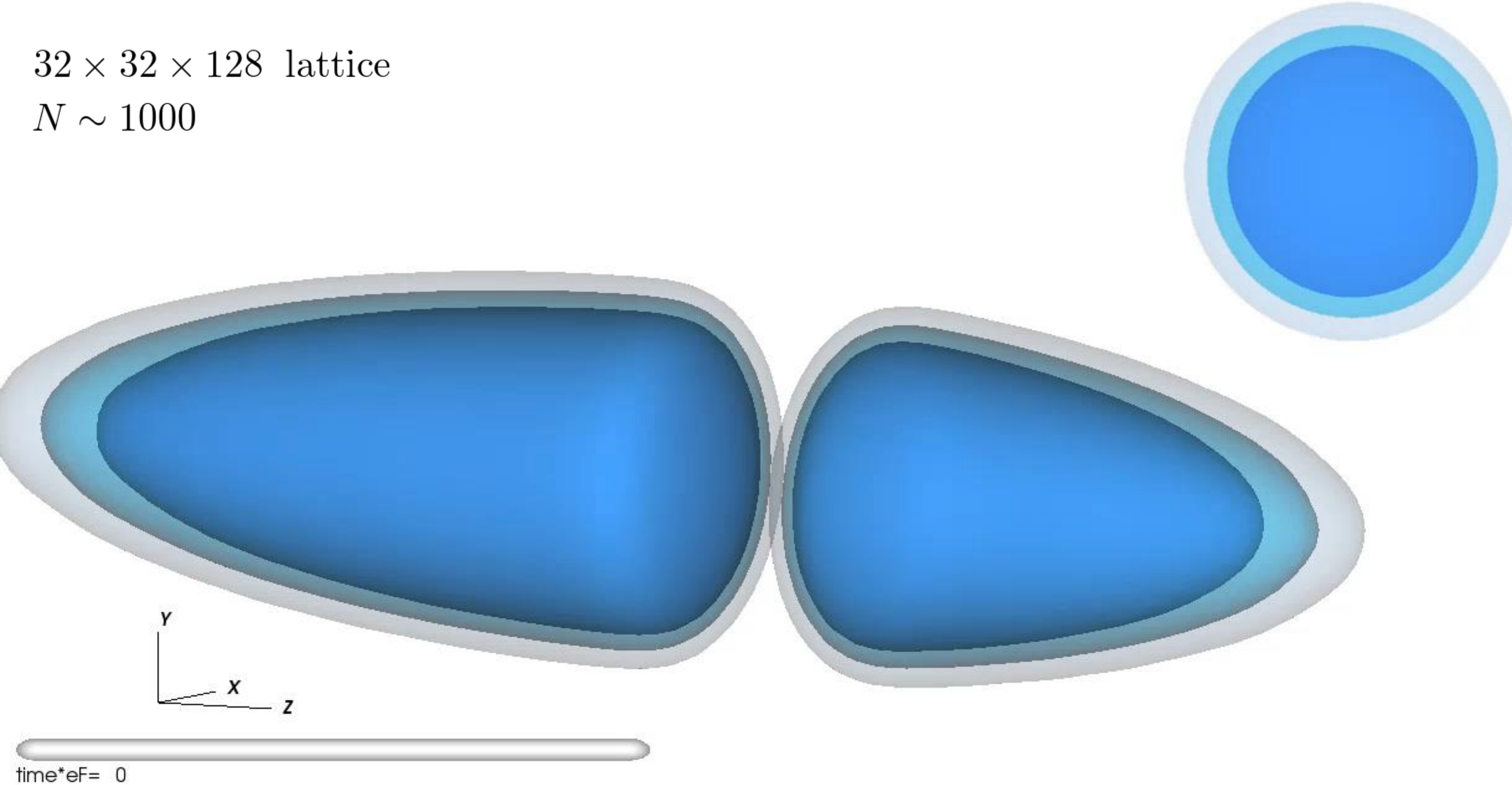
Quantum vortex

Result of TDSLDA simulation:

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

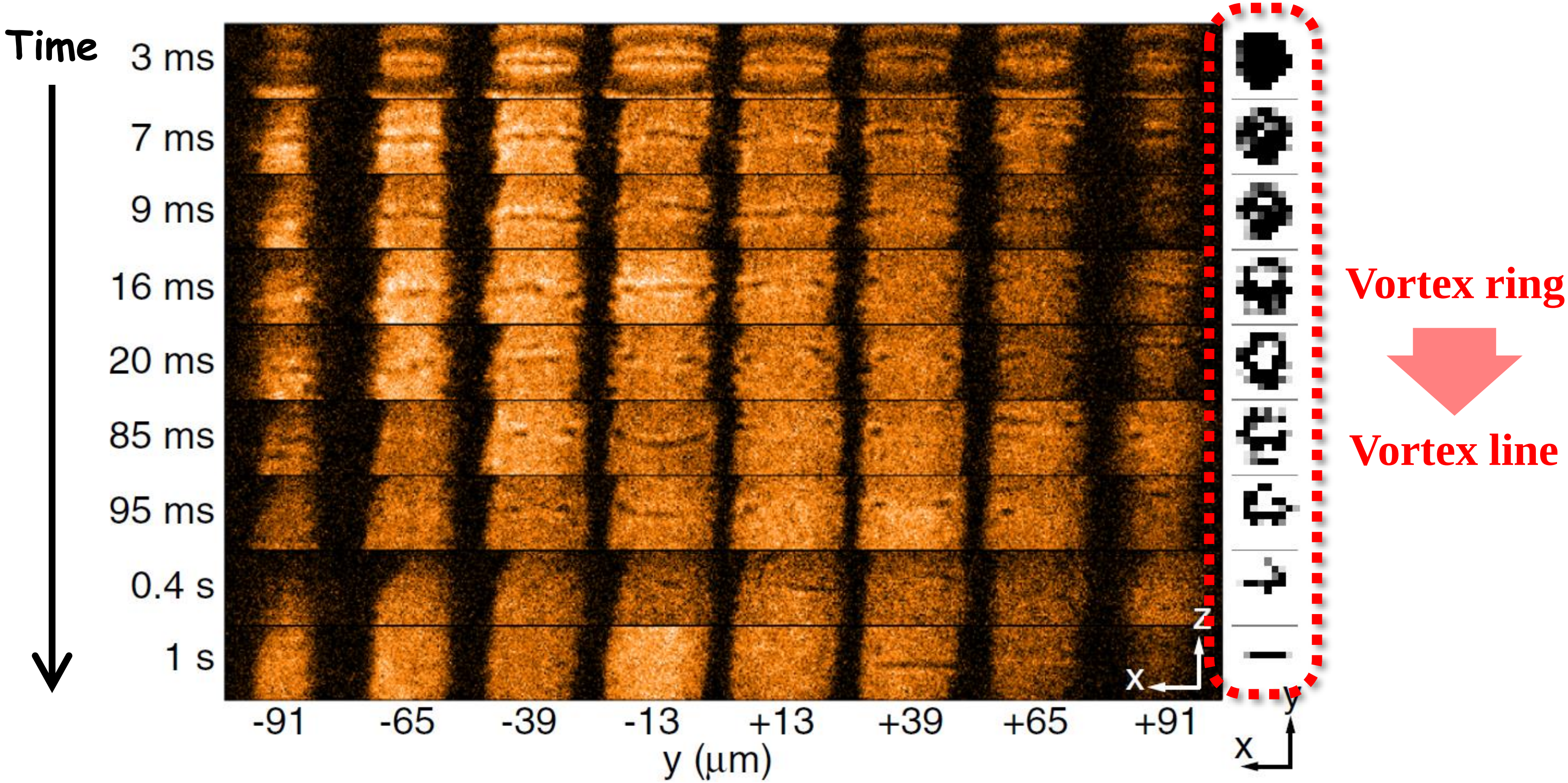
$32 \times 32 \times 128$ lattice

$N \sim 1000$



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



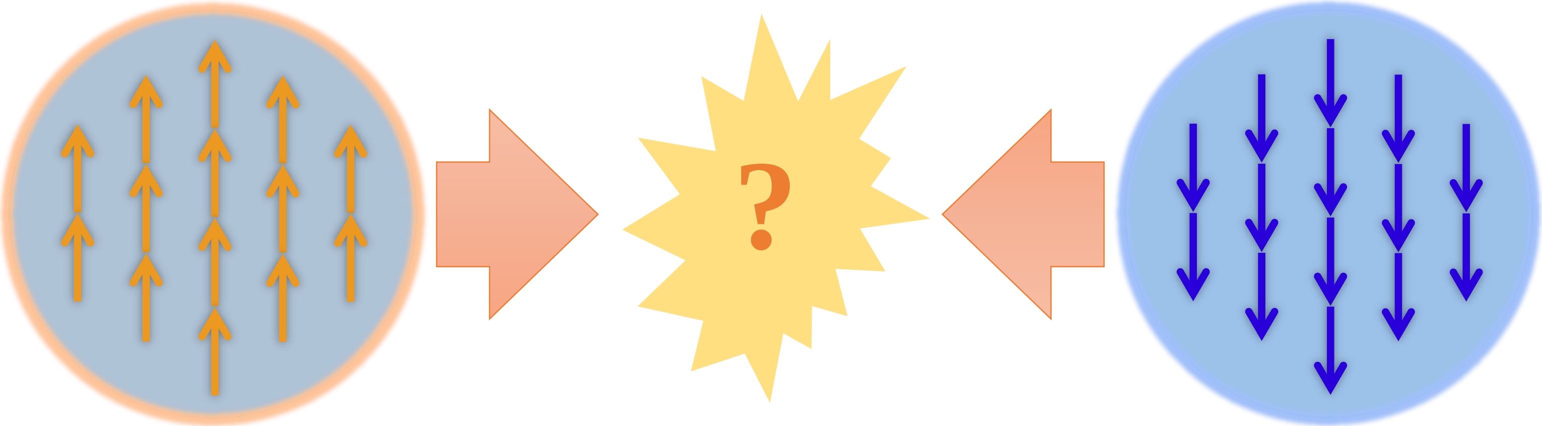
M.J.H. Ku, B. Mukherjee, T. Yefsah, and M.W. Zwierlein, Phys. Rev. Lett. **116**, 045304 (2016)

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

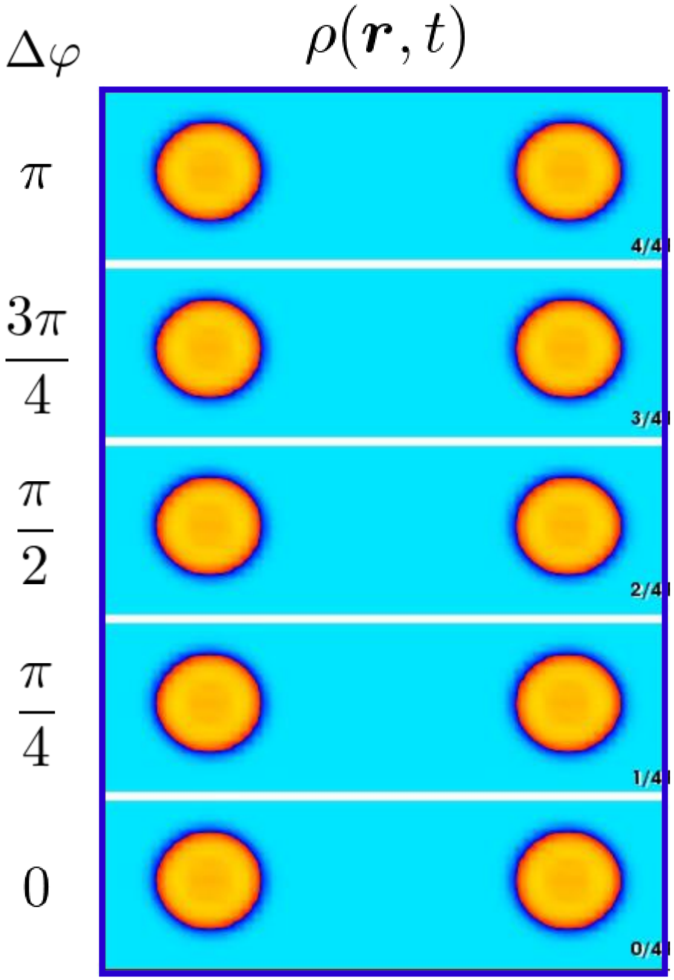
Q. What happens when two **superfluid** nuclei with different **phases** collide??

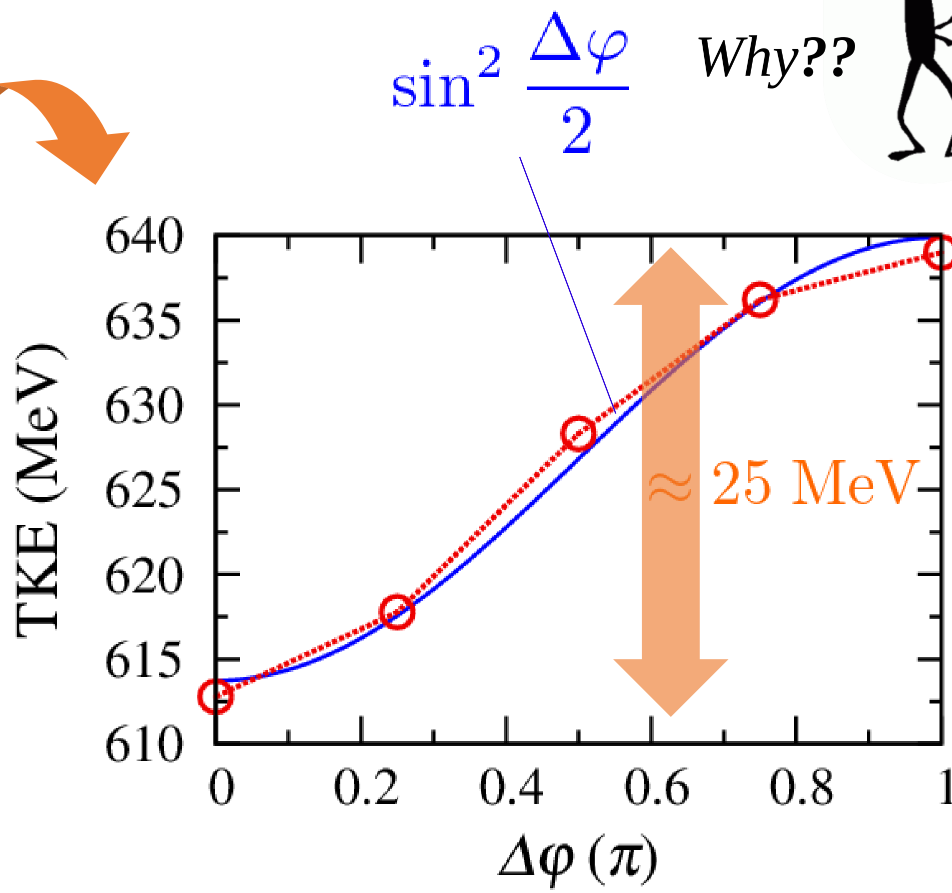
$$\Delta\varphi \ (\equiv \varphi_1 - \varphi_2)$$

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

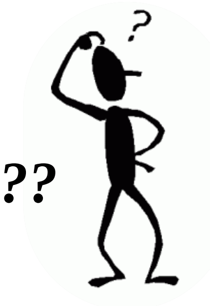


The phase difference changes **kinetic energy** of the fragments





Why??

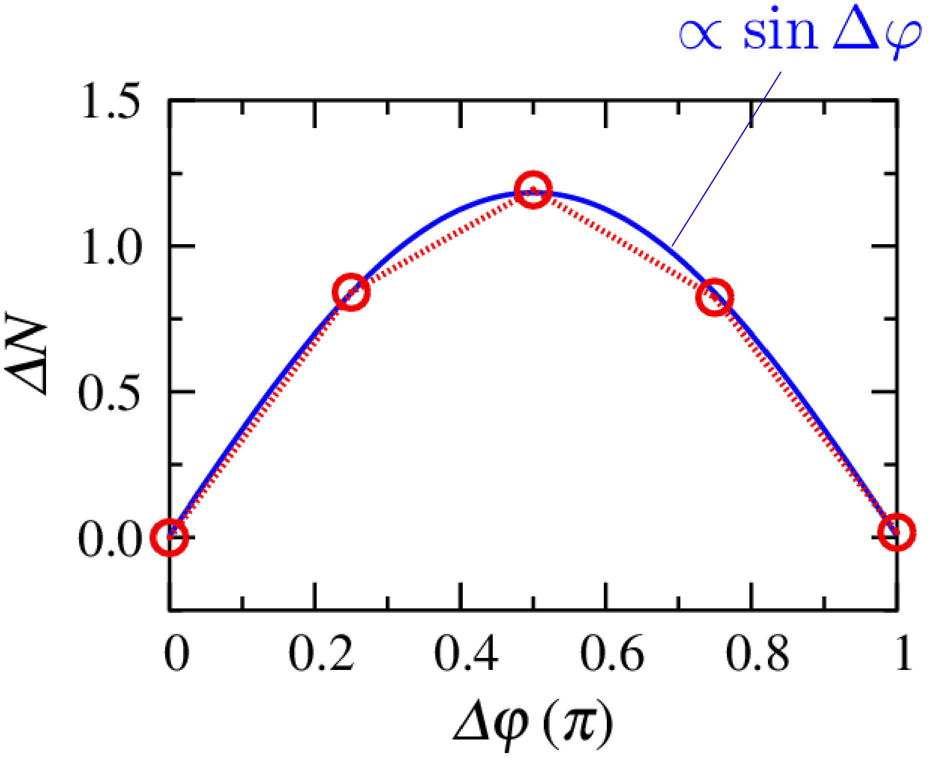


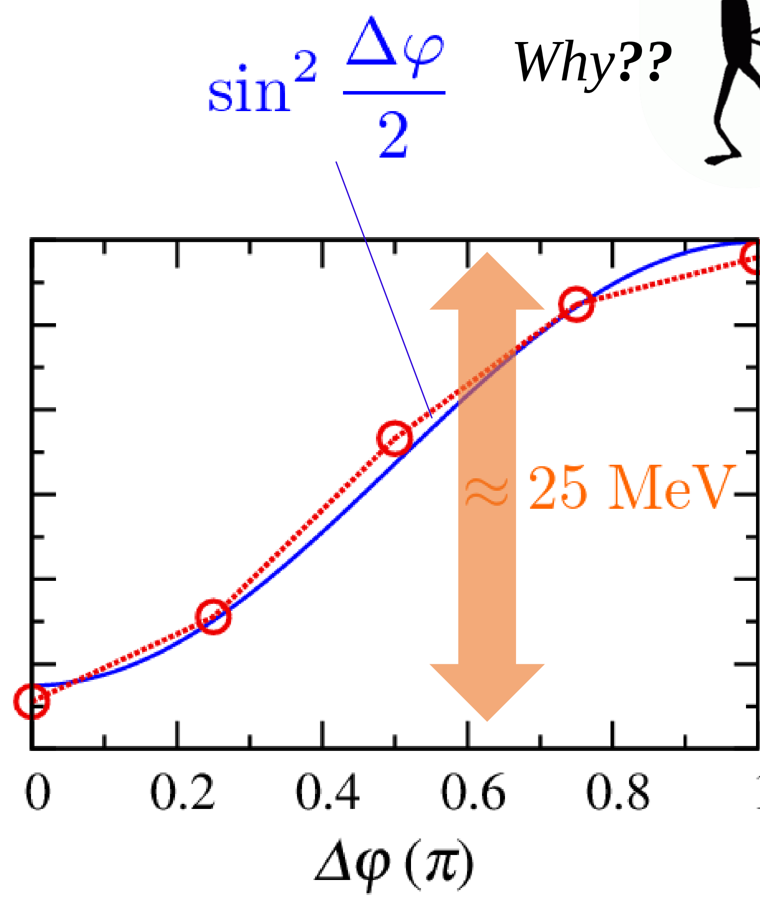
P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

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!





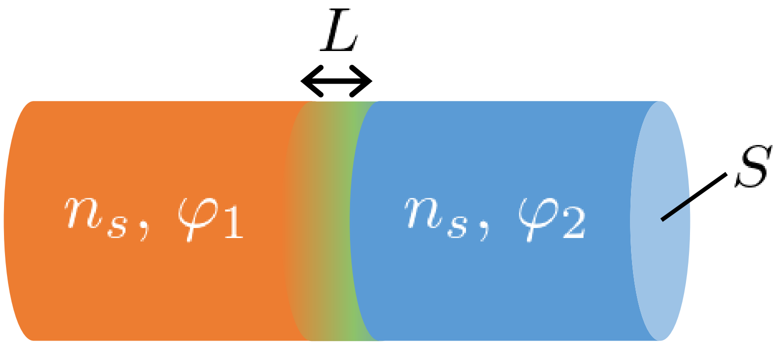
Why??

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

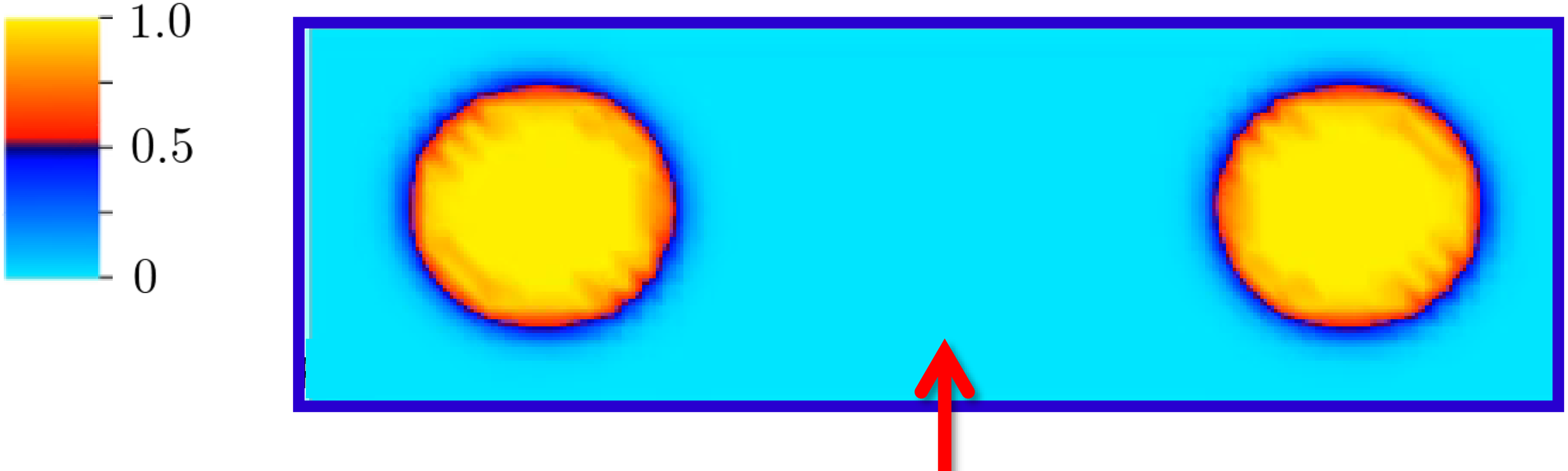
n_s: Superfluid density

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

Additional energy is required to attach two superfluids with different phases

$\Delta_n(\boldsymbol{r}, t)$ (MeV)

^{240}Pu+^{240}Pu (E/V_{Bass}=1.1), $\Delta\varphi = \pi$

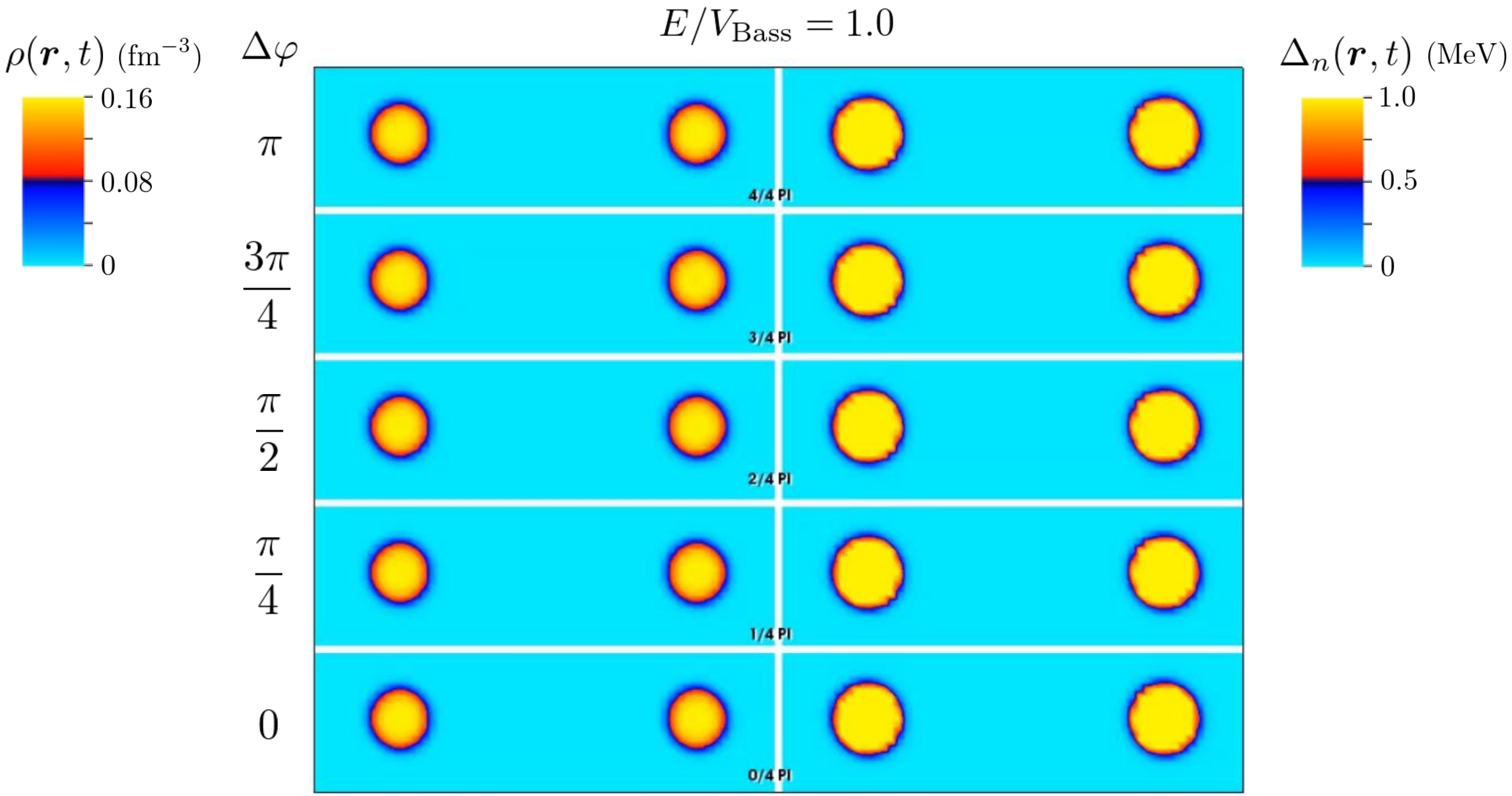


Pairing field is vanishing!
(due to phase discontinuity)

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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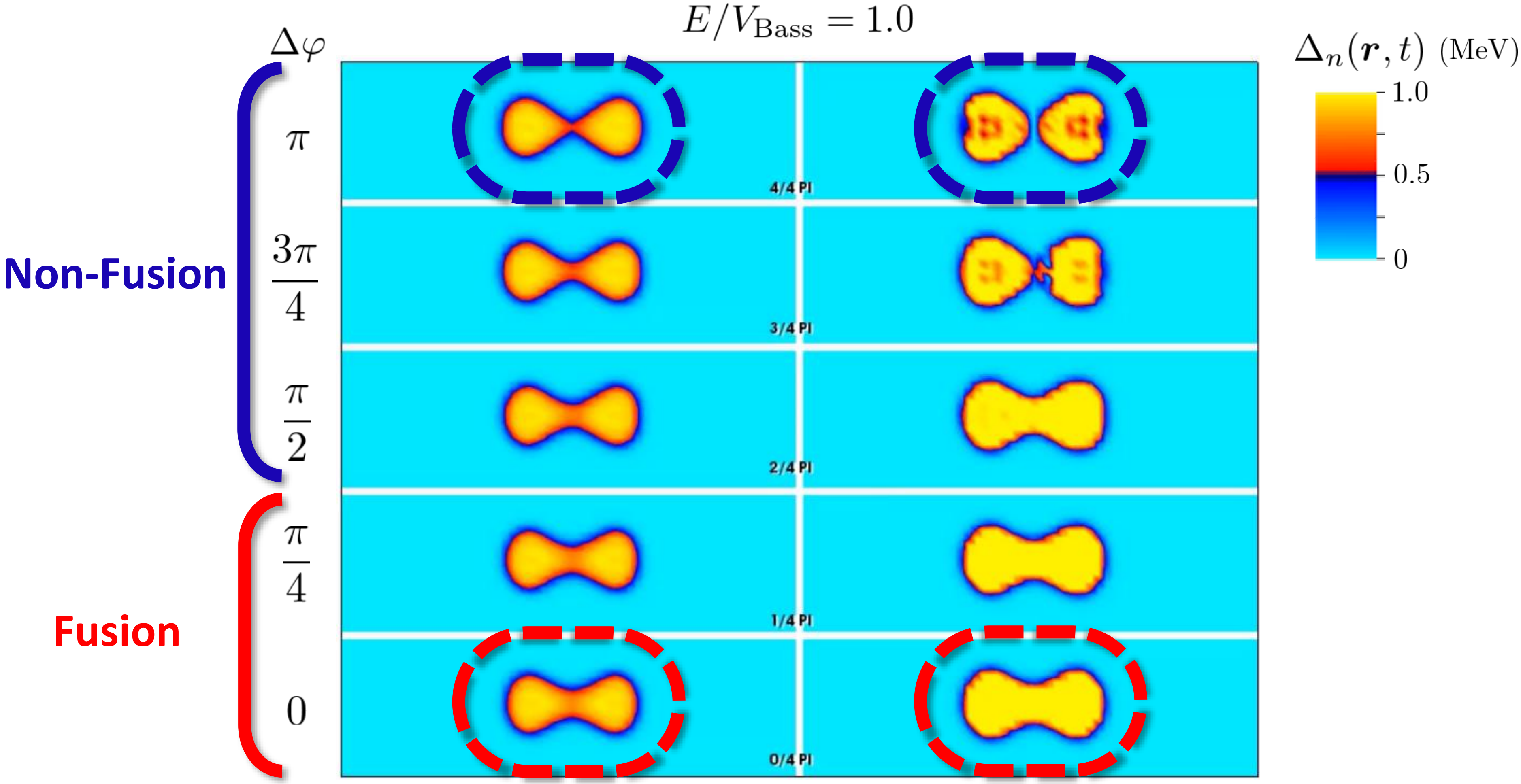
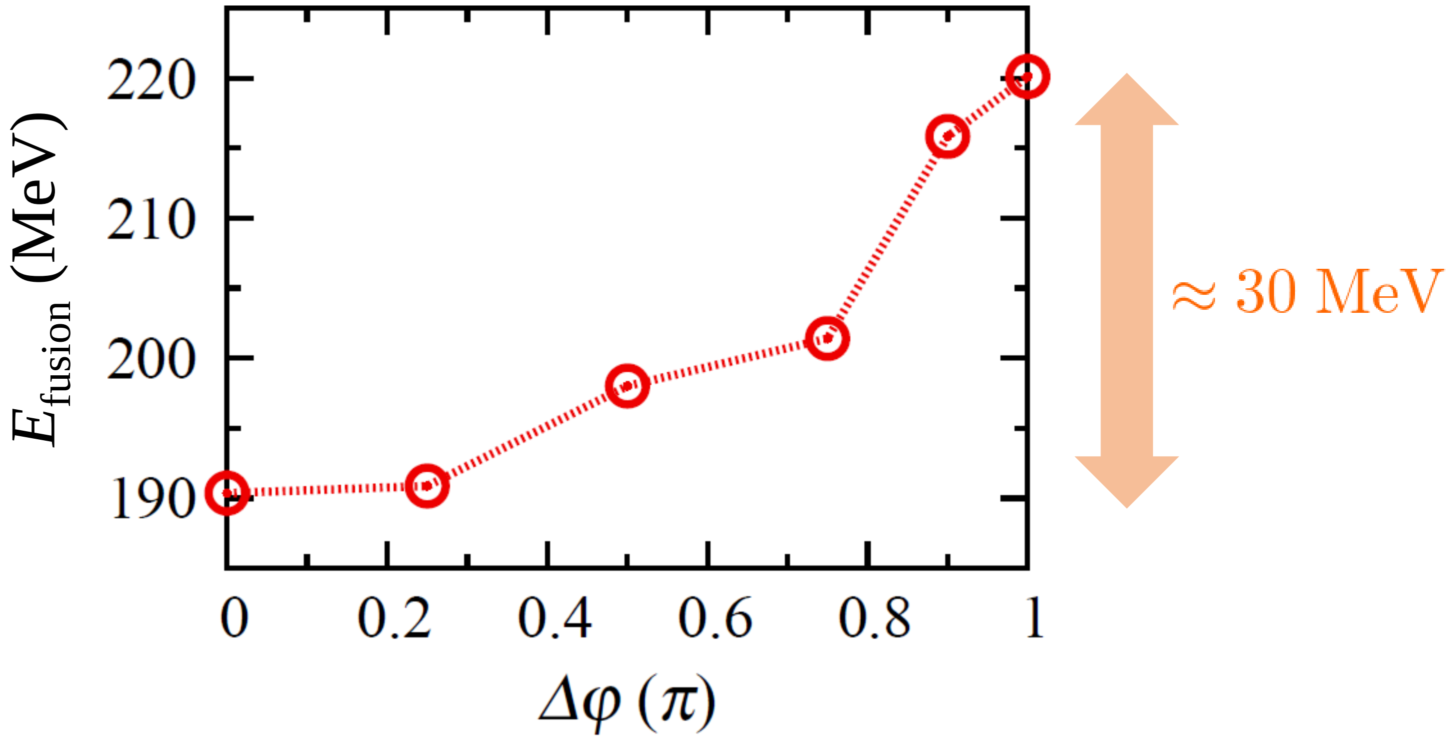


P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

Fusion reaction is suppressed by the phase difference

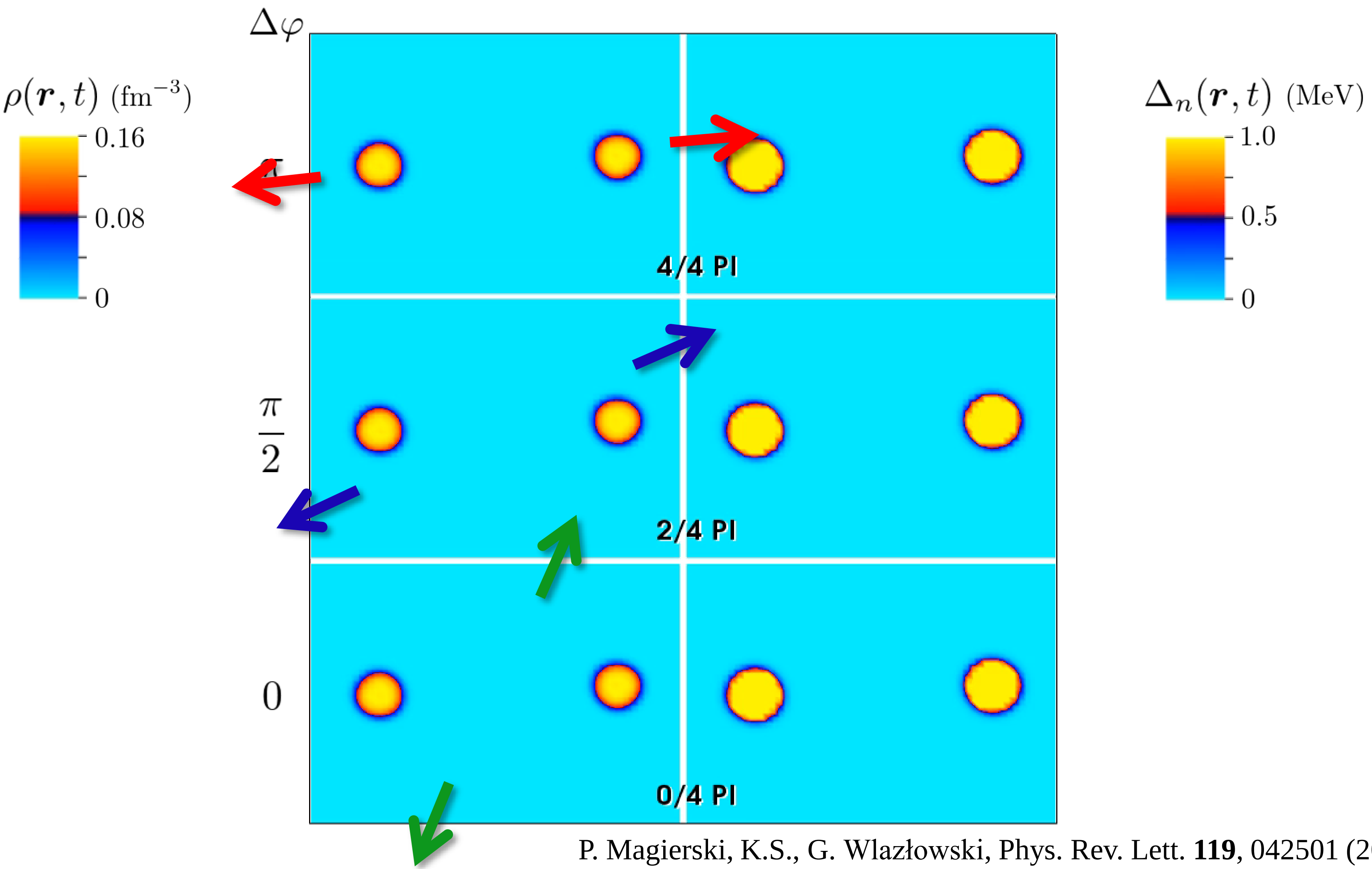
*$E_{\mathbf{fusion}}$: the lowest energy at which fusion reaction is observed



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

TDSLDA results: $^{90}Zr + ^{90}Zr$ non-central collisions

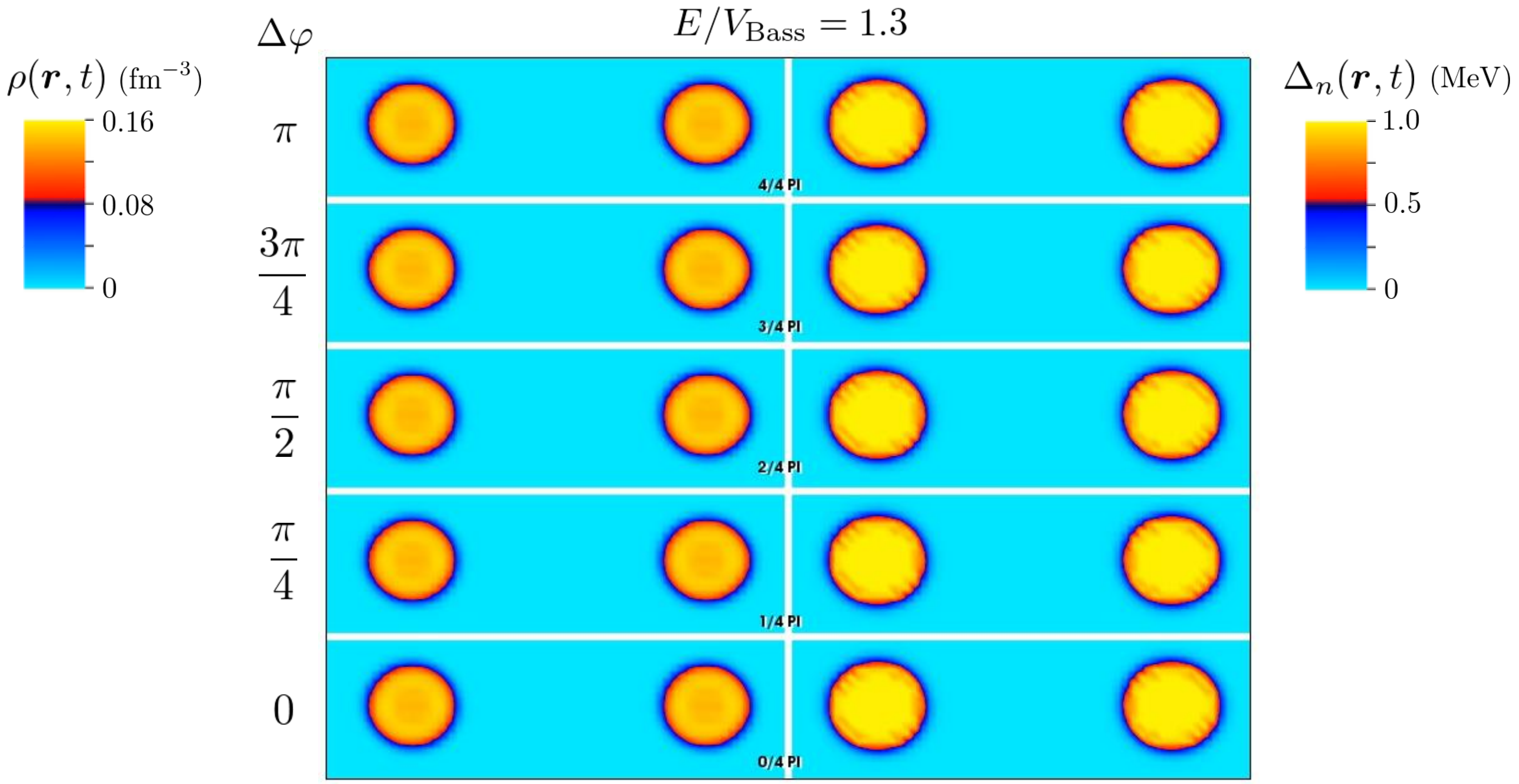
For non-central collisions, contact time & scattering angle are also affected



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

TDSLDA results: ^{240}Pu+^{240}Pu head-on collisions

Phase difference prevents ternary quasifission



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

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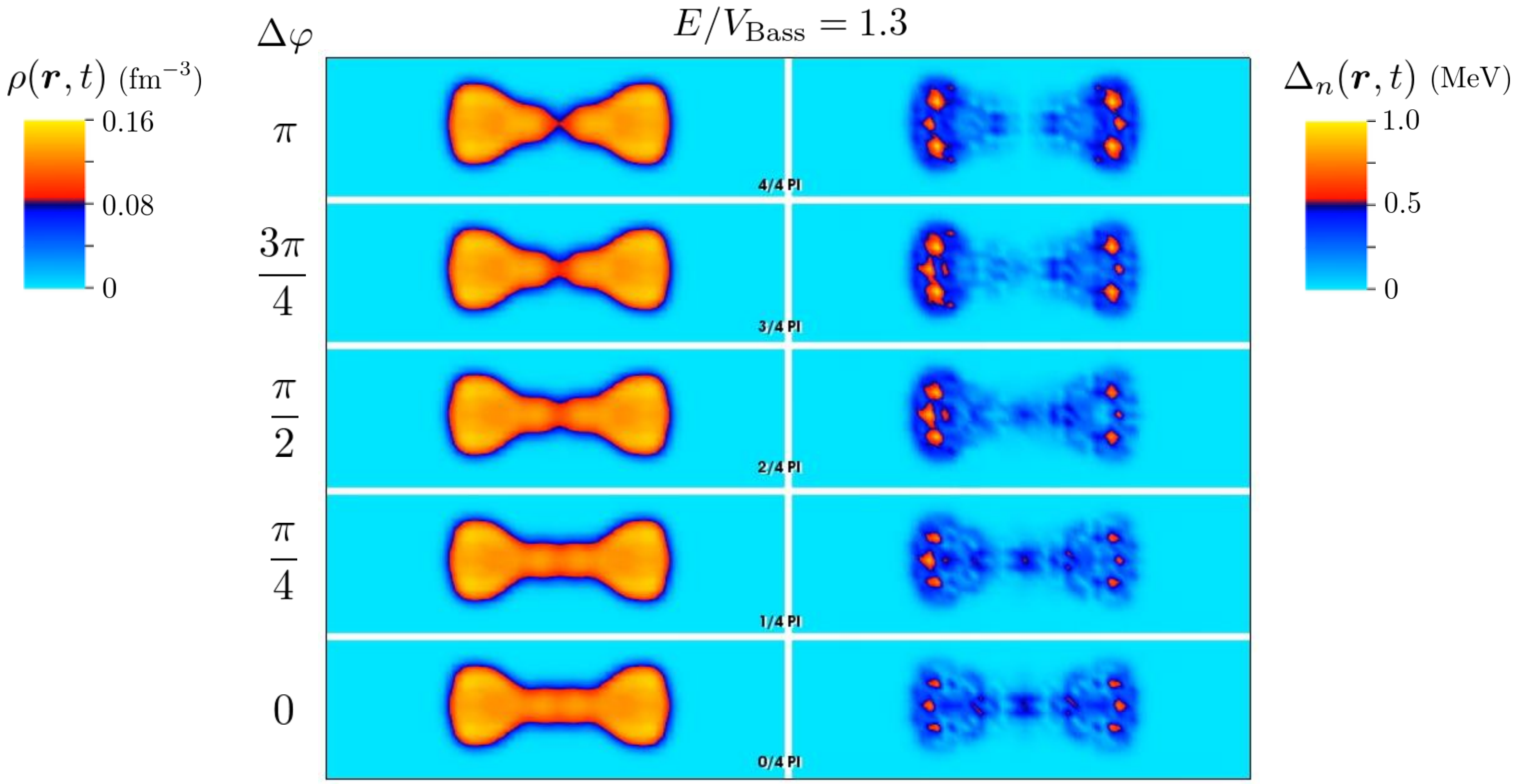


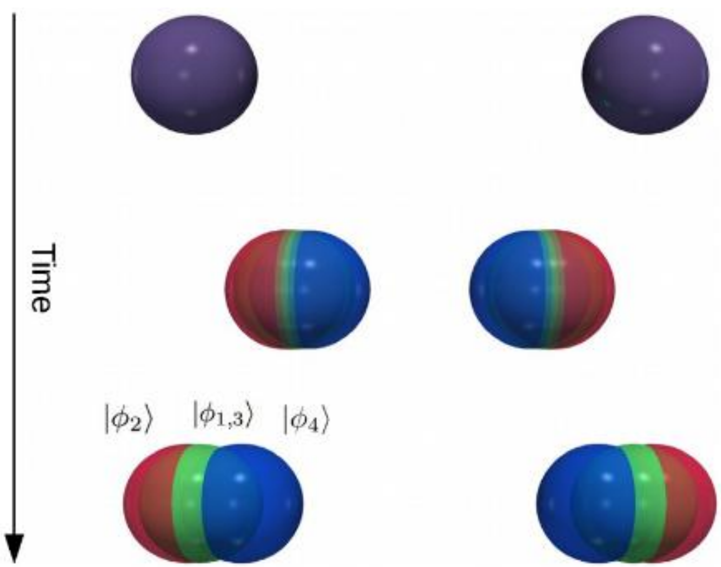
P. Magierski, K.S., G. Wlazłowski, Phys. Rev. Lett. **119**, 042501 (2017)

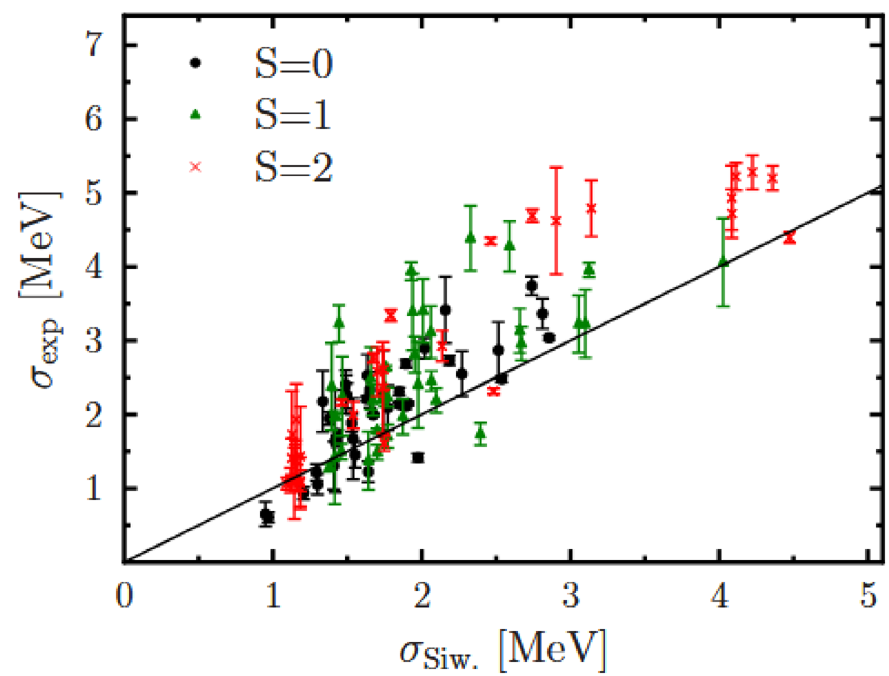
Things to be clarified

Y. Hashimoto and G. Scamps, Phys. Rev. C **94**, 014610 (2016).

G. Scamps and Y. Hashimoto, Phys. Rev. C **96**, 031602(R) (2017).

G. Scamps, Phys. Rev. C **97**, 044611 (2018).





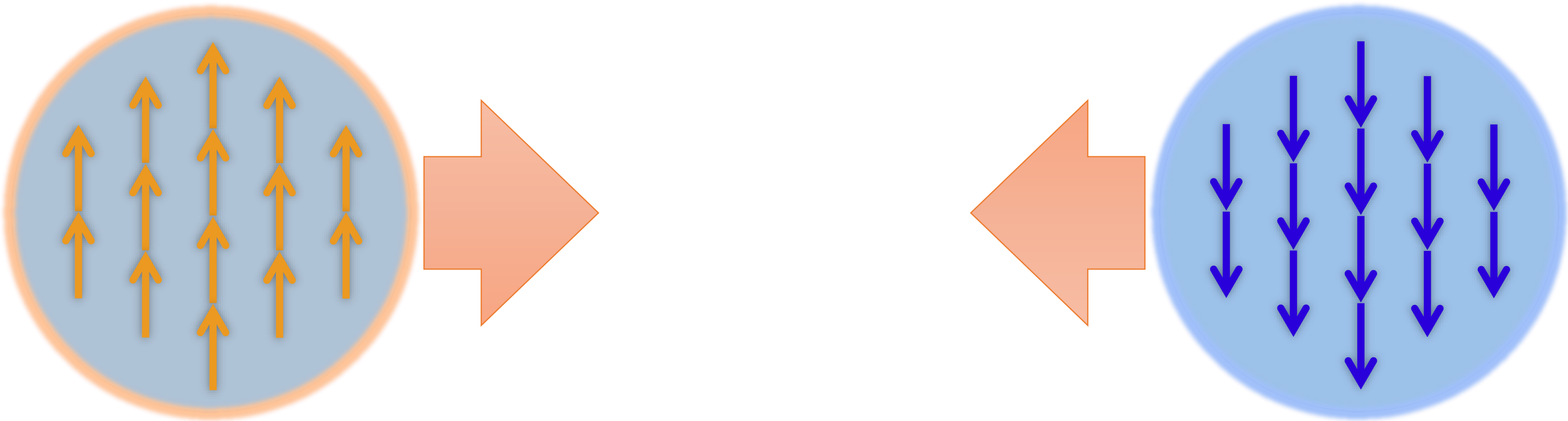
Conclusion

Conclusion

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

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

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



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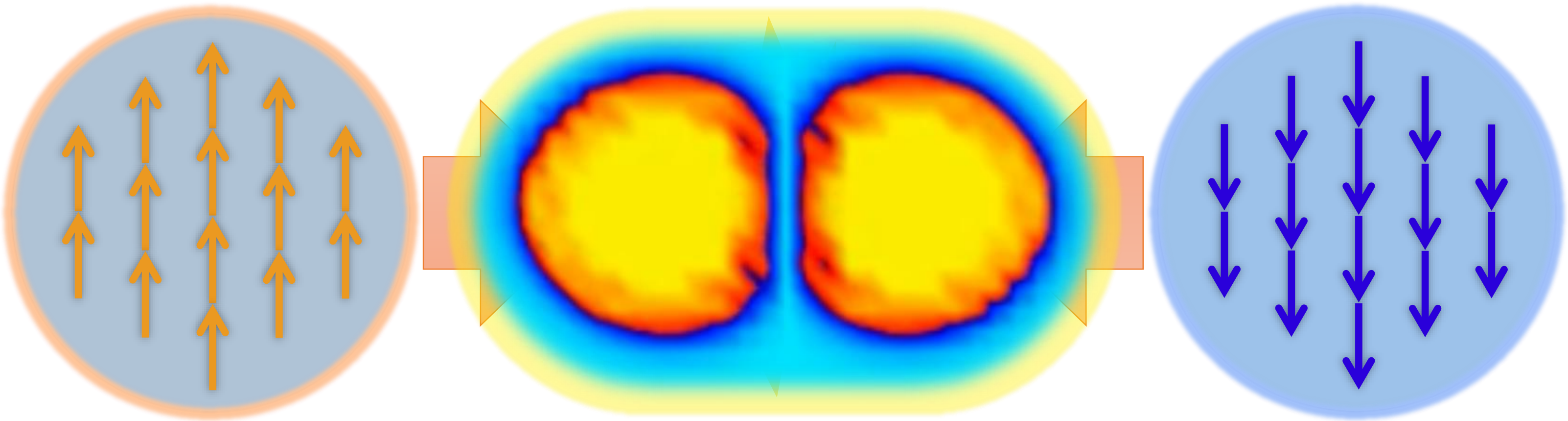

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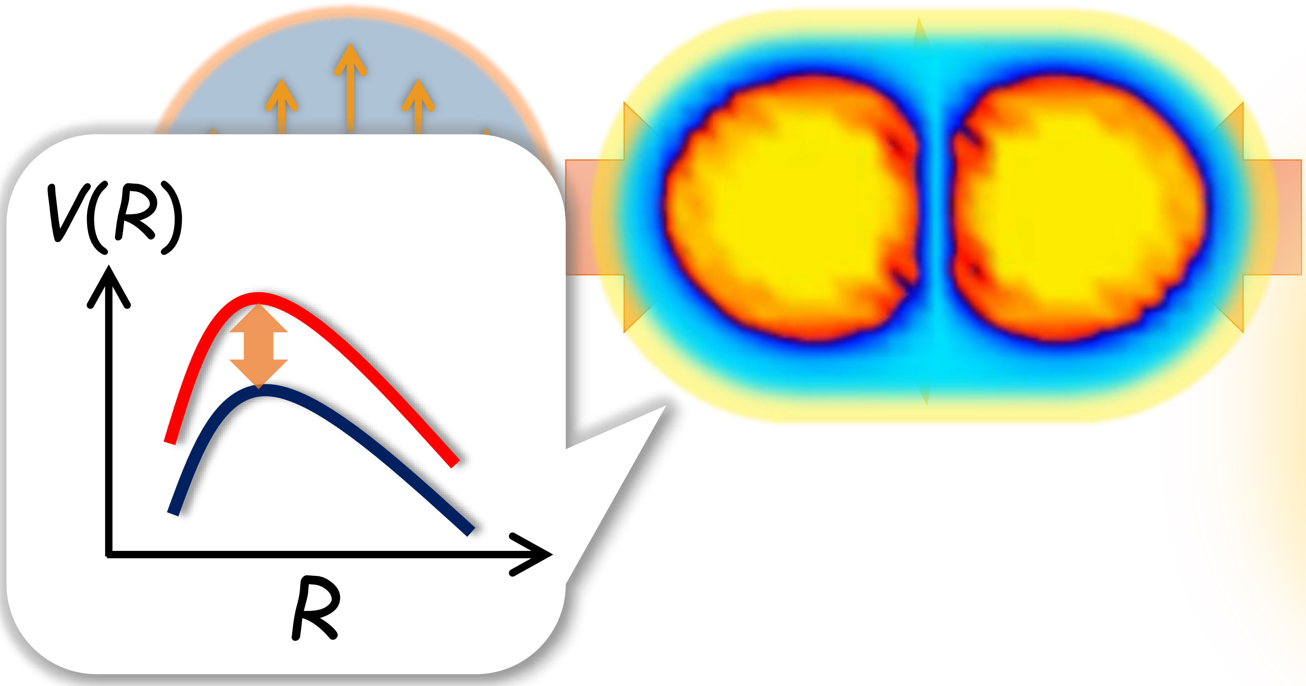

It may affect:

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

Kazuyuki Sekizawa
Specially Appointed Assistant Professor
Center for Transdisciplinary Research
Institute for Research Promotion, Niigata University
8050, Ikarashi Ninoho, Nishi-ku, Niigata City, Niigata 950-2181, Japan
sekizawa @ phys.sc.niigata-u.ac.jp
http://sekizawa.fizyka.pw.edu.pl/english/