

Solitonic excitations in nuclear reactions and their counterparts in ultracold Fermi gases

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https://www.youtube.com/watch?v=k5bNybqvRRc

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The results (may) depend on:

1) Energy Density Functional (we use Skyrme type functional)



- DFT is in principle exact theory Hohenberg-Kohn theorem (1964) implies that
- ... solving Schrödinger equation \leftrightarrow minimization of the energy density $E[\rho]$...
- ... however no mathematical recipe how to construct $\mathbf{E}[\rho]$.
- In practice we postulate the functional form!

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2) Broken symmetries: superfluidity/superconductivity \rightarrow

particle number symmetry is broken

Density-Functional Theory for Superconductors

L. N. Oliveira, E. K. U. Gross, and W. Kohn Phys. Rev. Lett. **60**, 2430 – Published 6 June 1988

- DFT has been extended to superfluid/superconducting systems...
- ... energy density functional $E[\rho,\nu]$...
- ... where ν is anomalous density \leftrightarrow order parameter

(quantity well defined in thermodynamic limit)

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3) Adiabatic approximation:
$$H\varphi_n = E_n\varphi_n \rightarrow i\hbar \frac{\partial \varphi_n}{\partial t} = H\varphi_n$$

Density-Functional Theory for Time-Dependent Systems

Erich Runge and E. K. U. Gross Phys. Rev. Lett. **52**, 997 – Published 19 March 1984

Time-Dependent Density-Functional Theory for Superconductors

O. -J. Wacker, R. Kümmel, and E. K. U. Gross Phys. Rev. Lett. **73**, 2915 – Published 21 November 1994

• For time-dependent case the "exact" functional is in general different from the one that is used in static calculations...

https://www.youtube.com/watch?v=k5bNybqvRRc

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- For time-dependent case the "exact" functional is in general different from the one that is used in static calculations...
- ... but if the evolution is slow (adiabatic), the system follows instantaneous ground state \rightarrow use the functional taken from static considerations.

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- Uncertainty quantification needed...
 - ... presently no well defined methodology how to do it in case of timedependent phenomena.
- Experiments provide info only about final states, no detailed info about time-evolution.

Fig. From: J. D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz, Phys. Rev. Lett. 114, 122501 (2015)



The real-time dynamics is given by equations, which are formally equivalent to the Time-Dependent HFB (TDHFB) or Time-Dependent Bogolubov-de Gennes (TDBdG) equations

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

where h and Δ depends on "densities" (their explicit form depends on the functional):

$$\rho_{\sigma}(\boldsymbol{r},t) = \sum_{E_n < E_c} |v_{n,\sigma}(\boldsymbol{r},t)|^2, \qquad v(\boldsymbol{r},t) = \sum_{E_n < E_c} u_{n,\uparrow}(\boldsymbol{r},t) v_{n,\downarrow}^*(\boldsymbol{r},t), \quad \text{etc.}$$

- Mathematically: large set of nonlinear coupled 3D PDEs; Number of PDEs is of the order of the number of spatial lattice points, typically 10⁵-10⁶.
- We use coordinate space solvers (system is placed on a 3D spatial lattice of size N_x×N_y×N_z)
- Codes are publicly accessible: *Nuclear* → The LISE Package: Comput. Phys. Commun. 269, 108130 (2021). *Cold atoms* → W-SLDA Toolkit, https://wslda.fizyka.pw.edu.pl



- Ultracold atomic systems offer alternative possibility to test predictive power of TDDFT.
- The (bare) interaction is simple $V(r-r')=g\delta(r-r')...$
- ... but the interaction strength g can be tuned at will!







Modeling nuclear vs ultracold systems

1) Energy Density Functional

The energy functional for cold atoms is much simpler than for nuclear cases (no gradient terms, no spin-orbit, ...) [We use SLDA functional, originally derived by A. Bulgac, Phys. Rev. A 76, 040502(R)]

2) Broken symmetries: superfluidity/superconductivity

→ can be easily justified since number of atoms in the cloud is 10^5 - 10^6

... but systems with "small" number of atoms are also accessible





Remark: transition from few-body to many-physics is also active area of researches with ultracold atoms...



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- 3) Adiabatic approximation: $H\varphi_n = E_n\varphi_n \rightarrow i\hbar \frac{\partial \varphi_n}{\partial t} = H\varphi_n$ No change
- 4) Practical/Numerical implementation (discretization scheme, regularization,) No change





Superfluidity: U(1) order parameter

Order parameter = "pairing" Δ

 $\Delta(\boldsymbol{r}) = |\Delta(\boldsymbol{r})|e^{i\theta(\boldsymbol{r})}$



In a ground state the phase is uniform across the system...

... and since it is closely connected with phase of the wave-function it can be absorbed by normalization factor $\Delta({m r}) o |\Delta({m r})|$



Excited states





Fig. from: A. Munoz Mateo and J. Brand, PRL 113, 255302 (2014)



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Coherence length:
$$\xi = {\hbar v_F \over \pi \Delta}$$

Cold atoms at unitarity: $\xi \sim n^{-1/3} \ll L$

Nuclear systems (n=0.08fm-3):

 $\xi pprox 17\,{
m fm} pprox 2R$ where R is radius of heavy nucleus

GENERAL REMARKS:

- Δ(r) should be treated as dynamical field...
- Ithe ∆(r) field introduces new excitation modes to the system (enormous number of new modes)
 - fluctuations (waves) of $|\Delta(r)|$...
 - fluctuations (waves) of $\theta(\mathbf{r})$...
 - Solitonic excitations..

How to excite "solitonic" modes?



1. Start with a cloud in ground state...



How to excite "solitonic" modes?



1. Start with a cloud in ground state...

2. Split into two fragments ...



How to excite "solitonic" modes?



MIT experiments: Nature 499, 426 (2013); Phys. Rev. Lett. 113, 065301(2014); Phys. Rev. Lett. 116, 045304 (2016);

- ⁶Li atoms near a Feshbach resonance (N≈10⁶) cooled in harmonic trap
- Step potential used to imprint a soliton (evolve to π phase shift)

 $-\pi -\pi/2 \ 0 \ \pi/2 \ \pi$

- Let system evolve...
- Take picture (subtle imaging with tomography)



PHYSICS, WUT

Experimental results – Cascade of Solitary Waves

Figures taken from: M. Zwierlein talk, (http://en.sif.it/activities/fermi_school/mmxiv) School of Physics E. Fermi – Quantum Matter at Ultralow Temperatures Varenna, July 9th, 2014





 \rightarrow remarkable agreement between theory and data!

Movie 2

For other comparison of TDDF vs exp see: https://wslda.fizyka.pw.edu.pl/index.php/Gallery No adjusting parameters to the experiment!

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



Note: we find that effective approaches, like GPE, are able to predict correctly the final state, however the states inbetween are different from TDDFT predictions.

From: G. Wlazłowski, A. Bulgac, M.M. Forbes, K.J. Roche, Phys. Rev. A 91, 031602(R) (2015).

"Pairing" as the dynamical field in nuclear physics?

Remarks:

- The phase φ (gauge angle) has well defined meaning only for systems with broken U(1) symmetry: N↔φ conjugate variables!
- In nuclear experiments the phase cannot be controlled.
- Possible signal should be extracted after averaging over the phase differences.
- Proper way of "averaging" is by projecting on a good particle number.

$$P^N = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{i\varphi(\hat{N}-N)}$$

Estimate of energy scales \rightarrow energy needed to excite the "soliton"

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

e.g.) $S=\pi R^2$, $L \sim R = 6 \text{ fm},$ $n_{\rm s}$ =0.08 fm⁻³ $\rightarrow E \sim 30 \text{ MeV}$

- *S*: Attaching area
- *L*: Length scale over which the phase varies
- *n*_s: Superfluid density

The

"²⁴⁰Pu+²⁴⁰Pu" head-on collisions (E/V_{Bass}=1.1, E=980MeV)

Movie 3

To simplify calcs:

- We used Fayans EDF (FaNDF⁰) S.A. Fayans, JETP Letters 68, 169 (1998);
- We neglected spin-orbit term;
- These are "^AX nuclei" in sense that these objects have requested number of protons and neutrons (average value).

From: P. Magierski, K. Sekizawa, G. Wlazłowski, Phys. Rev. Lett. 119, 042501 (2017) "240Pu+240Pu" head-on collisions (E/V_{Bass}=1.1, E=980MeV)

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

Fusion reaction: ⁹⁰Zr+⁹⁰Zr

suppressed by the phase difference

Related studies:

Y. Hashimoto and G. Scamps,

Gauge angle dependence in TDHFB calculations of ²⁰O+²⁰O head-on collisions with the Gogny interaction, Phys. Rev. C 94, 014610 (2016).

Examining empirical evidence of the effect of superfluidity on the fusion barrier

Guillaume Scamps Phys. Rev. C **97**, 044611 – Published 18 April 2018

In order to describe the fusion barrier, three parameters are defined, the centroid barrier,

$$B_0 = \frac{m_1^B}{m_0^B},$$
 (5)

the fusion radius, defined in order to normalize the barrier distribution,

$$R_B = \sqrt{\frac{m_0^B}{\pi}},\tag{6}$$

and the barrier width,

$$\sigma_B = \sqrt{\frac{m_2^B}{m_0^B} - \left(\frac{m_1^B}{m_0^B}\right)^2}.$$
 (7)

These three parameters are computed from the moment of the barrier distribution,

$$m_n^B = \int_0^{E_M} B^n \frac{d^2}{dE^2} (E\sigma(E)) \bigg|_{E=B} dB.$$
 (8)

This method is applied to 115 fusion reactions and compared to a model that does not include the expected effect of superfluidity. An enhancement of the fluctuations of the barrier of about 1 MeV is found in several reactions between superfluid nuclei. This result proves that the effect predicted by TDHFB calculation is real. Nevertheless, this empirical result is in contradiction with the idea of a very strong effect of superfluidity in the fusion barrier.

Simulations with (complete) Skyrme SkM*

P. Magierski, A. Makowski, M.C. Barton, K. Sekizawa, and G. Wlazłowski Phys. Rev. C 105, 064602 (2022)

- In the frozen density approximation the dynamical effects are neglected ...
- ... density of each fragment is fixed to be its ground-state one...
- ... the contribution from the pairing fields were also taken into account:

$$\Delta_{q,\text{tot}}(\mathbf{r}) = \Delta_{q,1}(\mathbf{r} - R/2) + \Delta_{q,2}(\mathbf{r} + R/2)$$

35

Simulations with (complete) Skyrme SkM*

P. Magierski, A. Makowski, M.C. Barton, K. Sekizawa, and G. Wlazłowski Phys. Rev. C 105, 064602 (2022)

The effect is of dynamic origin, which cannot be grasped in the static calculations.

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 $\Delta_{q,\text{tot}}(\mathbf{r}) = \Delta_{q,1}(\mathbf{r} - R/2) + \Delta_{q,2}(\mathbf{r} + R/2)$

⁹⁶Zr+⁹⁶Zr, E_{cm}=178MeV

density:

n

р

n

р

paring field:

 $\Delta\phi{=}0$

Related talk: Wiktor Kragiel

MPHYSICS.WUT

P. Magierski, A. Makowski, M.C. Barton, K. Sekizawa, and G. Wlazłowski Phys. Rev. C 105, 064602 (2022)

Pairing emergence during the collision

Large-amplitude oscillations of pairing field \rightarrow similarity to the pairing Higgs mechanism.

P. Magierski, A. Makowski, M.C. Barton, K. Sekizawa, and G. Wlazłowski Phys. Rev. C 105, 064602 (2022)

SUMMARY

Ultracold atomic gases can be used as a playground for testing predictive power of TDDFT...

... still, complex nature of nuclear interaction/energy density functional rises many questions about trustability of TDDFT in context of nuclear reactions.

- Solitonic excitations:
 - their dynamics have been properly reproduced by TDDFT for ultracold Fermi gases...
 - ... and analog of them is predicted to be present for nuclear reactions.
- Nuclear analog of "solitonic excitation" impacts:
 - Barrier for fussion;
 - TKE of fragments;
 - Dynamics of neck formation;

Collaborators: P. Magierski, A. Makowski, W. Kragiel (WUT); K. Sekizawa (Tokyo); A. Bulgac (UW);

$i\hbar \frac{\partial}{\partial t}$	$(U_{\uparrow n}(\mathbf{r},t))$	=	$\int h_{\uparrow\uparrow}(\mathbf{r},t)$	$h_{\uparrow\downarrow}({f r},t)$	0	$\Delta_{\uparrow\downarrow}(\mathbf{r},t)$	$U_{\uparrow n}(\mathbf{r},t)$
	$U_{\downarrow n}({\bf r},t)$		$h_{\downarrow\uparrow}({\bf r},t)$	$h_{\downarrow\downarrow}({\bf r},t)$	$\Delta_{\downarrow\uparrow}({\bf r},t)$	0	$U_{\downarrow n}({\bf r},t)$
	$V_{\uparrow n}({\bf r},t)$		0	$\Delta^*_{\downarrow\uparrow}({\bf r},t)$	$-h^*_{\uparrow\uparrow}({\bf r},t)$	$-h^*_{\uparrow\downarrow}(\mathbf{r},t)$	$V_{\uparrow n}({f r},t)$
	$\left(V_{\downarrow n}(\mathbf{r},t)\right)$		$\left\{ \Delta_{\uparrow\downarrow}^{*}(\mathbf{r},t) \right\}$	0	$-h^*_{\downarrow\uparrow}({\bf r},t)$	$-h^*_{\downarrow\downarrow}(\mathbf{r},t)$	$\left(V_{\downarrow n}(\mathbf{r},t)\right)$

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Appendix

Phase diagram of ultracold Fermi gas

Experiments:

Josephson effect

$$i\hbar \frac{\partial \psi_1}{\partial t} = \mathcal{E}_1 \psi_1 - \mathcal{T} \psi_2,$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = \mathcal{E}_2 \psi_2 - \mathcal{T} \psi_1,$$

$$\psi_j = \sqrt{n_j} \,\mathrm{e}^{i\varphi_j}$$

Flow of particles maximized when phase diff. is $\pi/2$

$$= -\frac{\partial n_1}{\partial t} = \frac{2\mathcal{T}}{\hbar} \sqrt{n_1 n_2} \sin(\varphi_2 - \varphi_1),$$

$$\frac{\partial \left(\varphi_2 - \varphi_1\right)}{\partial t} = \frac{\mathcal{E}_2 - \mathcal{E}_1}{\hbar} + \frac{\mathcal{T}}{\hbar} \frac{n_1 - n_2}{\sqrt{n_1 n_2}} \cos(\varphi_2 - \varphi_1)$$

- \rightarrow BCS-BEC crossover
- \rightarrow spin-imbalanced systems
- \rightarrow mass-imbalanced systems
- \rightarrow finite temperature formalism

Ongoing extensions:

- → Bose-Fermi mixtures
- \rightarrow Fermi-Fermi mixtures (like nuclear systems: protons+neutrons)

Warsaw University W-SLDA of Technology Toolkit

http://wslda.fizyka.pw.edu.pl/

W-SLDA Toolkit

Self-consistent solver of mathematical problems which have structure formally equivalent to Bogoliubov-de Gennes equations.

$$\begin{pmatrix} h_a(\boldsymbol{r}) - \mu_a & \Delta(\boldsymbol{r}) \\ \Delta^*(\boldsymbol{r}) & -h_b^*(\boldsymbol{r}) + \mu_b \end{pmatrix} \begin{pmatrix} u_n(\boldsymbol{r}) \\ v_n(\boldsymbol{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\boldsymbol{r}) \\ v_n(\boldsymbol{r}) \end{pmatrix}$$

time-dependent problems: td-wslda

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_n(\boldsymbol{r},t)\\v_n(\boldsymbol{r},t)\end{pmatrix} = \begin{pmatrix}h_a(\boldsymbol{r},t)-\mu_a & \Delta(\boldsymbol{r},t)\\\Delta^*(\boldsymbol{r},t) & -h_b^*(\boldsymbol{r},t)+\mu_b\end{pmatrix}\begin{pmatrix}u_n(\boldsymbol{r},t)\\v_n(\boldsymbol{r},t)\end{pmatrix}$$

can run on "small" computing clusters as well as leadership supercomputers (depending on the problem size)

Application #1: Fermionic Josephson Junction

