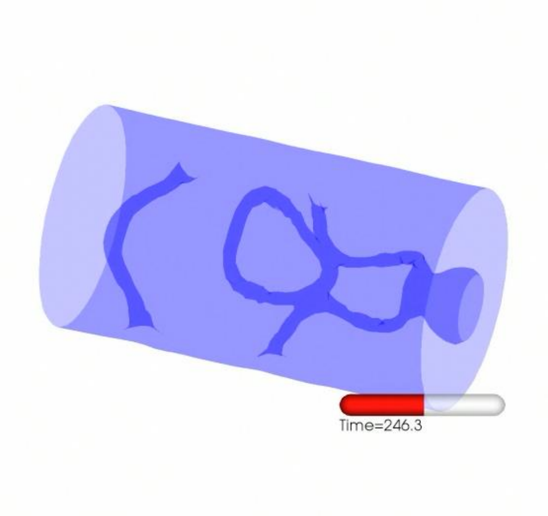
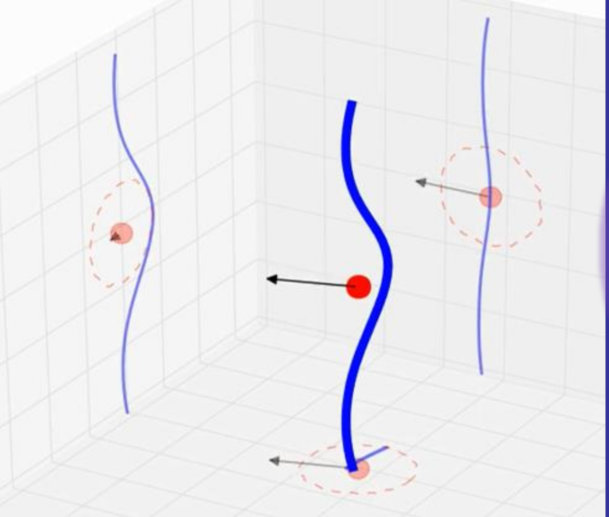
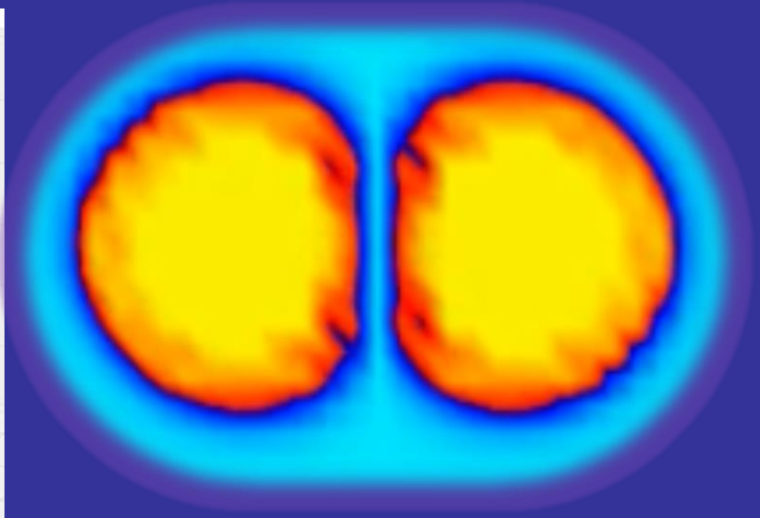
Solitonic excitations in collisions of superfluid nuclei.







Piotr Magierski
(Warsaw University of Technology & Univ. of Washington)

Collaborators:

Warsaw Univ. of Technology

- Janina Grineviciute
- **Kazuyuki Sekizawa**
- **Gabriel Wlazłowski**

- Aurel Bulgac (Univ. of Washington)
- Michael M. Forbes (Washington State U.)
- Kenneth J. Roche (PNNL)
- Ionel Stetcu (LANL)

GOAL:

Description of superfluid dynamics of fermionic systems far from equilibrium based on microscopic theoretical framework.

Microscopic framework = explicit treatment of fermionic degrees of freedom.

Why Time Dependent Density Functional Theory (TDDFT)?

We need to describe the time evolution of (externally perturbed) spatially inhomogeneous, superfluid Fermi system.

Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of hundred of thousands fermions.

Runge Gross mapping

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \quad |\psi_0\rangle = |\psi(t_0)\rangle$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0$$

$$\left.\begin{matrix}\rho(\vec{r},t)\\ |\psi(t_0)\rangle\end{matrix}\right\} \leftrightarrow e^{i\alpha(t)}|\psi(t)\rangle$$

Up to an arbitrary function α(t)

and consequently the functional exists:

$$F[\psi_0,\rho] = \int_{t_0}^{t_1}\langle\psi[\rho]|\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)|\psi[\rho]\rangle\,dt$$

E. Runge, E.K.U Gross, PRL 52, 997 (1984)
B.-X. Xu, A.K. Rajagopal, PRA 31, 2682 (1985)
G. Vignale, PRA77, 062511 (2008)

Kohn-Sham approach

Suppose we are given the density of an interacting system.
There exists a unique noninteracting system with the same density.

Interacting system

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = (\hat{T}+\hat{V}(t)+\hat{W})\left|\psi(t)\right\rangle$$

Noninteracting system

$$i\hbar\frac{\partial}{\partial t}\left|\varphi(t)\right\rangle = (\hat{T}+\hat{V}_{KS}(t))\left|\varphi(t)\right\rangle$$

$$\rho(\vec{r},t)=\left\langle\psi(t)\right|\hat{\rho}(\vec{r})\left|\psi(t)\right\rangle=\left\langle\varphi(t)\right|\hat{\rho}(\vec{r})\left|\varphi(t)\right\rangle$$

However as always there is a price to pay:

- No dissipation effects except for the one-body dissipation (justified if energies are not too large)
- Only one body observables can be reliably evaluated.

The extensions are possible and under progress (see e.g. talk on stochastic TDHF)

Superfluid extension of (TD)DFT

Triggered initially by the discovery of high-Tc supercondutors:

DFT for superconductors:
L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60 2430 (1988).
TDDFT for supercondutors:
O.-J. Wacker, R. Kummel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994).

Extensions required to introduce an anomalous density:

$$\Delta(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\frac{\delta E(\rho, \chi)}{\delta \chi^*(\mathbf{r}\sigma, \mathbf{r}'\sigma')}.$$

Problem:
Such formulation results in Kohn-Sham equations in a form of integro-differential equations of enormous computational complexity.

Pairing correlation in DFT

One may extend DFT to superfluid systems by defining the pairing field:

$$\Delta(\mathbf{r}\sigma, \mathbf{r}'\sigma') = -\frac{\delta E(\rho, \chi)}{\delta \chi^*(\mathbf{r}\sigma, \mathbf{r}'\sigma')}.$$

L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60 2430 (1988).

O.-J. Wacker, R. Kümmel, E.K.U. Gross, Phys. Rev. Lett. 73, 2915 (1994).

and introducing anomalous density $\chi(\mathbf{r}\sigma, \mathbf{r}'\sigma') = \langle \hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma}(\mathbf{r})\rangle$

However in the limit of the local field these quantities diverge unless one renormalizes the coupling constant:

$$\begin{aligned} \Delta(\mathbf{r}) &= g_{eff}(\mathbf{r})\chi_c(\mathbf{r}) \\ \frac{1}{g_{eff}(\mathbf{r})} &= \frac{1}{g(\mathbf{r})} - \frac{mk_c(\mathbf{r})}{2\pi^2\hbar^2}\left(1 - \frac{k_F(\mathbf{r})}{2k_c(\mathbf{r})}\ln\frac{k_c(\mathbf{r}) + k_F(\mathbf{r})}{k_c(\mathbf{r}) - k_F(\mathbf{r})}\right) \end{aligned}$$

which ensures that the term involving the kinetic and the pairing energy density is finite:

$$\frac{\tau_c(r)}{2m} - \Delta(r)\chi_c(r)$$

Bulgac, Yu, Phys. Rev. Lett. 88 (2002) 042504
Bulgac, Phys. Rev. C65 (2002) 051305

TDDFT equations with local pairing field (TDSLDA):

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

The form of $h(r,t)$ and $\Delta(r,t)$ is determined by EDF (Energy Density Functional)

- **The system is placed on a large 3D spatial lattice.**
- **No symmetry restrictions.**
- **Number of PDEs is of the order of the number of spatial lattice points.**

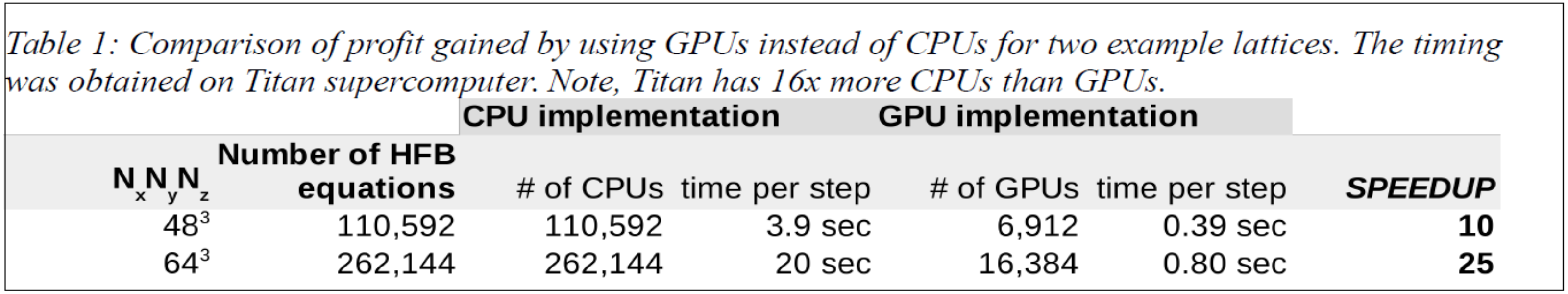


Table 1: Comparison of profit gained by using GPUs instead of CPUs for two example lattices. The timing was obtained on Titan supercomputer. Note, Titan has 16x more CPUs than GPUs.

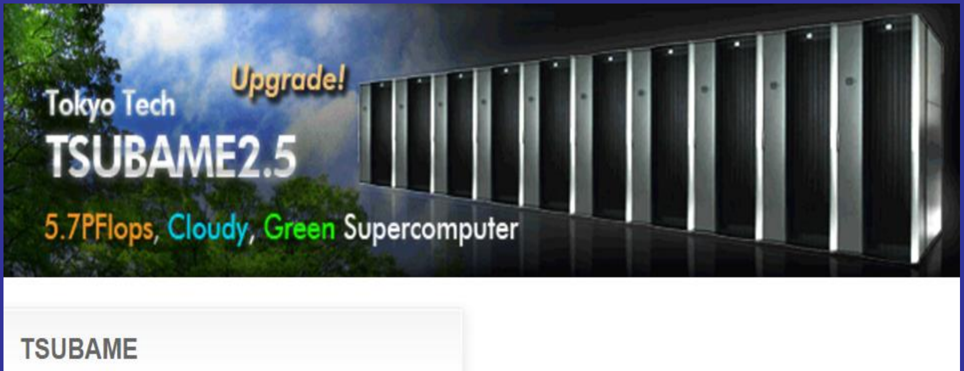
		CPU implementation		**GPU implementation**		
$N_xN_yN_z$	**Number of HFB equations**	# of CPUs	time per step	# of GPUs	time per step	***SPEEDUP***
48^3	110,592	110,592	3.9 sec	6,912	0.39 sec	**10**
64^3	262,144	262,144	20 sec	16,384	0.80 sec	**25**

The main advantage of TDSLDA over TDHF (+TDBCS) is related to the fact that in TDSLDA the pairing correlations are described as a true complex field which has its own modes of excitations, which include spatial variations of both amplitude and phase. Therefore in TDSLDA description the evolution of nucleon Cooper pairs is treated consistently with other one-body degrees of freedom.

Selected supercomputers (CPU+GPU) currently in use:

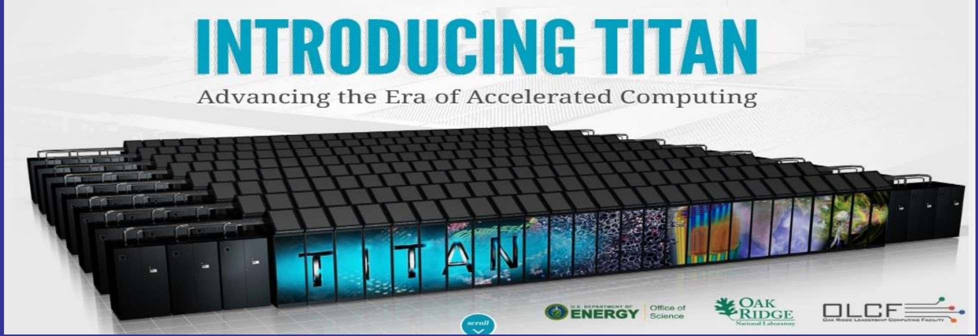
Piz Daint: 7.787 PFlops
(Swiss National Supercomputing Centre)

HA-PACS: 0.802 PFlops
(University of Tsukuba)



Tsubame: 5.7 PFlops
(Tokyo Institute of Technology)

Titan: 27 PFlops
(ORNL Oak Ridge)



Areas of applications

$$\frac{\Delta}{\varepsilon_F} \le 0.5$$

Ultracold atomic (fermionic) gases. Unitary regime.

Dynamics of quantum vortices, solitonic excitations, quantum turbulence.

$$\frac{\Delta}{\varepsilon_F} \le 0.1 - 0.2$$

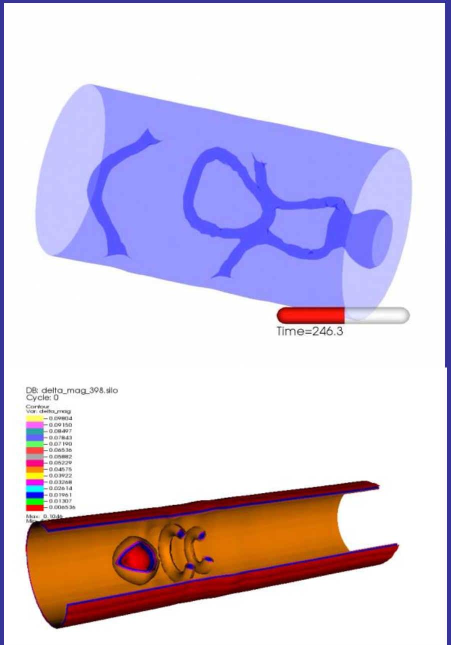
Astrophysical applications.

Modelling of neutron star interior (glitches): vortex dynamics, dynamics of inhomogeneous nuclear matter (in strong magnetic fields).

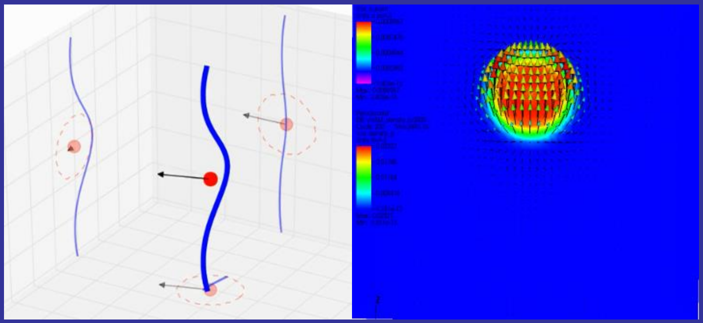
$$\frac{\Delta}{\varepsilon_F} \le 0.03$$

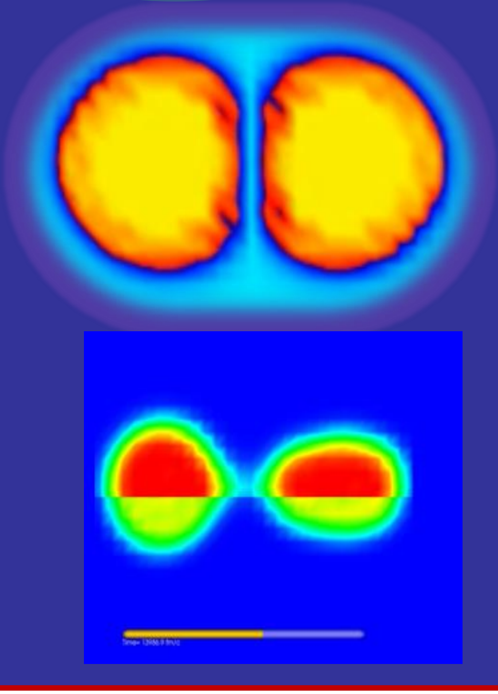
Nuclear physics.

Induced nuclear fission, fusion, collisions.



See Gabriel’s talk on Friday

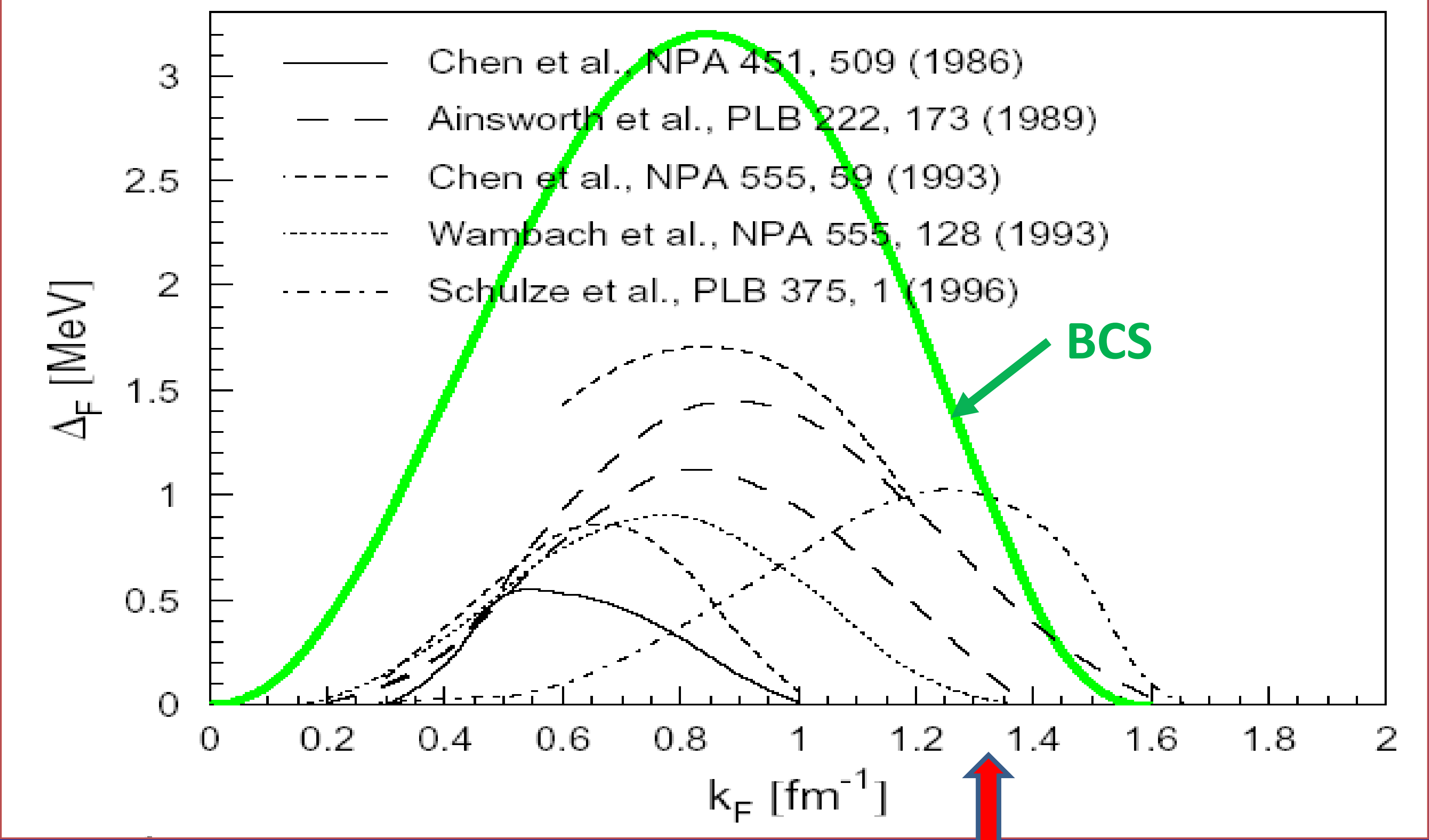




See Aurel’s talk on Friday

Pairing in nuclear systems

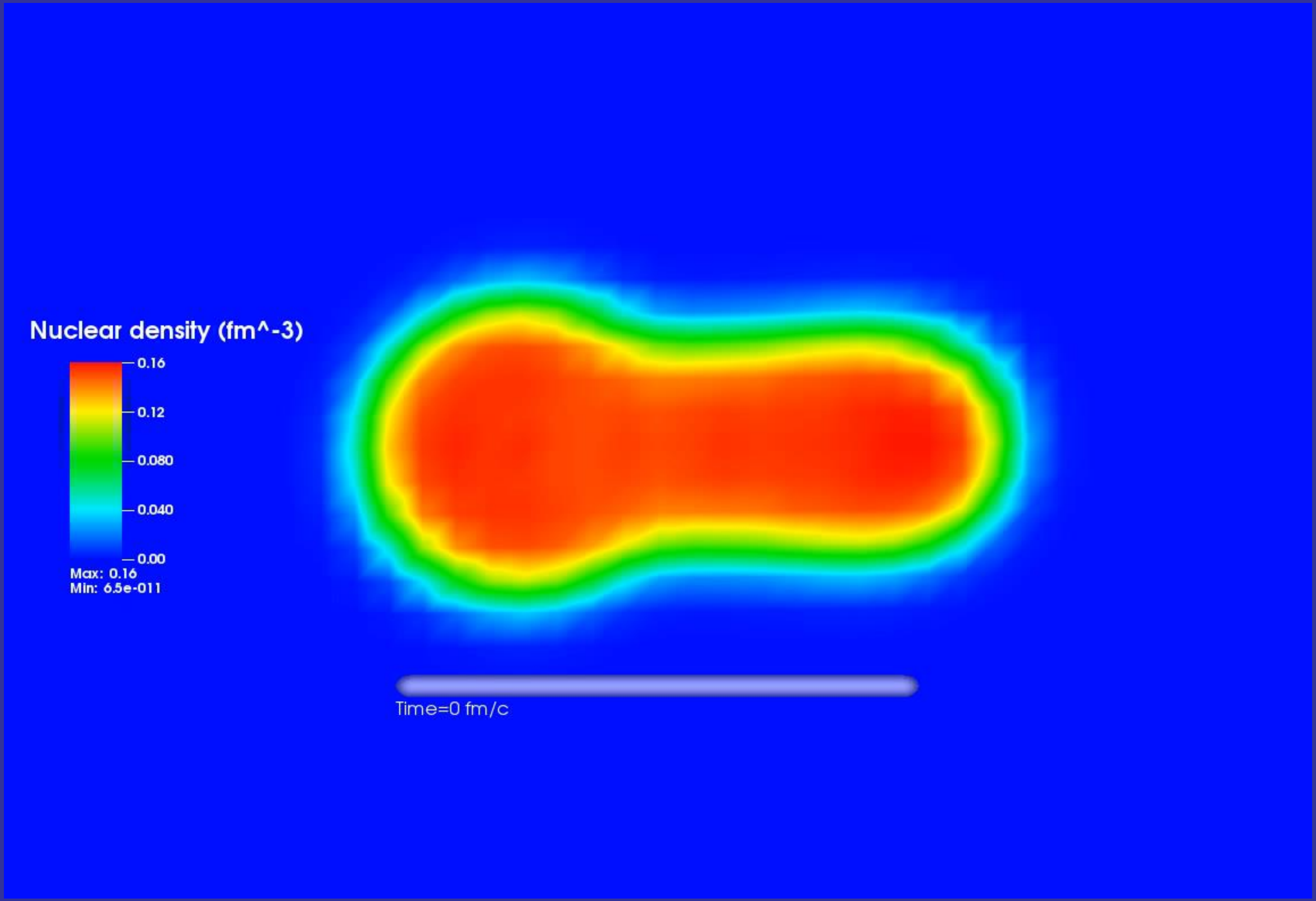
s-wave pairing gap in infinite uniform neutron matter with realistic NN-interactions.



Atomic nuclei: $\Delta \approx 1 MeV$

Nuclear fission dynamics

Initial configuration of ^{240}Pu is prepared beyond the barrier at quadrupole deformation *Q=165b* and excitation energy *E=8.08 MeV*:



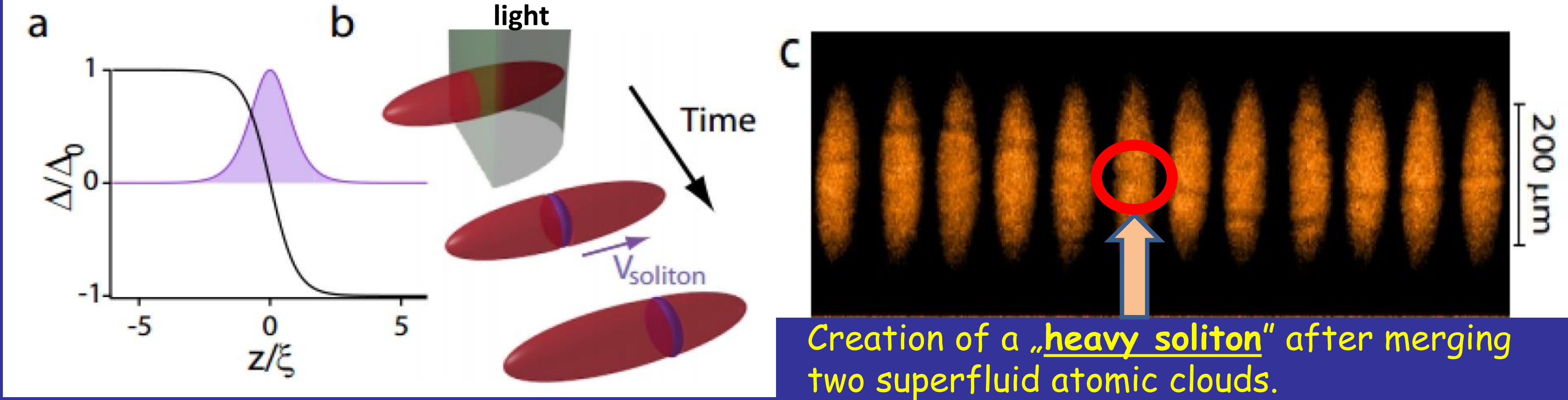
Without pairing correlations the nucleus does not fission!

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

Solitonic excitations nuclear collisions

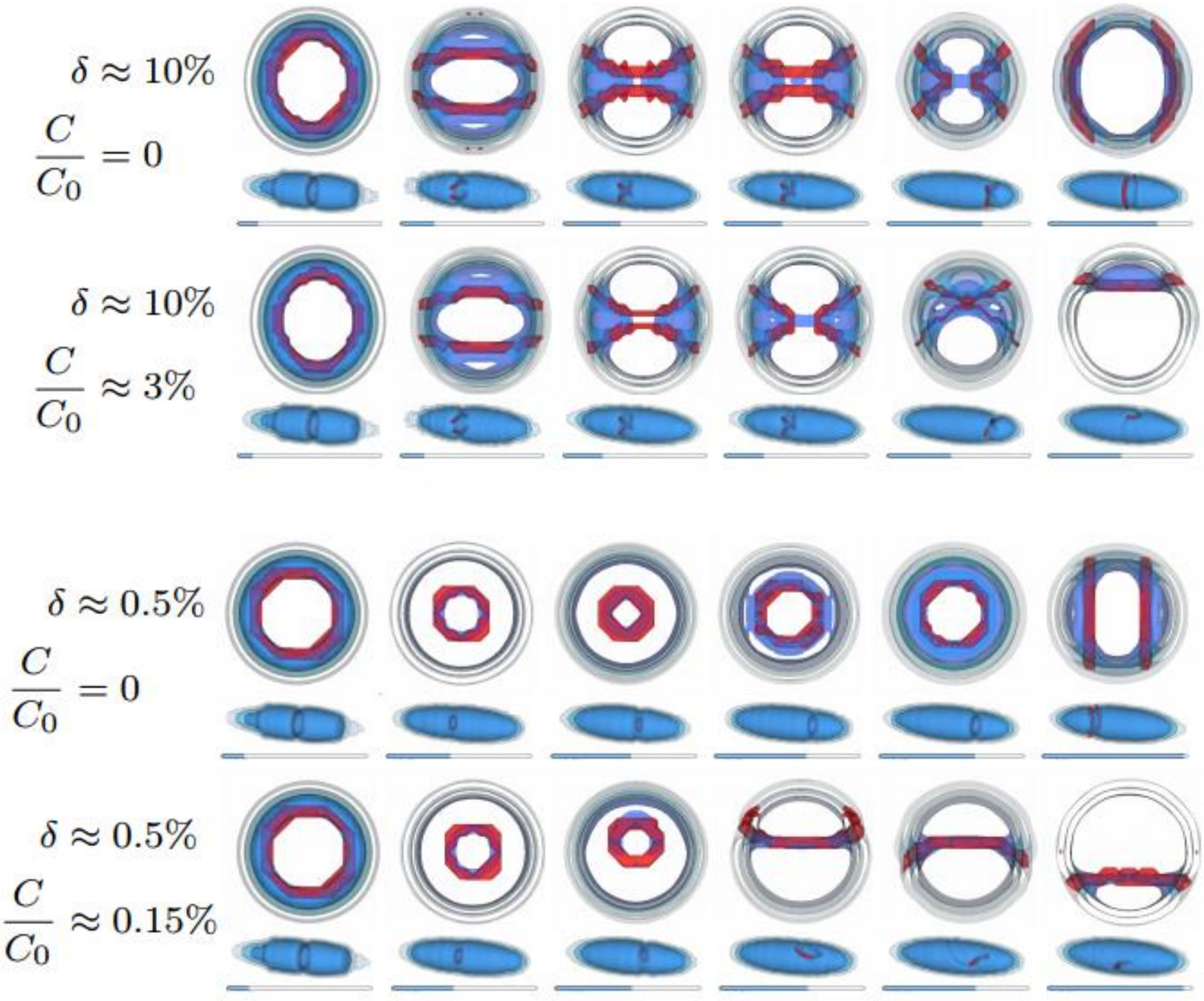
Collisions of superfluid nuclei having different phases of the pairing fields

Motivated by experiments on ultracold atomic gases: merging two 6Li clouds



Creation of a „**heavy soliton**" after merging two superfluid atomic clouds.

T. Yefsah et al., Nature 499, 426 (2013).



Moreover with TDDFT we can reproduce the sequence of topological excitations observed experimentally (M.H.J. Ku et al. Phys. Rev. Lett. 113, 065301 (2014)).

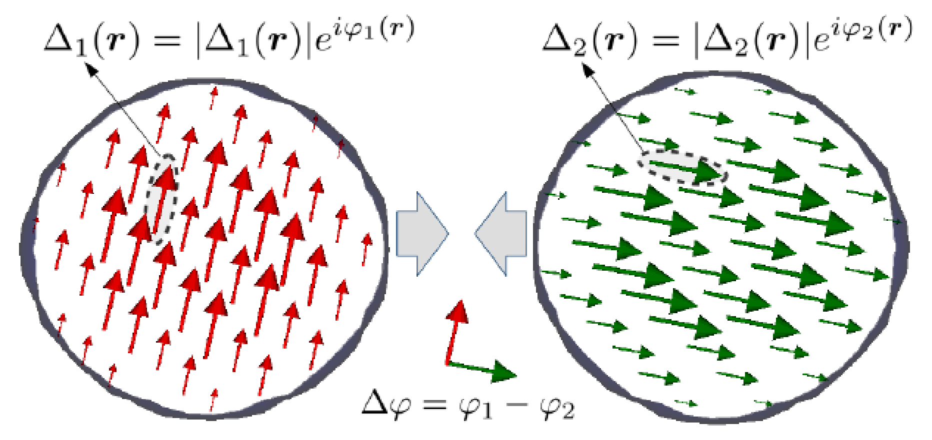
Wlazłowski, et al., Phys. Rev. A91, 031602 (2015)

In the context of nuclear systems the main questions are:

-how a possible solitonic structure can be manifested in nuclear system?

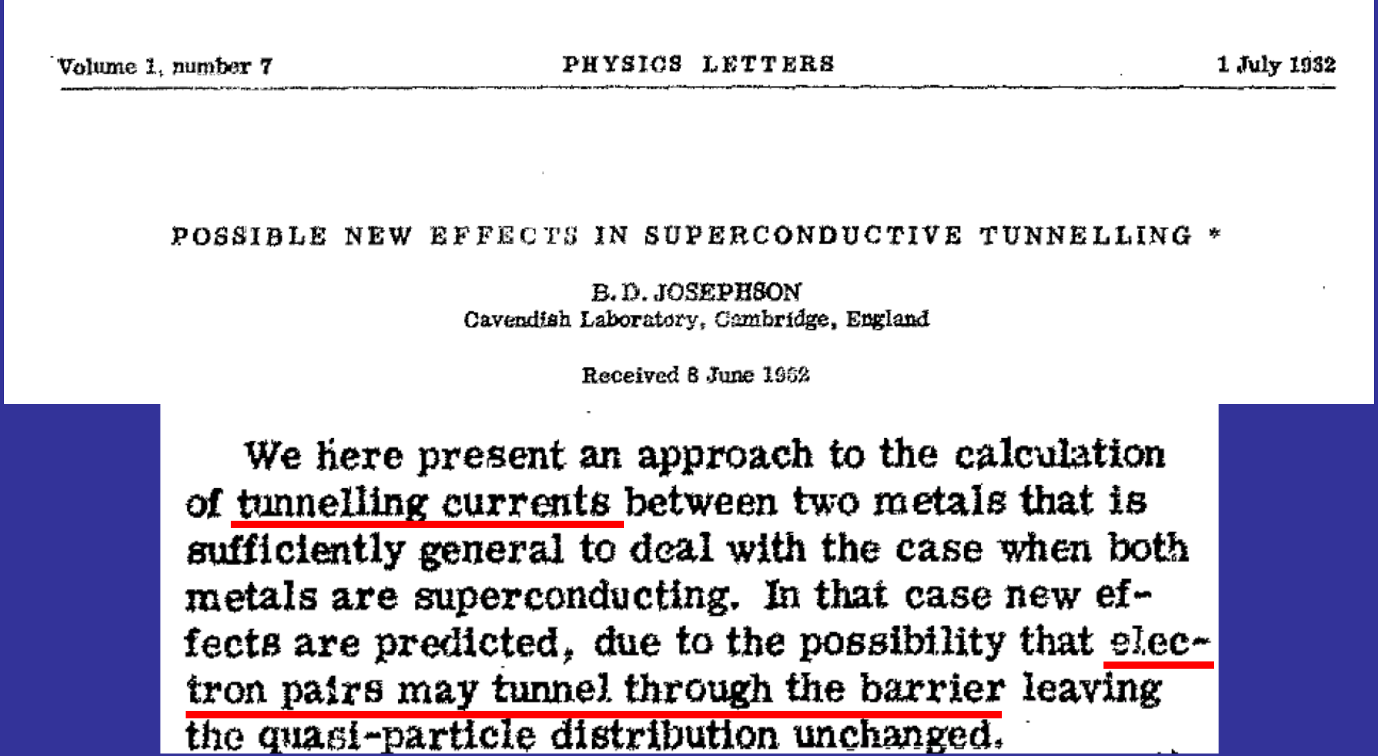
-what observable effect it may have on heavy ion reaction:
kinetic energies of fragments, capture cross section, etc.?

Clearly, we cannot control phases of the pairing field in nuclear experiments and the possible signal need to be extracted after averaging over the phase difference.



Digression: Physics of two nuclear, coupled superconductors

Little bit of history:



Volume 1, number 7 PHYSICS LETTERS 1 July 1962

POSSIBLE NEW EFFECTS IN SUPERCONDUCTIVE TUNNELLING *

B. D. JOSEPHSON
Cavendish Laboratory, Cambridge, England

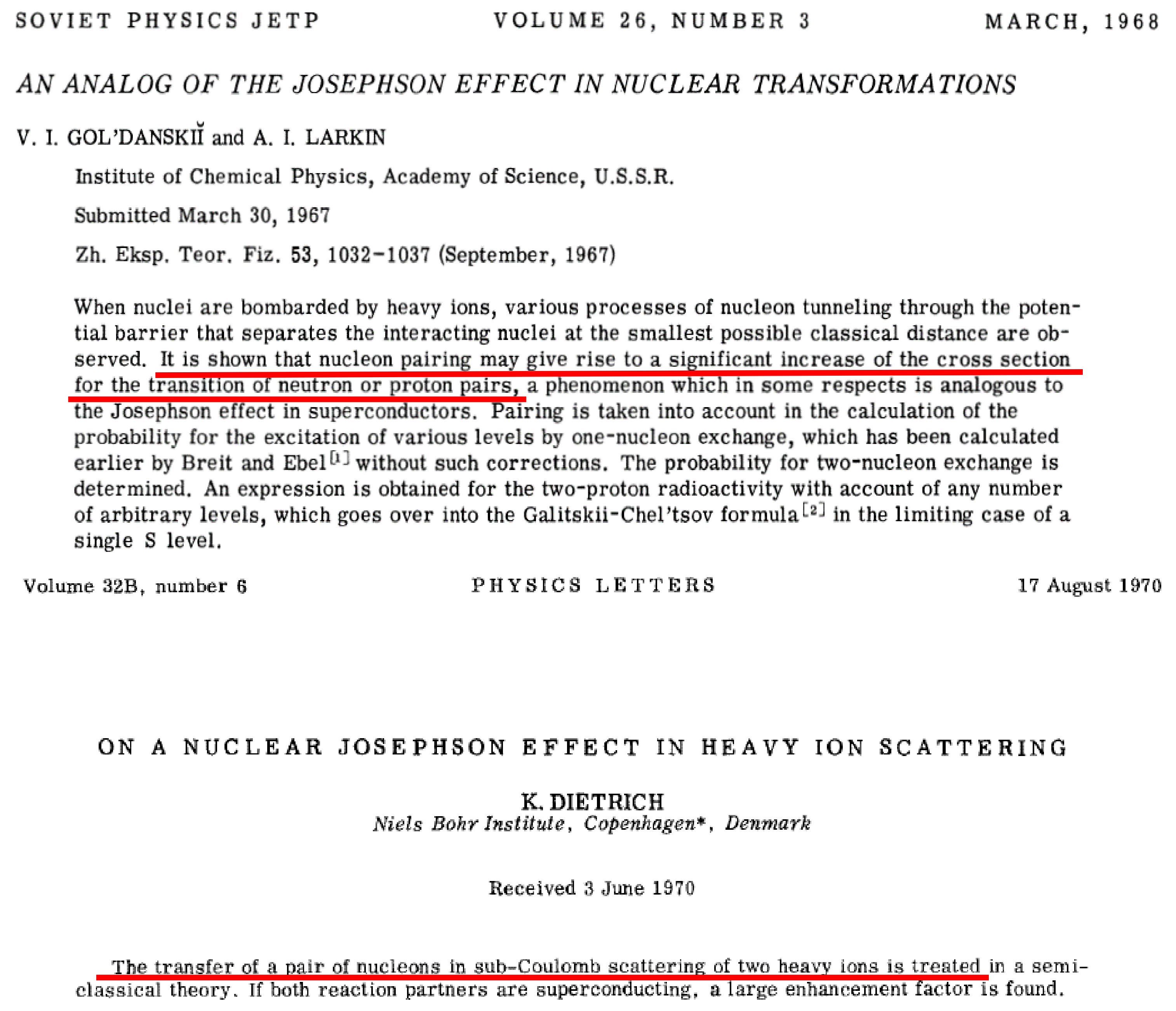
Received 8 June 1962

We here present an approach to the calculation of tunnelling currents between two metals that is sufficiently general to deal with the case when both metals are superconducting. In that case new effects are predicted, due to the possibility that electron pairs may tunnel through the barrier leaving the quasi-particle distribution unchanged.

Dynamics of the Josephson effect:

$$\boxed{\begin{gathered} J(t) = J_c \sin\left(\Delta\varphi(t)\right) \\ \frac{d\left(\Delta\varphi\right)}{dt} = \frac{2eU}{\hbar} \end{gathered}}$$

First applications to nuclear collisions:



SOVIET PHYSICS JETP VOLUME 26, NUMBER 3 MARCH, 1968

AN ANALOG OF THE JOSEPHSON EFFECT IN NUCLEAR TRANSFORMATIONS

V. I. GOL'DANSKIĬ and A. I. LARKIN

Institute of Chemical Physics, Academy of Science, U.S.S.R.

Submitted March 30, 1967

Zh. Eksp. Teor. Fiz. 53, 1032–1037 (September, 1967)

When nuclei are bombarded by heavy ions, various processes of nucleon tunneling through the potential barrier that separates the interacting nuclei at the smallest possible classical distance are observed. It is shown that nucleon pairing may give rise to a significant increase of the cross section for the transition of neutron or proton pairs, a phenomenon which in some respects is analogous to the Josephson effect in superconductors. Pairing is taken into account in the calculation of the probability for the excitation of various levels by one-nucleon exchange, which has been calculated earlier by Breit and Ebel[1] without such corrections. The probability for two-nucleon exchange is determined. An expression is obtained for the two-proton radioactivity with account of any number of arbitrary levels, which goes over into the Galitskii-Chel'tsov formula[2] in the limiting case of a single S level.

Volume 32B, number 6 PHYSICS LETTERS 17 August 1970

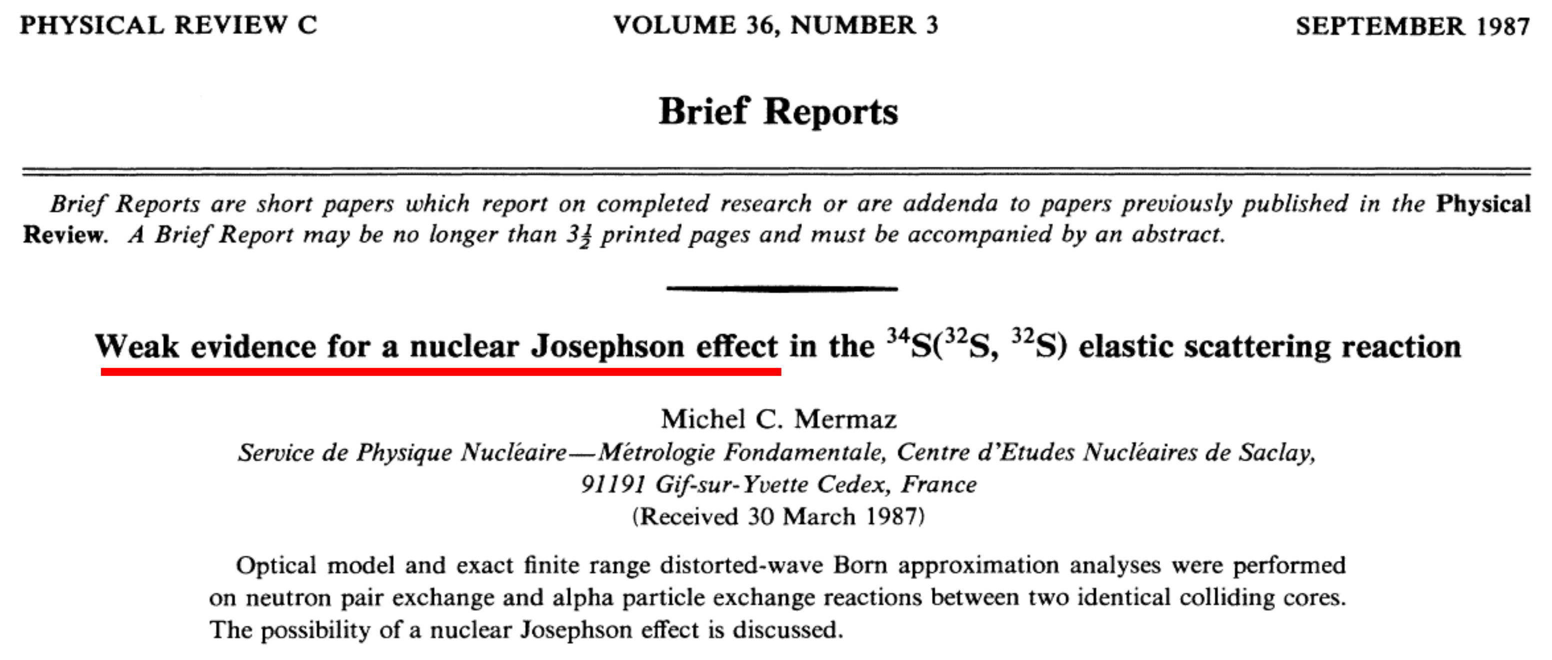
ON A NUCLEAR JOSEPHSON EFFECT IN HEAVY ION SCATTERING

K. DIETRICH
Niels Bohr Institute, Copenhagen, Denmark*

Received 3 June 1970

The transfer of a pair of nucleons in sub-Coulomb scattering of two heavy ions is treated in a semi-classical theory. If both reaction partners are superconducting, a large enhancement factor is found.

Some evidence for a nuclear Josephson effect has been gathered over the years:



PHYSICAL REVIEW C VOLUME 36, NUMBER 3 SEPTEMBER 1987

Brief Reports

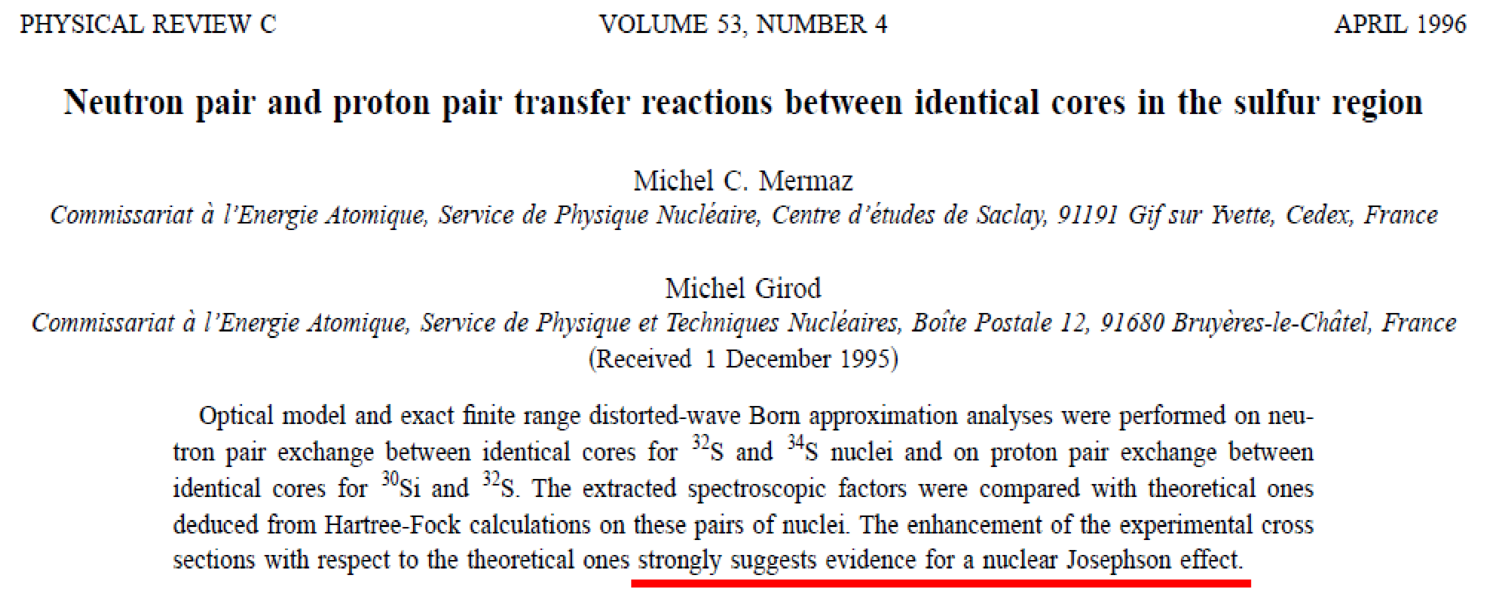
Brief Reports are short papers which report on completed research or are addenda to papers previously published in the **Physical Review**. *A Brief Report may be no longer than $3\frac{1}{2}$ printed pages and must be accompanied by an abstract.*

Weak evidence for a nuclear Josephson effect in the ^{34}S(^{32}S, ^{32}S) elastic scattering reaction

Michel C. Mermaz
Service de Physique Nucléaire—Métrologie Fondamentale, Centre d'Etudes Nucléaires de Saclay,
91191 Gif-sur-Yvette Cedex, France

(Received 30 March 1987)

Optical model and exact finite range distorted-wave Born approximation analyses were performed on neutron pair exchange and alpha particle exchange reactions between two identical colliding cores. The possibility of a nuclear Josephson effect is discussed.



PHYSICAL REVIEW C VOLUME 53, NUMBER 4 APRIL 1996

Neutron pair and proton pair transfer reactions between identical cores in the sulfur region

Michel C. Mermaz
Commissariat à l'Energie Atomique, Service de Physique Nucléaire, Centre d'études de Saclay, 91191 Gif sur Yvette, Cedex, France

Michel Girod
Commissariat à l'Energie Atomique, Service de Physique et Techniques Nucléaires, Boîte Postale 12, 91680 Bruyères-le-Châtel, France

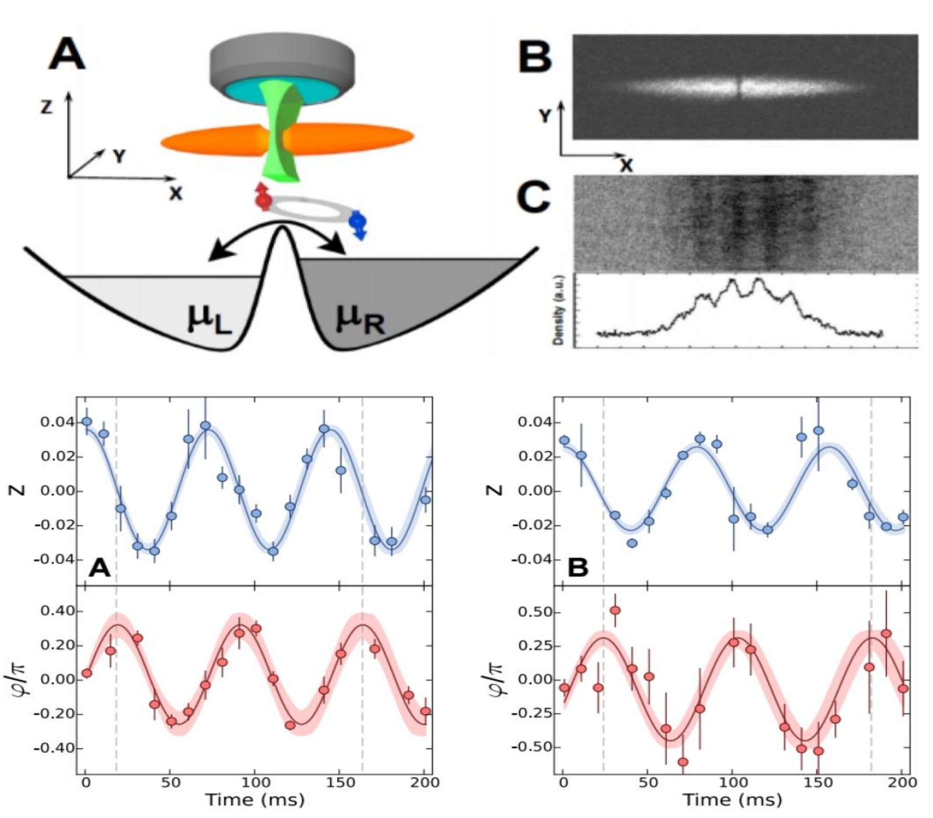
(Received 1 December 1995)

Optical model and exact finite range distorted-wave Born approximation analyses were performed on neutron pair exchange between identical cores for ^{32}S and ^{34}S nuclei and on proton pair exchange between identical cores for ^{30}Si and ^{32}S. The extracted spectroscopic factors were compared with theoretical ones deduced from Hartree-Fock calculations on these pairs of nuclei. The enhancement of the experimental cross sections with respect to the theoretical ones strongly suggests evidence for a nuclear Josephson effect.

Ultracold atomic gases: two regimes for realization of the Josephson junction

Weak coupling (weak link)

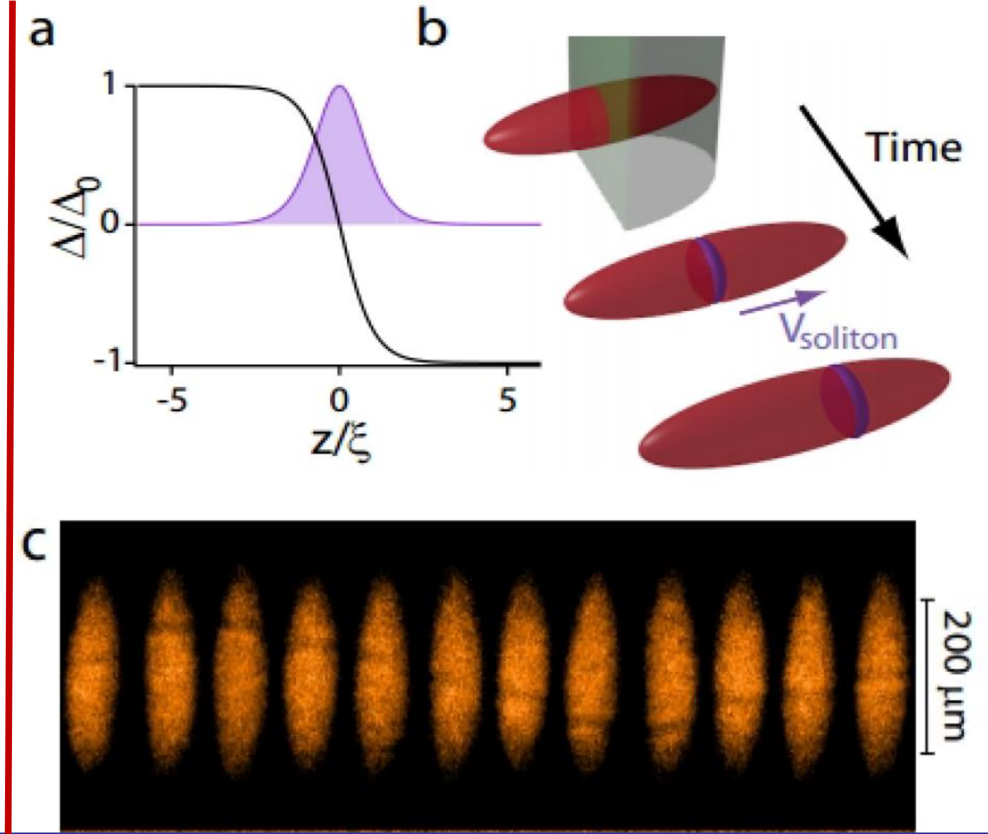
Strong coupling



Observation of ***AC Josephson effect*** between two 6Li atomic clouds.

It need not to be accompanied by creation of a topological excitation.

G. Valtolina et al., Science 350, 1505 (2015).



Creation of a „heavy soliton" after merging two superfluid atomic clouds.

T. Yefsah et al., Nature 499, 426 (2013).

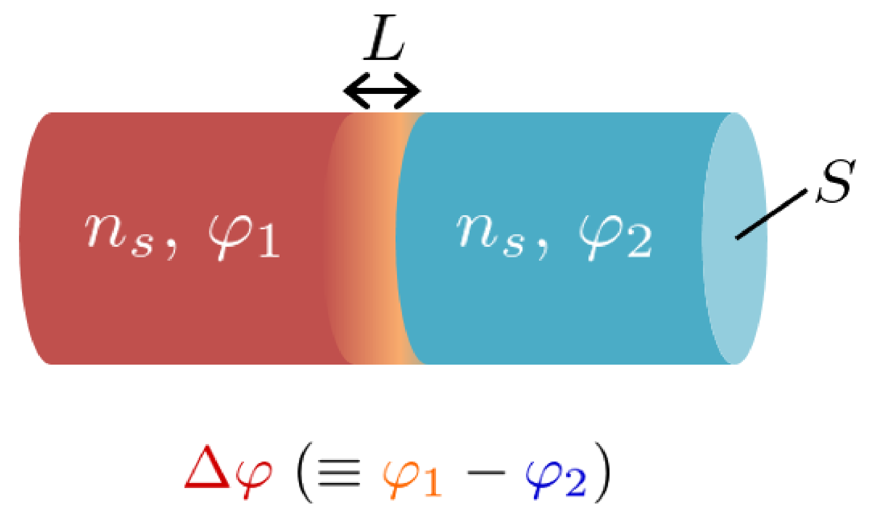
End of digression

Estimates for the magnitude of the effect

At first one may think that the magnitude of the effect is determined by the nuclear pairing energy which is of the order of MeV's in atomic nuclei (according to the expression):

$$\frac{1}{2}g(\varepsilon_F)|\Delta|^2; \quad g(\varepsilon_F) \text{ - density of states}$$

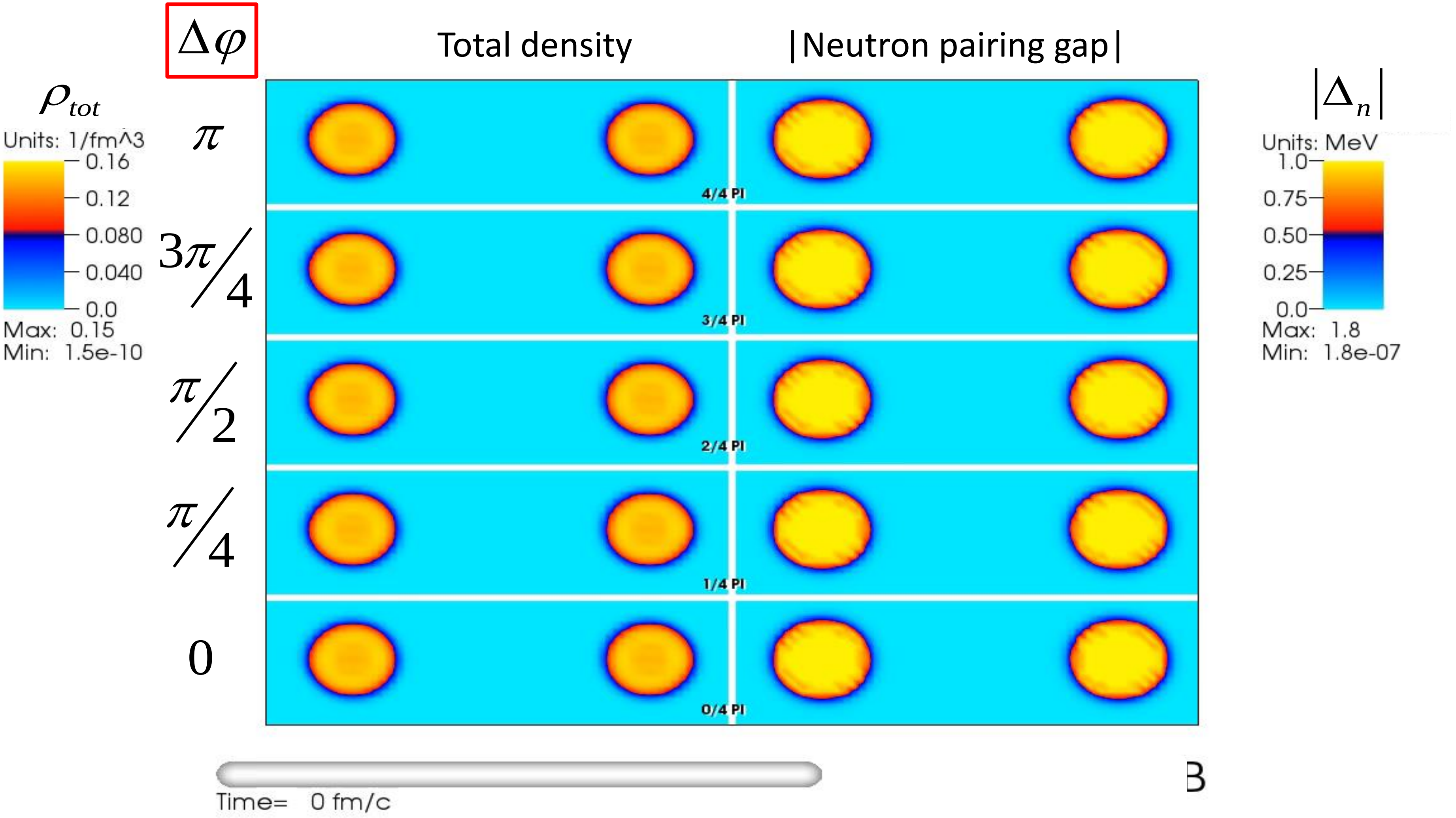
On the other hand the energy stored in the junction can be estimated from Ginzburg-Landau (G-L) approach:



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

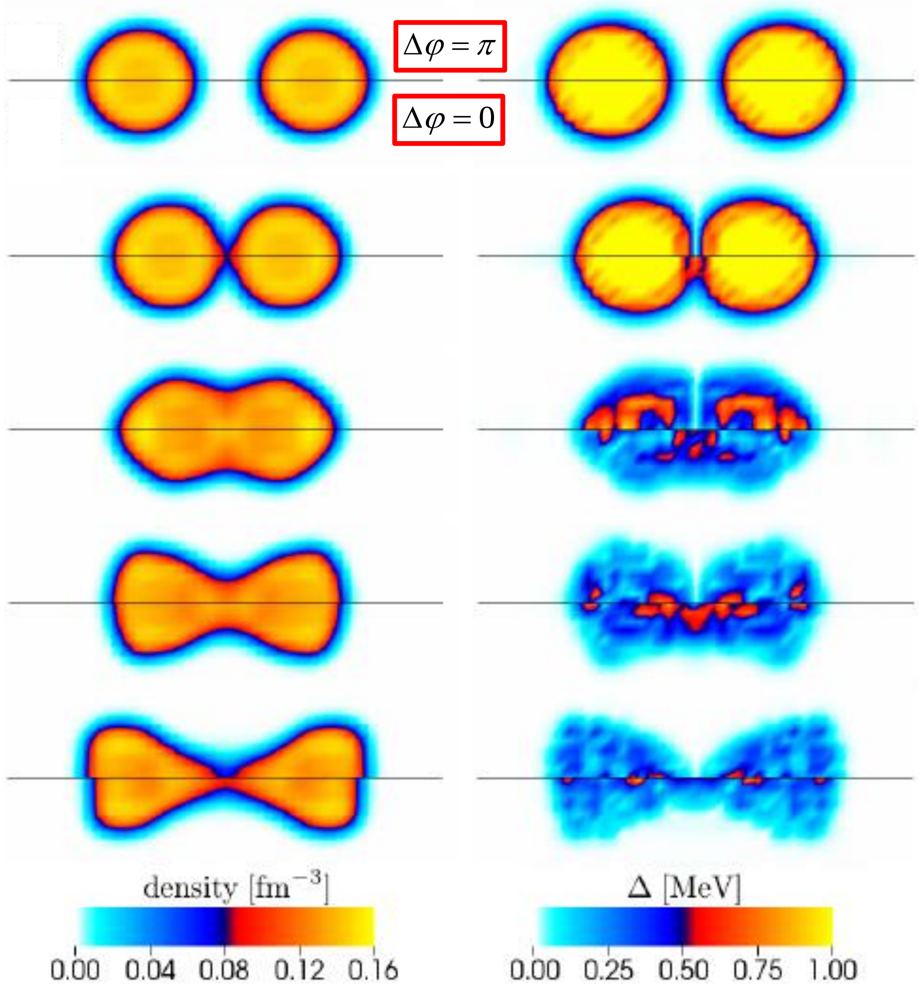
For typical values characteristic for two heavy nuclei: $E_j \approx 30 MeV$

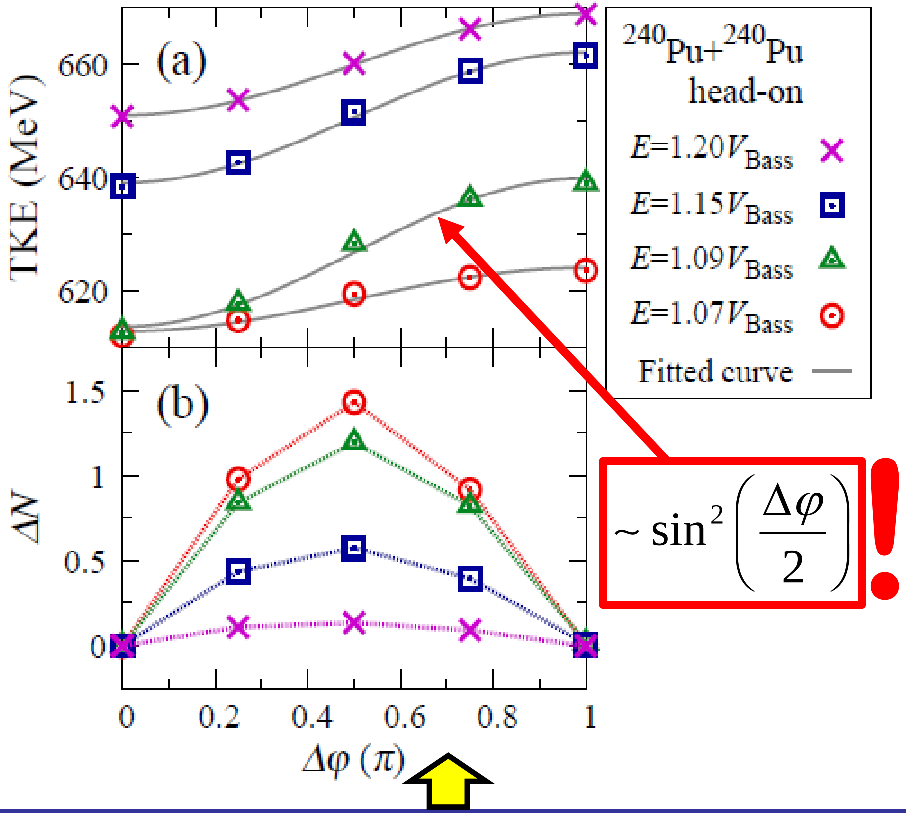
$^{240}Pu + ^{240}Pu$ at energy $E \simeq 1.1 V_{Bass}$



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

Total kinetic energy of the fragments (TKE)





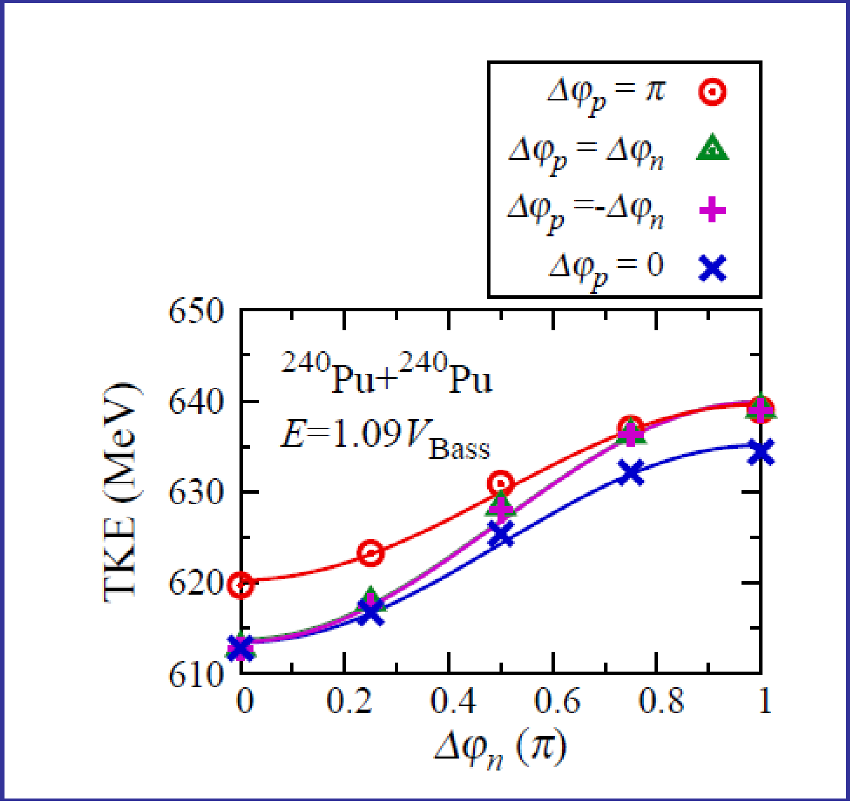
$$\sim \sin^2\left(\frac{\Delta\varphi}{2}\right)$$!

Average particle transfer between fragments.

Creation of the solitonic structure between colliding nuclei prevents energy transfer to internal degrees of freedom and consequently enhances the kinetic energy of outgoing fragments.
Surprisingly, the gauge angle dependence from the G-L approach is perfectly well reproduced in the kinetic energies of outgoing fragments!

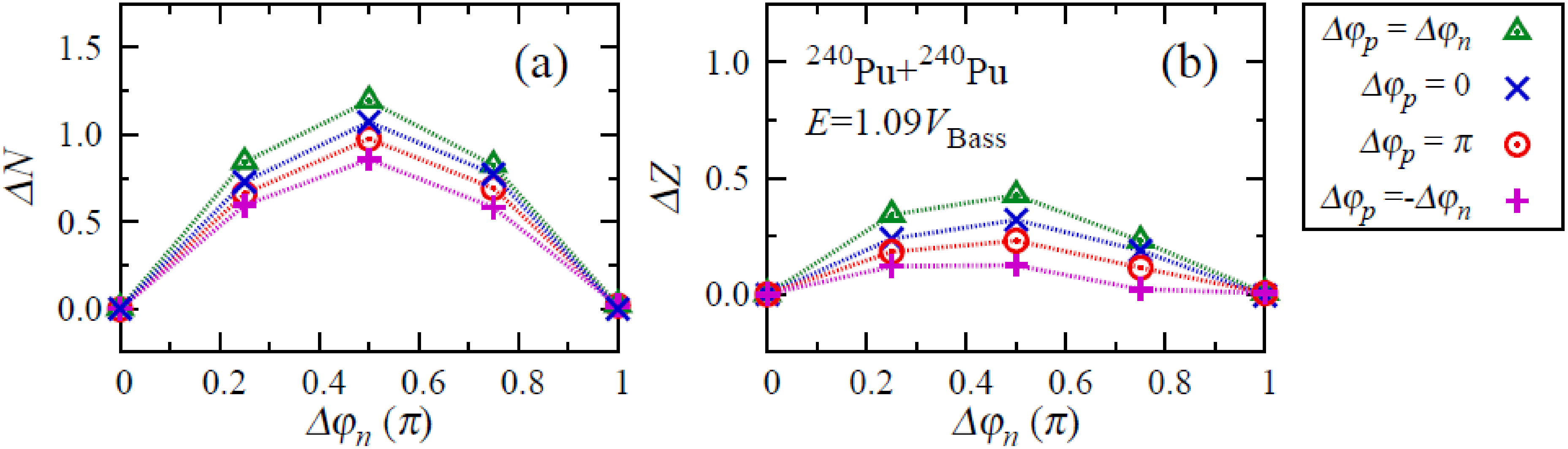
Proton pairing gap contribution to TKE

The effect is predominantly due to neutron pairing.

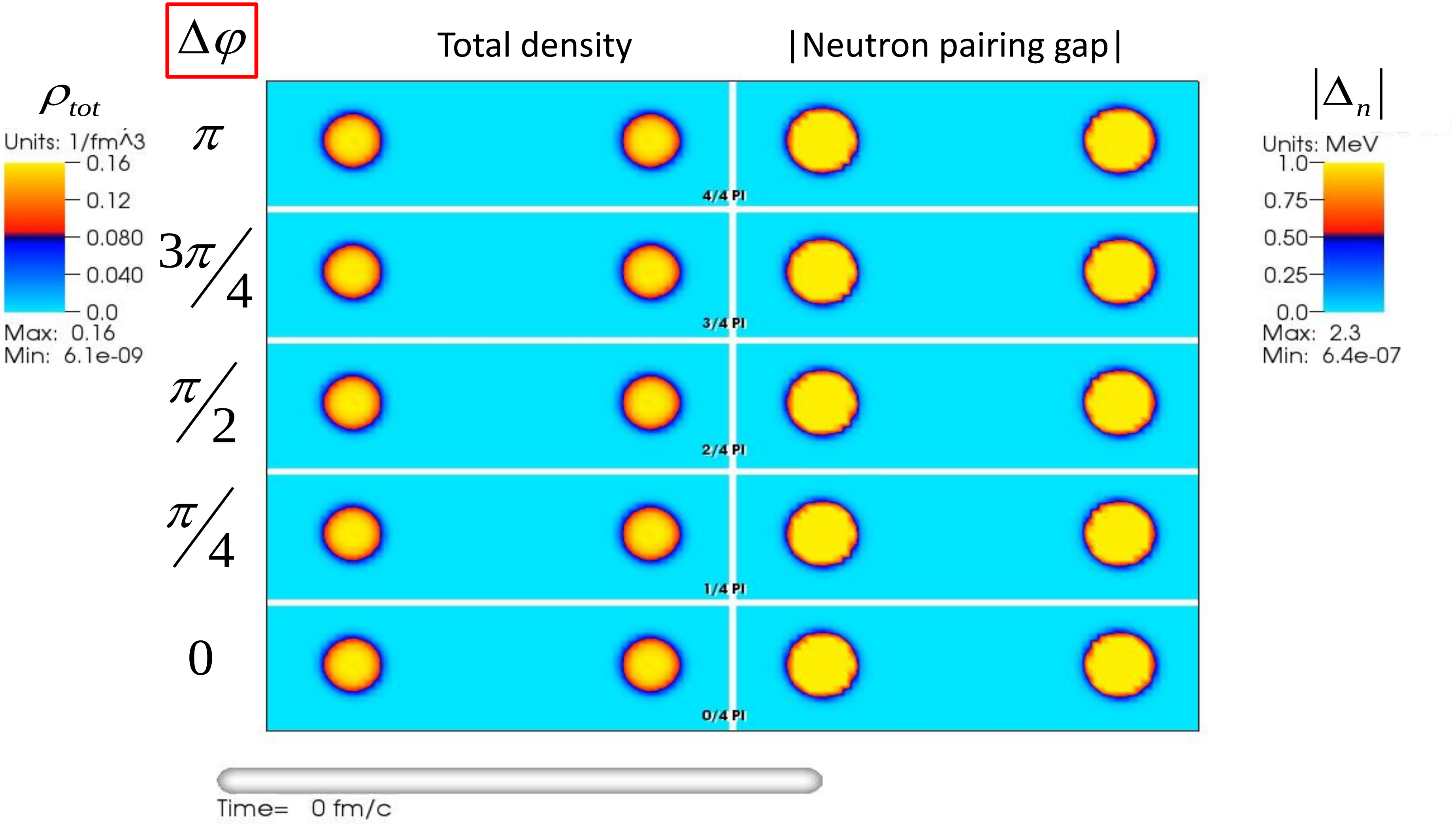


Neutron transfer

Proton transfer



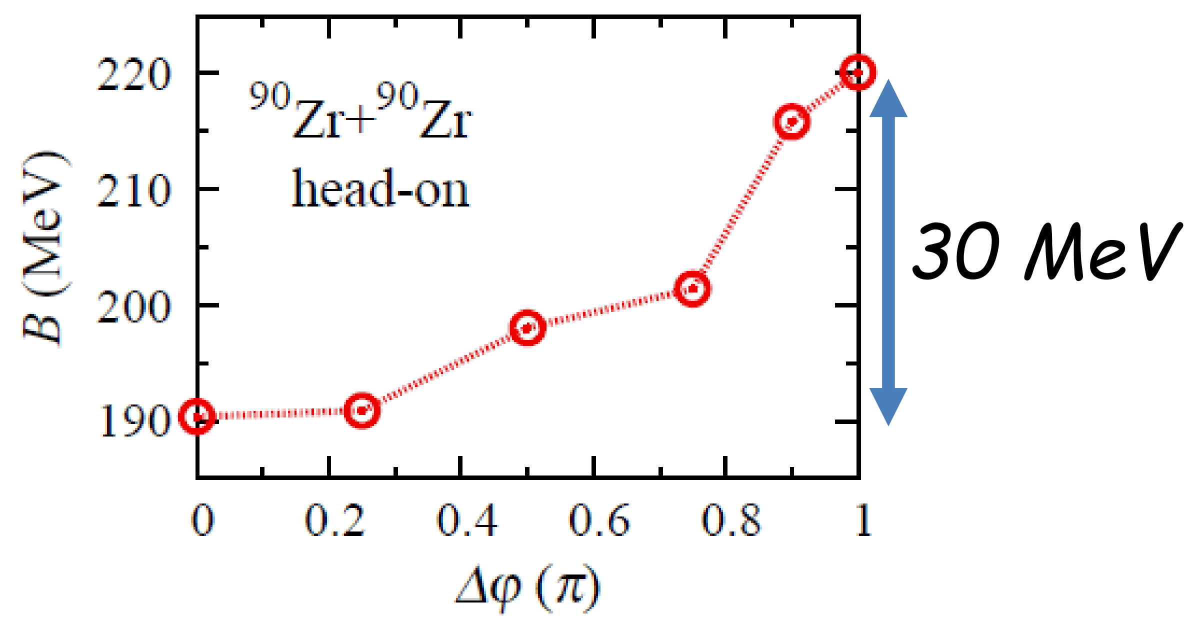
$^{90}Zr + {}^{90}\mathrm{Zr}$ at energy $E \simeq V_{Bass}$



Modification of the capture cross section!

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

Effective barrier height for fusion as a function of the phase difference



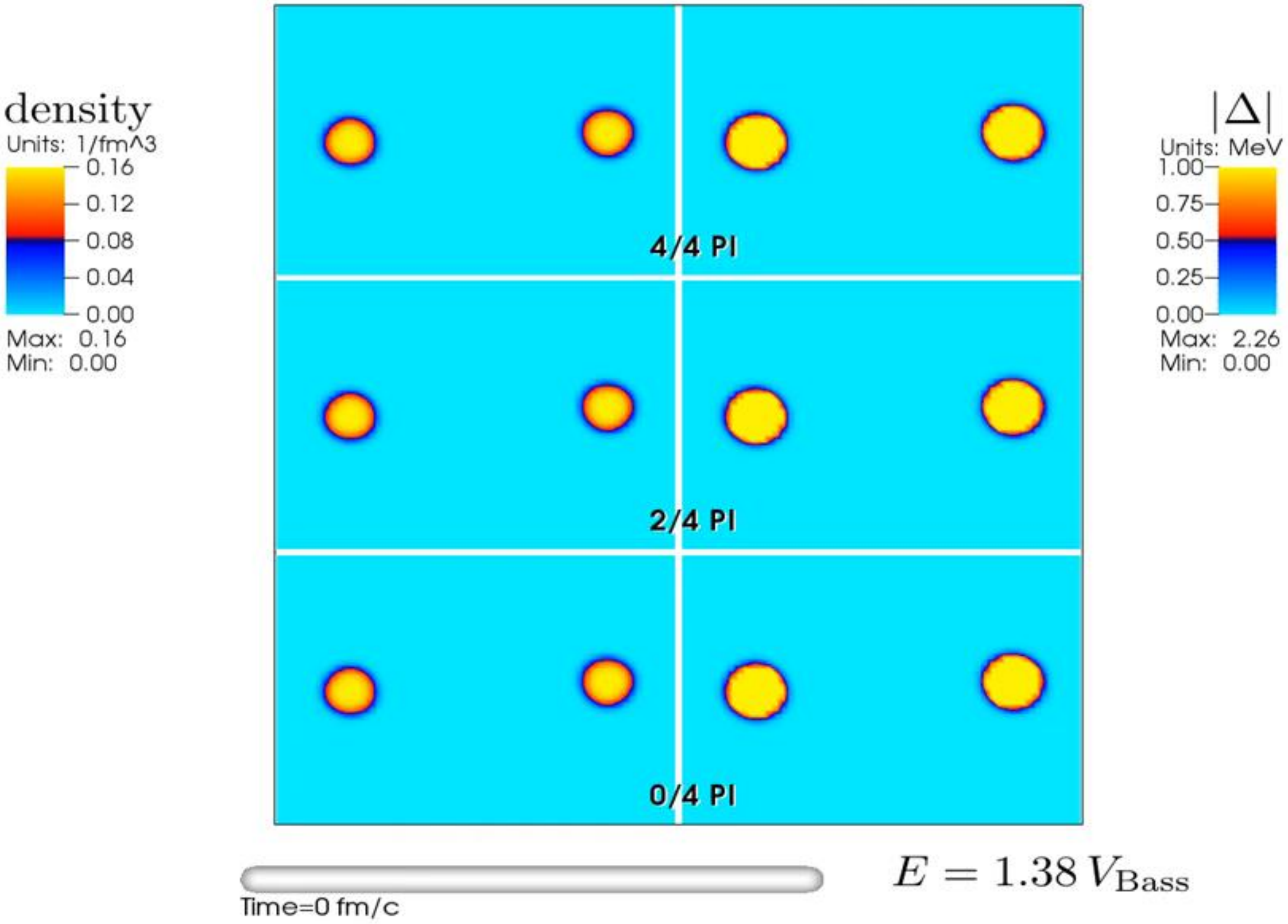
What is an average extra energy needed for the capture?

$$\boxed{E_{extra} = \frac{1}{\pi}\int_0^\pi \left(B(\Delta\varphi) - V_{Bass}\right) d(\Delta\varphi) \approx 10MeV}$$

How the angle dependence affects the shape of the excitation function?

$$\boxed{\frac{d}{dE}\left(E\sigma(E)\right) \propto \Delta\varphi_{tr} + \ldots}$$

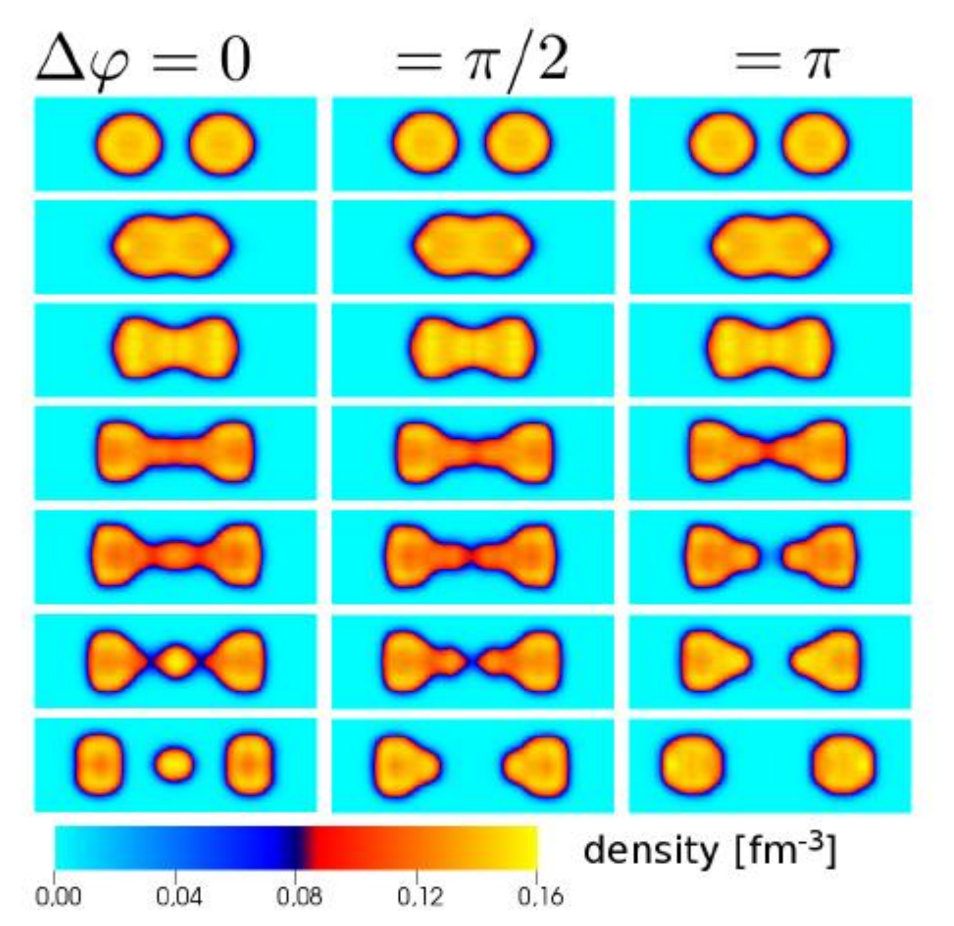
Noncentral collisions: ${}^{90}Zr + {}^{90}Zr$



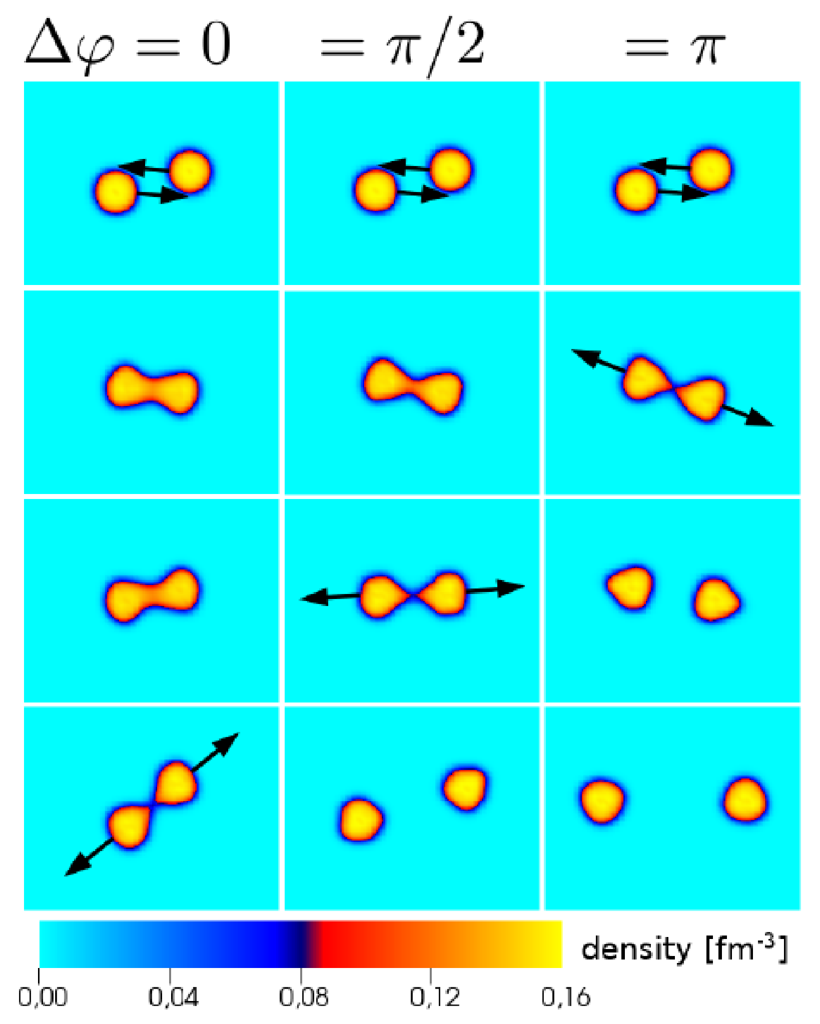
$E = 1.38\, V_{\mathrm{Bass}}$

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

Noncentral collisions



At higher energies (1.3-1.5 of the barrier height) the phase difference modifies the reaction outcomes suppressing the reaction channel leading to 3 fragments.



For noncentral collisions the trajectories of outgoing nuclei are affected due to the shorter contact time for larger phase differences.

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

Summarizing

Pairing field dynamics play an important role in nuclear dynamics including both induced fission (see Aurel's talk) and collisions.

Clearly the aforementioned effects CANNOT be grasped by any version of simplified (and commonly used) TDHF+BCS approach.

The phase difference of the pairing fields of colliding medium or heavy nuclei produces a similar solitonic structure as the system of two merging atomic clouds.

The energy stored in the created junction is subsequently released giving rise to an increased kinetic energy of the fragments and modifying their trajectories. The effect is found to be of the order of 30MeV for heavy nuclei and occur for energies up to 20-30% of the barrier height.

Consequently the effective barrier for the capture of medium nuclei is enhanced by about 10MeV.

Josephson current is weak and DOES NOT contribute noticeably to collision dynamics (consistent with other studies).

Open question

Time dependent DFT describes nuclear collision in the broken symmetry framework.

What is the effect of the particle nonconservation ?

Whether the broken symmetry framework provides a reasonable description depends on the time scale associated with the related Goldstone mode.

Here, the time scale is related to the inverse of the neutron separation energy. However, since both pairing fields rotate in gauge space it is rather the difference of the separation energy which matters (this can be made arbitrarily long in the case of symmetric collisions)

Summarizing

- TDDFT extended to superfluid systems and based on the local densities offers a flexible tool to study quantum superfluids far from equilibrium.
- TDDFT offers an unprecedented opportunity to test the nuclear energy density functional for large amplitude collective motion, non-equilibrium phenomena, and in new regions of the collective degrees of freedom.

- **Interesting research topics:**

- Ultracold atoms: investigation of quantum turbulence in Fermi systems; topological excitations in spin-polarized atomic gases in the presence of LOFF phase (see Gabriel's talk).
- Neutron star: Provide a link between large scale models of neutron stars and microscopic studies; towards the first simulation of the glitch phenomenon based on microscopic input.
- Nuclear physics: induced fission and fusion processes based directly on Energy Density Functional (see also Aurel's talk); search for new effects related to pairing dynamics in nuclear processes.