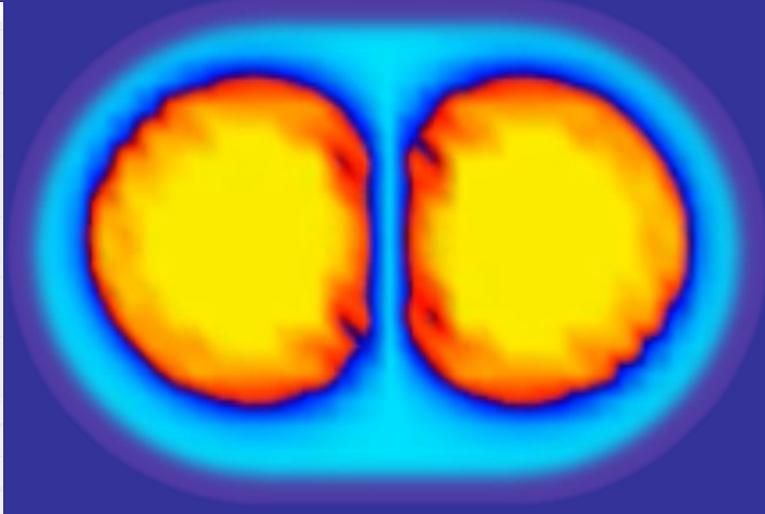
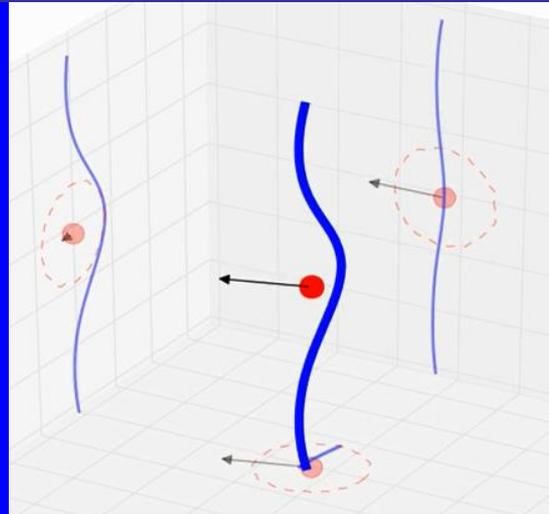
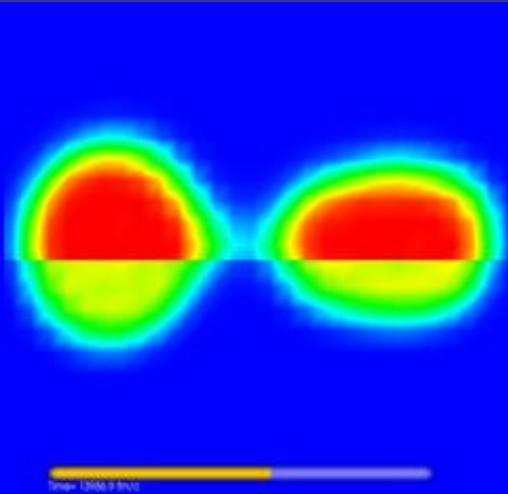


Pairing dynamics in low energy nuclear reactions.



Piotr Magierski

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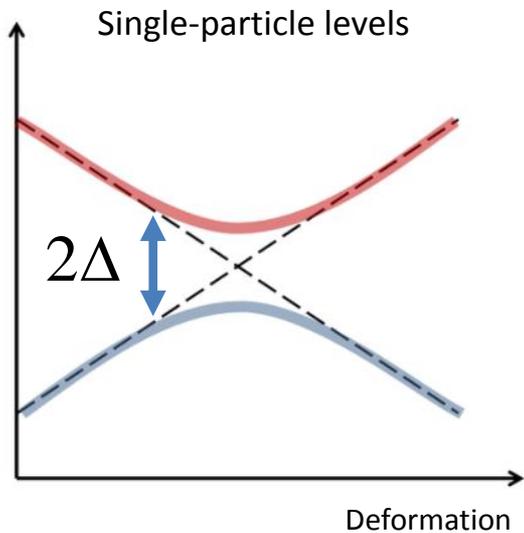
Michael M. Forbes (Washington State U.)

Kenneth J. Roche (PNNL)

Ionel Stetcu (LANL)

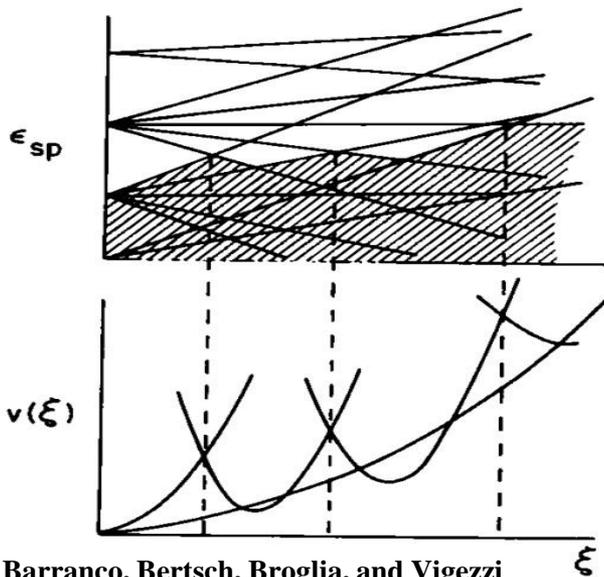
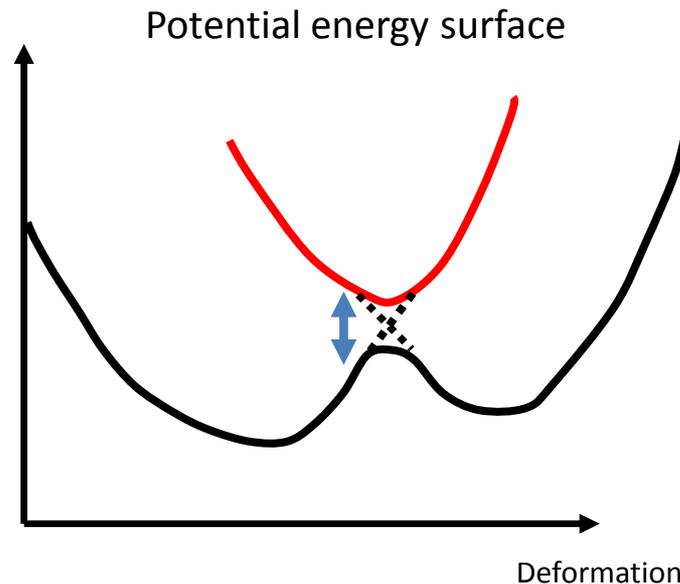
Shi Jin (Univ. of Washington, Ph.D. student)

Pairing as an energy gap



Quasiparticle energy:

$$E_{qp} = \sqrt{(\varepsilon - \mu)^2 + |\Delta|^2}$$



As a consequence of pairing correlations large amplitude nuclear motion becomes more adiabatic.

While a nucleus elongates its Fermi surface becomes oblate and its sphericity must be restored
 Hill and Wheeler, PRC, 89, 1102 (1953)
 Bertsch, PLB, 95, 157 (1980)

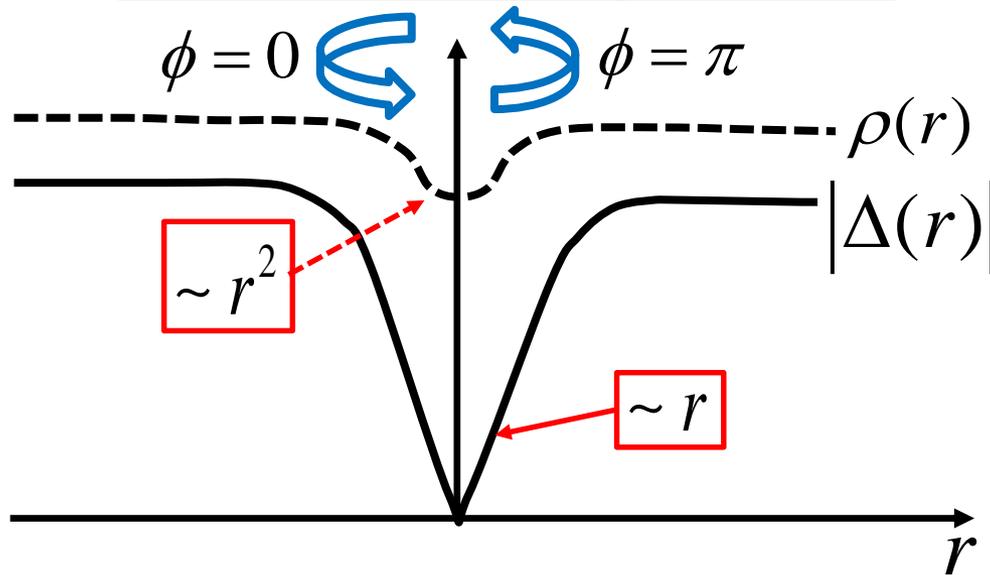
Pairing as a field

$$\Delta(\vec{r}, t) = |\Delta(\vec{r}, t)| e^{i\phi(\vec{r}, t)}$$

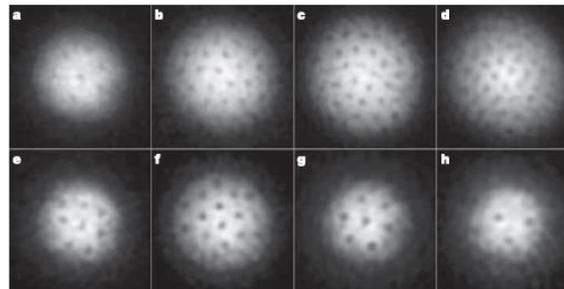
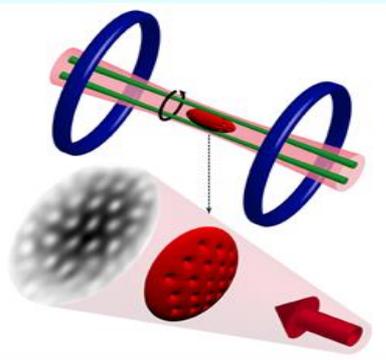
Both magnitude and phase may have a nontrivial spatial and time dependence.

Example of a nontrivial spatial dependence: *quantum vortex*

Vortex structure – section through the vortex core



Example of a topological excitation: magnitude of the pairing gap vanishes in the vortex core.



Experiments with ultracold Li6 atoms: pictures of the vortex lattice.

Figure 2 | Vortices in a strongly interacting gas of fermionic atoms on the BEC- and the BCS-side of the Feshbach resonance. At the given field, the cloud of lithium atoms was stirred for 300 ms (a) or 500 ms (b–h) followed by an equilibration time of 500 ms. After 2 ms of ballistic expansion, the

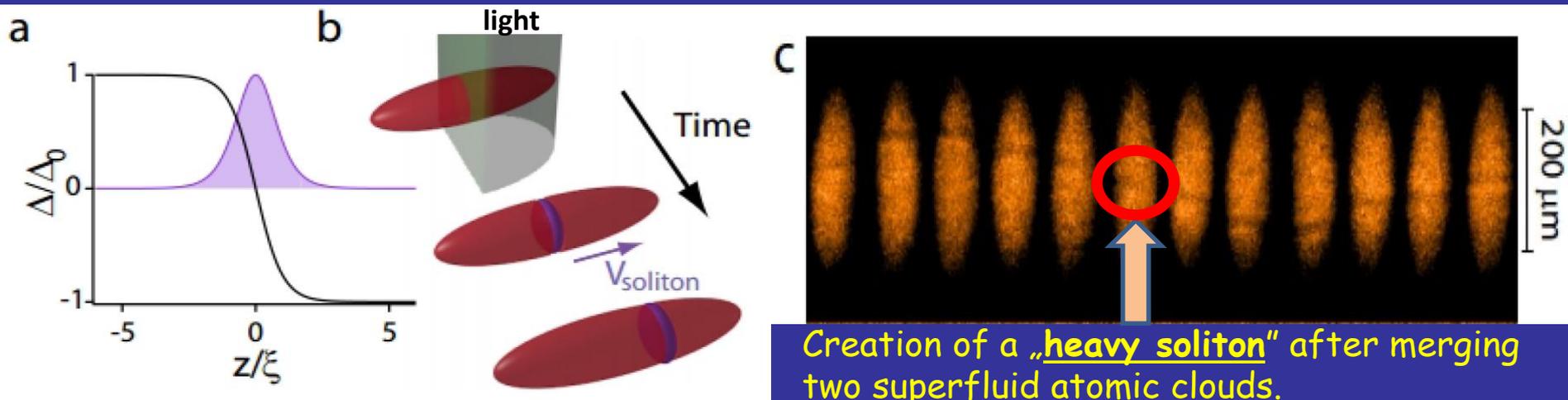
magnetic field was ramped to 735 G for imaging (see text for details). The magnetic fields were 740 G (a), 766 G (b), 792 G (c), 812 G (d), 833 G (e), 843 G (f), 853 G (g) and 863 G (h). The field of view of each image is $880 \mu\text{m} \times 880 \mu\text{m}$.

M.W. Zwierlein *et al.*,
Nature, 435, 1047 (2005)

Nuclear collisions

Collisions of superfluid nuclei having different phases of the pairing fields

Inspired by experiments on ultracold atomic gases: merging two atomic clouds.



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

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

M.J.H. Ku et al. Phys. Rev. Lett. 116, 045304 (2016)

Sequence of topological excitations reproduced in TDDFT: Wlazłowski, Sekizawa, Marchwiany, Magierski, arXiv:1711.05803

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.?

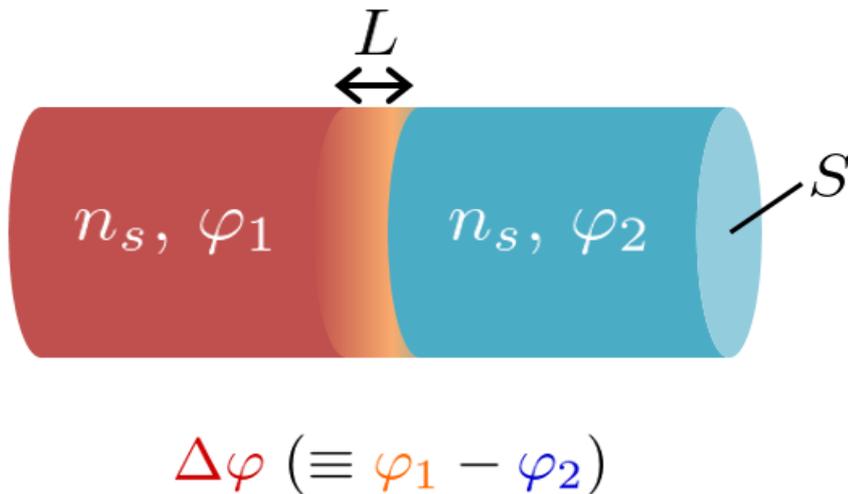
Clearly, we cannot control phases of the pairing field in nuclear experiments and the possible signal need to be extracted after averaging over the phase difference.

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):

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

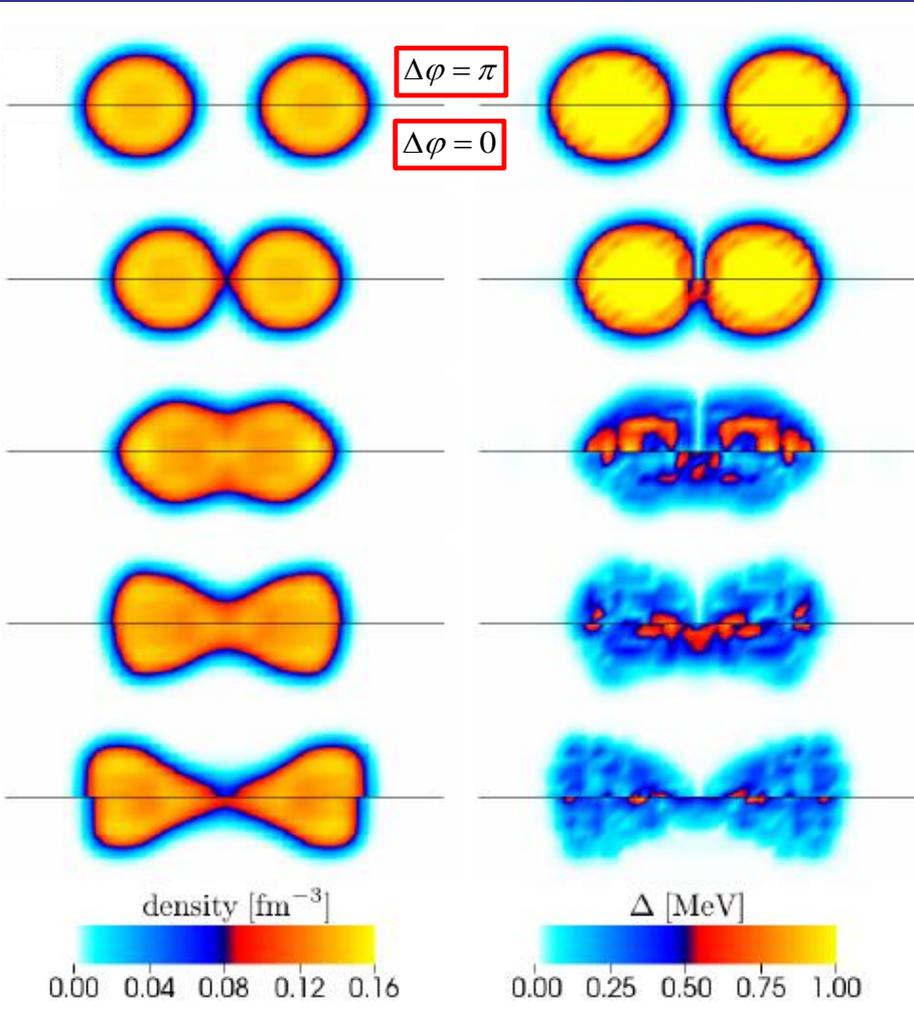
On the other hand the energy stored in the junction can be estimated from Ginzburg-Landau (G-L) approach:



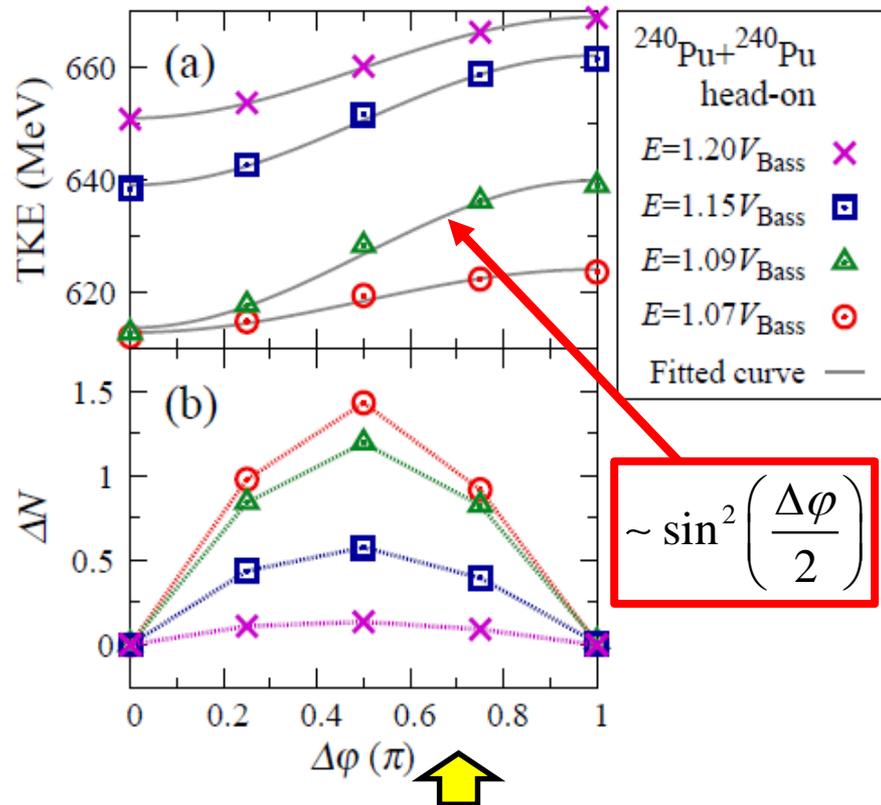
$$E_j = \frac{S \hbar^2}{L 2m} n_s \sin^2 \frac{\Delta\varphi}{2}$$

For typical values characteristic for two heavy nuclei:

$$E_j \approx 30 \text{ MeV}$$



Total kinetic energy of the fragments (TKE)



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.

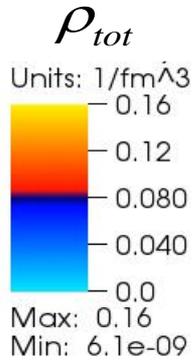
Surprisingly, the gauge angle dependence from the G-L approach is perfectly well reproduced in the kinetic energies of outgoing fragments!

$^{90}\text{Zr} + ^{90}\text{Zr}$ at energy $E \approx V_{\text{Bass}}$

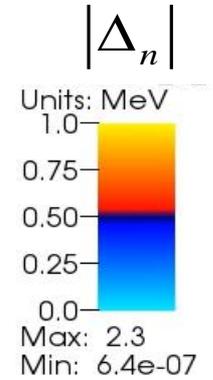
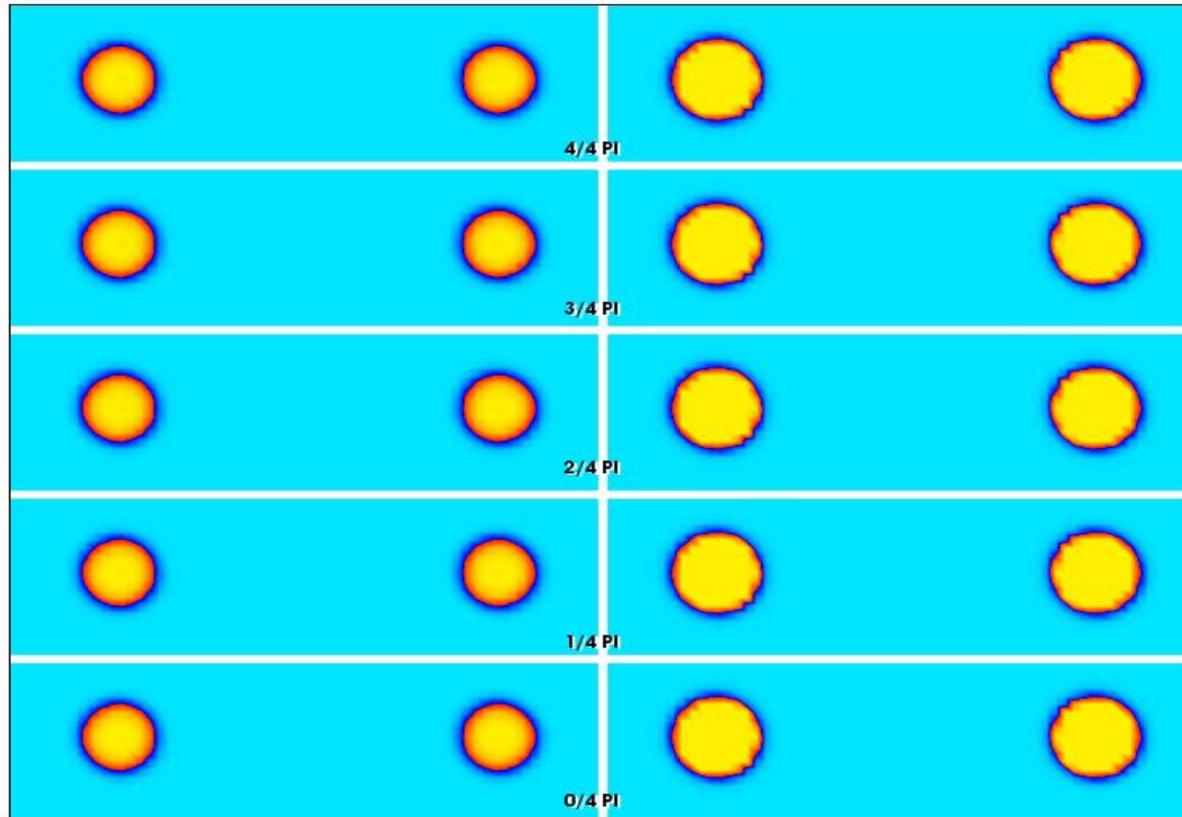
$\Delta\varphi$

Total density

|Neutron pairing gap|



π
 $3\pi/4$
 $\pi/2$
 $\pi/4$
0

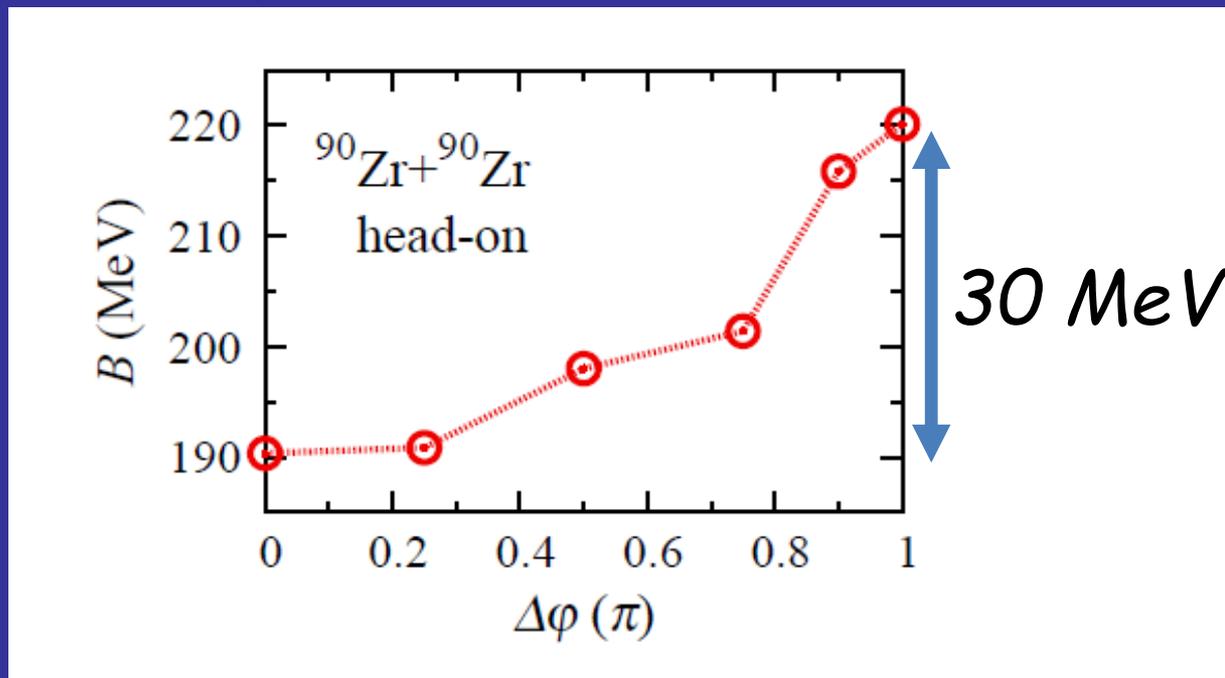


Time= 0 fm/c

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?

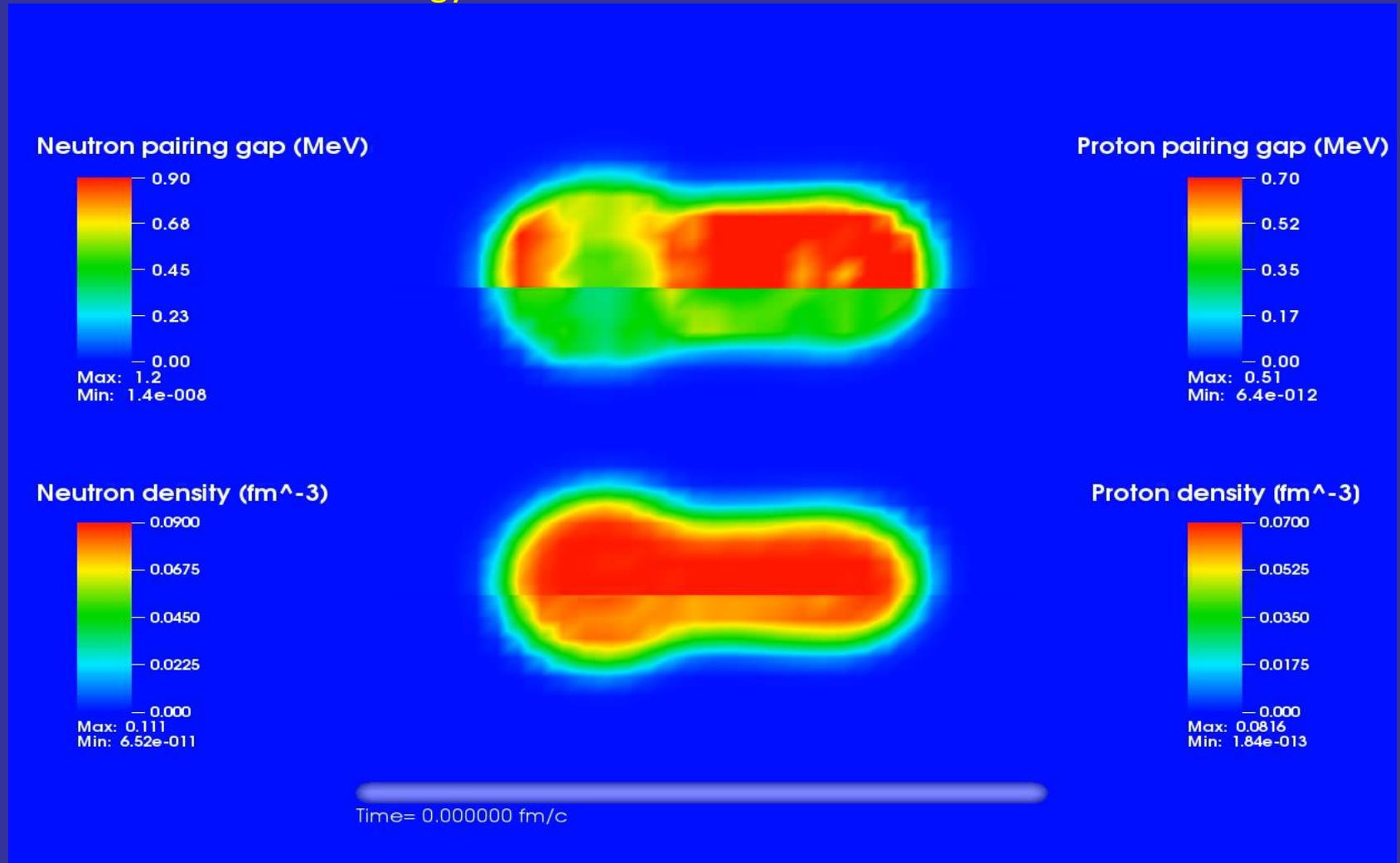
$$E_{extra} = \frac{1}{\pi} \int_0^{\pi} (B(\Delta\phi) - V_{Bass}) d(\Delta\phi) \approx 10 \text{ MeV}$$

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.

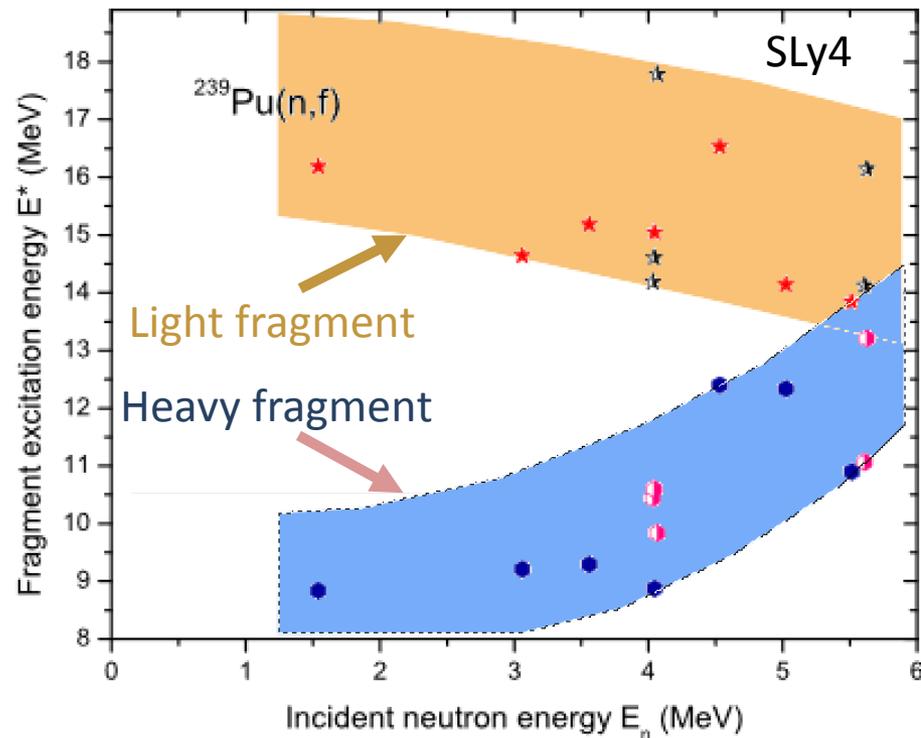
The energy stored in the created junction is subsequently released giving rise to an increased kinetic energy of the fragments. The effect is found to be of the order of 30 MeV for heavy nuclei and occur for energies up to 20-30% of the barrier height.

Fission dynamics of ^{240}Pu

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



Induced fission of ^{240}Pu



The lighter fragment is more excited (and strongly deformed) than the heavier one.

Energies are not shared proportionally to mass numbers of the fragments!

E^* (MeV)	E_n (MeV)	TKE_{TDSLDA} (MeV)	TKE_{syst} (MeV)	err (%)	Z_L	N_L
8.08	1.542	173.81	177.26	1.95	40.825	62.246
9.60	3.063	174.73	176.73	1.13	40.500	61.536
10.10	3.560	179.09	176.56	1.43	41.625	62.783
10.57	4.032	173.67	176.39	1.55	40.092	61.256
10.58	4.043	173.39	176.39	1.70	40.146	61.388
10.58	4.047	175.11	176.39	0.72	40.313	61.475
10.60	4.065	174.75	176.38	0.92	40.904	62.611
11.07	4.534	176.46	176.22	0.14	41.495	63.134
11.56	5.024	175.15	176.05	0.51	40.565	61.894
12.05	5.515	176.75	175.88	0.49	40.412	61.809
12.15	5.610	176.36	175.84	0.29	40.355	61.695
12.16	5.626	176.10	175.84	0.15	41.386	62.764

$$TKE = 177.80 - 0.3489E_n \quad [\text{in MeV}],$$

Nuclear data evaluation, Madland (2006)

Calculated TKEs slightly reproduce experimental data with accuracy < 2%

J. Grineviciute, et al. (in preparation)

see also:

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

Summarizing

Pairing field dynamics play an important role in nuclear dynamics including both induced fission 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).

TDDFT equations with local pairing field (TDSLDA):

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

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.

$N_x N_y N_z$	Number of HFB equations	CPU implementation		GPU implementation		SPEEDUP
		# of CPUs	time per step	# of GPUs	time per step	
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

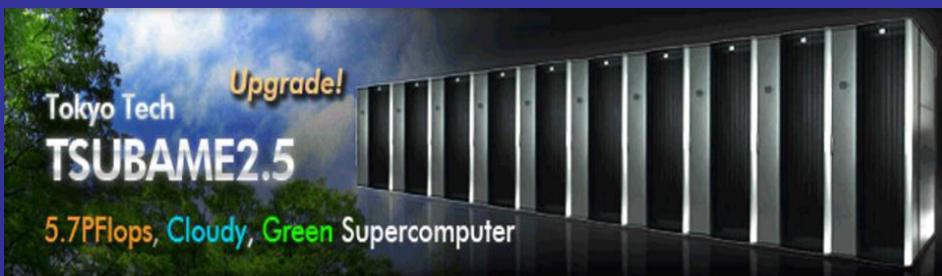
Within current computational capabilities TDDFT allows to describe real time dynamics of strongly interacting, superfluid systems of hundred of thousands fermions.

Selected supercomputers (CPU+GPU) currently in use:



Piz Daint: 25.3 PFlops
(Swiss National Supercomputing Centre)

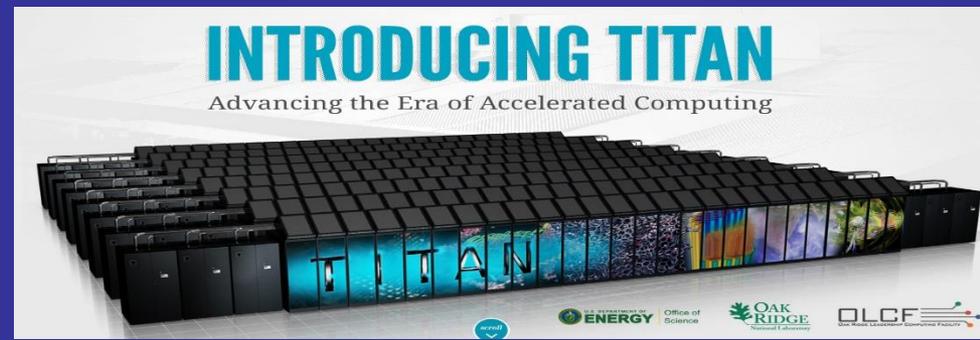
HA-PACS: 0.802 PFlops
(University of Tsukuba)



Tsubame: 5.7 Pflops
Upgraded recently to Tsubame3.0: 12.2 PFlops
(Tokyo Institute of Technology)

TSUBAME

Titan: 27 PFlops
(ORNL Oak Ridge)



Collaborators:



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WUT -> Niigata Univ.



Aurel Bulgac
(U. Washington)



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