TDDFT with pairing correlations in nuclear reactions:

Induced fission and low-energy collisions of superfluid nuclei

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Slides (pptx) with movies will be available for download from http://www.faculty.washington.edu/bulgac/Pu240/
This presentation is a perfect illustration of Dave Barry’s suggestion:

Never be afraid to try something new. Remember that amateurs built the Ark and professionals built the Titanic.

I definitely could not call myself a fission or high-performance computing expert at the time when this project started around late 2006. At that time nuclear fission looked to me like a good problem to try, being unaware of how complex really is and not having someone around to warn me.

Now I know a bit more.

But then again, as Sydney Brenner (Nobel prize 2002) said:

I’m a strong believer that ignorance is important in science. If you know too much, you start seeing why things won’t work. That is why it’s important to change your field to collect more ignorance.
While in this presentation I will concentrate on a couple of issues, it is important to summarize that so far TDSLDA has lead to many qualitative new developments:

- The first microscopic description of structure and creation, and decay of quantized vortices in a Fermi superfluid predicted by Feynman and Onsager in 1950’s.
- The demonstration of supercritical flow and of superfluid to normal transition.
- The first microscopic description of the incipient phases of quantum turbulence in Fermi superfluids predicted in 1954 by Feynman.
- Demonstrated the existence of the Larkin-Ovchinnikov phase in cold fermion atoms at unitarity.
- The creation of Anderson-Higgs mode, domain walls, and the correct identification of the vortex rings, their dynamics and decay, and of the quantum shock waves in experiments.
- Described the microscopic structure of quantized vortices in neutron matter.
- Described microscopically the interaction of quantized vortices with nuclei in neutron star crust (see talk by Wlazłowski).
- Described microscopically the Coulomb excitation of nuclei with relativistic nuclei (see talk by Magierski).
- Described induced nuclear fission and revealed unexpected qualitative aspects.
- Has been applied to collisions of heavy superfluid nuclei and revealed new qualitative phenomena (see also talk by Magierski).
Nuclear fission is unquestionably one of the most challenging quantum many-body problems. (Do not be fooled by some misleading titles which include “microscopic approach!” The bar is much higher than some would like to admit.)

Superconductivity needed less than 50 years to reach a microscopic understanding, from 1911 to 1957. Nuclear fission is almost 80 years old!

Several recent developments have radically changed our prospects of attaining a microscopic description of nuclear fission.

Nuclear fission was the impetus for funding big science in the second part of the 20th century and it is important for fundamental nuclear theory, origin of elements, applications, …
Critical new developments

• **In THEORY:**

  Formulation of a local extension of the Density Functional Theory (DFT), in the spirit of the Local Density Approximation (LDA) formulation of DFT due to Kohn and Sham, to superfluid time-dependent phenomena, the Superfluid Local Density Approximation (SLDA).

  Validation and verification of (TD)SLDA against a large set of theoretical and experimental data for systems of strongly interacting fermions.

• **In HIGH PERFORMANCE COMPUTING:**

  Emergence of very powerful computational resources, non-trivial numerical implementation of TDSLDA, advanced capabilities of leadership class computers, in particular tens of thousands of GPUs.

  SLDA and TDSLDA are problems of extreme computational complexity, requiring the solution of 10,000s … 1,000,000s coupled complex non-linear time-dependent 3D partial differential equations.
- How nuclei change their shape at a microscopic level? (beyond the liquid drop phenomenology)
- The potential energy surface is a bit more complicated than a liquid drop model would naively suggest! It is not very smooth, it has a certain degree of “roughness.”

- 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)

- Each single-particle level is double degenerate (Kramers’ degeneracy) and at each level crossing two nucleons must jump simultaneously!

  $$(m, -m) \Rightarrow (m', -m')$$

  “Cooper pair” $\Rightarrow$ “Cooper pair”

- Pairing interaction/superfluidity is the most effective mechanism at performing shape changes.

It requires the breaking of axial symmetry and it was never really shown to be the correct mechanism. Here is the problem.

- Occupied single-particle orbitals m-quantum numbers in initial and final configurations. Notice the different number of 1/2 and 5/2 orbitals, which incompatible with conserved axial symmetry.
- One more problem!
  Different parities of initial and final sp fields.
  Initial nucleus: 20 positive + 12 negative parity sp orbitals
  Final nuclei: 16 positive + 16 negative parity sp orbitals

Our Main Theoretical Tool: DFT!

THEOREM: There exist an universal density functional of particle density.

DFT provides the framework, the equivalent of the Schrödinger equation.
(We might not have the “exact potential” yet!)
This is a mathematical theory which is more than 50 years old: DFT - Kohn and Hohenberg, 1964 and LDA - Kohn and Sham, 1965.

DFT has been developed and used mainly to describe normal (non-superfluid) electron systems. But not everyone is normal! Hence, a new local extension of DFT to superfluid systems and time-dependent phenomena was developed.
Kohn-Sham theorem (1965)

\[
H = \sum_{i}^{N} T(i) + \sum_{i<j}^{N} U(ij) + \sum_{i<j<k}^{N} U(ijk) + \cdots + \sum_{i}^{N} V_{\text{ext}}(i)
\]

\[
H \Psi_0(1,2,...N) = E_0 \Psi_0(1,2,...N)
\]

\[
n(\vec{r}) = \langle \Psi_0 \mid \sum_{i}^{N} \delta(\vec{r} - \vec{r}_i) \mid \Psi_0 \rangle
\]

\[
\Psi_0(1,2,...N) \iff V_{\text{ext}}(\vec{r}) \iff n(\vec{r})
\]

\[
E_0 = \min_{n(\vec{r})} \int d^3r \left\{ \frac{\hbar^2}{2m^*(\vec{r})} \tau(\vec{r}) + \varepsilon \left[ n(\vec{r}) \right] + V_{\text{ext}}(\vec{r}) n(\vec{r}) \right\}
\]

\[
n(\vec{r}) = \sum_{i}^{N} |\varphi_i(\vec{r})|^2, \quad \tau(\vec{r}) = \sum_{i}^{N} |\nabla \varphi_i(\vec{r})|^2
\]

THEOREM: There exist an universal functional of particle density alone independent of the external potential.

The wave function of \(^{240}\text{Pu}\) depends on 720 coordinates and has 1.77E72 spin components!!!
SLDA Extension to Superfluids and Time-Dependent Phenomena, and its Verification and Validation

Since DFT/SLDA is not an approximation, but in principle an exact theoretical framework (unlike HF, HFB, etc.) and one has to convincingly show that:

• its specific realization is equivalent to the Schrödinger equation! Namely, both the Schrödinger equation and DFT should lead to identical outcomes.

(This is theory versus theory and not theory versus experiment validation! This aspect has been tested in normal electronic systems and also in superfluid cold atom systems.)

• it correctly describes Nature!

• the numerical implementation faithfully reproduces the theory.
  (This particular aspect is particularly important in the case of superfluid systems, due to their complex mathematical structure.)
The SLDA energy density functional for unitary Fermi gas (infinite scattering length and zero effective range)

*Dimensional arguments, renormalizability, Galilean invariance, and symmetries determine the functional form of the energy density.*

In this respect this system is perhaps unique in Nature. It describes cold atoms and to a large extent dilute neutron matter, making it an ideal testing ground for DFT.

\[
\varepsilon(\vec{r}) = \frac{\hbar^2}{m} \left\{ \alpha \frac{\tau_c(\vec{r})}{2} + \gamma \left( \frac{V_c(\vec{r})}{n^{1/3}(\vec{r})} \right)^2 \right\} + \beta \frac{3(3\pi^2)^{2/3} n^{5/3}(\vec{r})}{5} \right\} - \frac{\hbar^2}{m} (\alpha - 1) \frac{j^2(\vec{r})}{2n(\vec{r})}
\]

\[
n(\vec{r}) = 2 \sum_{0<E_k<E_c} \left| v_k(\vec{r}) \right|^2, \quad \tau_c(\vec{r}) = 2 \sum_{0<E_k<E_c} \left| \nabla v_k(\vec{r}) \right|^2,
\]

\[
v_c(\vec{r}) = \sum_{0<E_k<E_c} u_k(\vec{r}) v^*_k(\vec{r}) \quad \Leftarrow \text{divergent without a cutoff, need RG}
\]

- Surprisingly, the gradient corrections are negligible!
- Three dimensionless constants \(\alpha, \beta,\) and \(\gamma\) determining the functional are extracted from Quantum Monte Carlo for homogeneous systems and they determine the total energy, the pairing gap and the effective mass.
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<th>(E_{FNDMC})</th>
<th>(E_{ASLDA})</th>
<th>error</th>
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<td>(3, 1)</td>
<td>6.6 ± 0.01</td>
<td>6.687</td>
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<td>13.3 ± 0.1</td>
<td>13.54</td>
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</tr>
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<td>15.8 ± 0.1</td>
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<td>26.73</td>
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<td>(10, 2)</td>
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<td>(10, 6)</td>
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<td>35.93</td>
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<td>(35, 20)</td>
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<th>((N_a, N_b))</th>
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<th>(E_{ASLDA})</th>
<th>error</th>
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<td>12.573 ± 0.03</td>
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<td>34.87</td>
<td>3.1%</td>
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<td>(10, 10)</td>
<td>41.302 ± 0.08</td>
<td>40.54</td>
<td>1.8%</td>
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<tr>
<td>(11, 11)</td>
<td>46.889 ± 0.09</td>
<td>46.45</td>
<td>4%</td>
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<td>(12, 12)</td>
<td>52.624 ± 0.2</td>
<td>51.23</td>
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<tr>
<td>(13, 13)</td>
<td>58.545 ± 0.18</td>
<td>56.25</td>
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<td>(14, 14)</td>
<td>64.388 ± 0.31</td>
<td>62.52</td>
<td>2.9%</td>
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<td>(15, 15)</td>
<td>70.927 ± 0.3</td>
<td>68.72</td>
<td>3.1%</td>
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</table>

Bulgac, Forbes, and Magierski, Ch.9 in Lecture Notes in Physics, vol. 836 (2012)
Red line: Larkin-Ovchinnikov phase (unitary Fermi supersolid)

Black line: normal part of the energy density


\[
E(n_a, n_b) = \frac{3}{5} \frac{(6\pi^2)^{2/3}}{2m} \hbar^2 \left[ n_a g \left( \frac{n_b}{n_a} \right) \right]^{5/3}
\]
Cray XK7, ranked at peak $\approx 27$ Petaflops ($\text{Peta} = 10^{15}$)

On Titan there are 18,688 GPUs which provide 24.48 Petaflops !!! and 299,008 CPUs which provide only 2.94 Petaflops.

A single GPU on Titan performs the same amount of FLOPs as approximately 134 CPUs.
TDSLDA equations

\[
\begin{pmatrix}
    u_n^\uparrow(\vec{r},t) \\
    u_n^\downarrow(\vec{r},t) \\
    v_n^\uparrow(\vec{r},t) \\
    v_n^\downarrow(\vec{r},t)
\end{pmatrix}
\frac{i\hbar}{\partial t}
\begin{pmatrix}
    \hat{h}^\uparrow\uparrow(\vec{r},t) - \mu \\
    \hat{h}^\uparrow\downarrow(\vec{r},t) - \mu \\
    -\Delta^*(\vec{r},t) \\
    \Delta^*(\vec{r},t)
\end{pmatrix}
\begin{pmatrix}
    \hat{h}^\uparrow\downarrow(\vec{r},t) \\
    \hat{h}^\downarrow\uparrow(\vec{r},t) + \mu \\
    -\hat{h}^\downarrow\downarrow(\vec{r},t) + \mu \\
    -\hat{h}^\uparrow\uparrow(\vec{r},t) + \mu
\end{pmatrix}
\begin{pmatrix}
    0 \\
    0 \\
    -\Delta(\vec{r},t) \\
    \Delta(\vec{r},t)
\end{pmatrix}
\begin{pmatrix}
    u_n^\uparrow(\vec{r},t) \\
    u_n^\downarrow(\vec{r},t) \\
    v_n^\uparrow(\vec{r},t) \\
    v_n^\downarrow(\vec{r},t)
\end{pmatrix}
\]

Index “n” is practically a continuous variable!

- The system is placed on a large 3D spatial lattice (adequate representation of continuum)
- Derivatives are computed with FFTW (this insures machine accuracy) and is very fast
- Fully self-consistent treatment with fundamental symmetries respected (isospin, gauge, Galilean, rotation, translation, parity)
- Adams-Bashforth-Milne fifth order predictor-corrector-modifier integrator which is effectively a sixth order method
- No symmetry restrictions for the solutions
- Number of PDEs is of the order of the number of spatial lattice points – from 10,000s to 1-2,000,000
- SLDA/TDSLDA (DFT) is formally by construction like meanfield HFB/BdG
- The code was implemented on Jaguar, Titan, Franklin, Hopper, Edison, Hyak, Athena
  - Initially Fortran 90, 95, 2003 …, presently C, CUDA, and obviously MPI, threads, etc.
- Extremely efficient I/O for Check-Point Restart
$^{240}$Pu on a spatial lattice $18^2 \times 30$

(Sky3D is TDHF+TDBCS)

Sky3D $\Rightarrow$ \( \frac{(\text{number of CPUs}) \times (\text{wall time})}{(\text{number of time-steps}) \times (\text{number of PDES})} = \frac{128 \times 300}{1000 \times 1024} = 0.0375 \text{ sec.} \)

TDSLDA $\Rightarrow$ \( \frac{(\text{number of GPUs}) \times (\text{wall time})}{(\text{number of time-steps}) \times (\text{number of PDES})} = \frac{128 \times 468.5}{1909 \times 52792} = 0.000595 \text{ sec.} \)

Sky3D $\Rightarrow$ \( \frac{(\text{wall time})}{(\text{number of time-steps})} = \frac{300}{1000} = 0.333 \text{ sec.} \)

TDSLDA $\Rightarrow$ \( \frac{(\text{wall time})}{(\text{number of time-steps})} = \frac{468.5}{1909} = 0.245 \text{ sec.} \)

On a $20^2 \times 40$ spatial lattice 256,000 3D TD PDEs are integrated for 400,000 time steps in 47 hours on 512 GPUs or in 24 hours on 1602 GPUs.
Our main achievement was that we were able to reach scission starting from the outer saddle (as typical in Langevin/Brownian Motion models too) in a microscopic framework without making any assumptions, or uncontrolled approximations, or fitting of Parameters, and using a realistic (as everyone else does too, but albeit still a phenomenological, but quite accurate) energy density functional!

At last!

Remember, fission is controlled mainly by the competition between surface and Coulomb energies.
$1 \text{ zs} = 10^{-21} \text{ sec.} = 300 \text{ fm/c}$
How reasonable are the results though?
Evolution of the average magnitude of the pairing fields.

Hexadecapole (dashed), octupole (dotted), and quadrupole (solid) mass moments.
The most surprising finding was that the saddle-to-scission time was significantly longer than expected from any previous treatments, approximately by a factor of ten.

Why???

One cause: all collective degrees of freedom present.

2D classical analog model of the Drude model for electron conduction in metals.

On the left side there is no “ion lattice” present, only electrons in an “uniform electric field.”

On the right side the electrons, again in the presence of an “uniform electric field,” collide elastically with the “ions” in the lattice.

Another reason: fluctuating pairing field.

Note that the kinetic energy is not dissipated and in both cases the “electrons” at any height have the same speed and but arrive at the bottom at different times!
We know by now that without pairing nuclear fission is hindered, if not even completely stopped.

Collisions can help, but not of any kind, as only pairing provides the most efficient mechanism which maintains the sphericity of the Fermi surface.

(Otherwise the potential energy surface will have a large volume contribution, and not only the surface and Coulomb terms mainly as the liquid drop model suggests. Two-body collisions of general type will be less efficient, especially when the nucleus is cold.)

So, how important pairing really is?
$^{240}\text{Pu fission}$

$^{240}\text{Pu fission in the normal pairing gap}$

$^{240}\text{Pu fission in a larger pairing gap}$

Normal pairing strength
Saddle-to-scission 14,000 fm/c

Enhanced pairing strength
Saddle-to-scission 1,400 fm/c !!!
First Set of Conclusions

• While pairing is not the engine driving the fission dynamics, pairing provides the essential lubricant, without which the evolution will come quickly to a screeching halt.

• The quality of the agreement with experimental observations is surprisingly good, especially taking into account the fact that we made no effort to reproduce any measured data.

• TDSLDA predicts long saddle-to-scission time scales and the systems behaves superficially as a very viscous one, while at the same time the collective motion is not overdamped. There is no thermalization and the “temperatures” of the fission fragments are not equal. As W. Mittig discussed at a recent meeting, this could be a key mechanism to create long lived large (Z >> 100) nuclear systems.

• TDSLDA will offer insights into nuclear processes and quantities which are either not easy or impossible to obtain in the laboratory:

  fission fragments excitation energies and angular momenta distributions (mean and width),
  element formation in astrophysical environments, other nuclear reactions …

• TDSLDA offers an unprecedented opportunity to test the nuclear energy density functional for large amplitude collective motion, non-equilibrium phenomena, in new regions of the collective degrees of freedom.
“Nuclear Josephson junction”

Novel role of superfluidity in low-energy nuclear reactions
Magierski, Sekizawa, and Wlazłowski, arXiv:1611.10261

Gauge angle dependence in TDHFB calculations of $^{20}\text{O}+^{20}\text{O}$ head-on collisions with the Gogny interaction
Can the phase of the condensate affect observables?

Related questions have been raised by many over the years, in connection with superfluid liquid helium, cold Bose and Fermi gases:

- B.D. Josephson, Rev. Mod. Phys. 36, 216 (1964), *Coupled Superconductors*
P.W. Anderson (1986) considered two types of Gedanken experiments:

✓ Take a bucket of liquid helium above the lambda transition, cool it down to close to absolute zero, separate into two parts, keep them at a temperature close to absolute zero, subject them to different external conditions while both are still below the lambda point, and bring them together.

  Will they interfere? Yes, they remain entangled!

The experiments with Bose and Fermi gases performed so far are of this kind.

✓ Take two buckets of liquid helium above the lambda point, cool them down independently, and bring them together.

  Will they interfere? Yes, but with different phases every time the experiment is performed. After a short contact however they get entangled and the initial state becomes impossible to be recovered.

Josephson junctions are likely of this type (depending on preparation however).
Experiments of the first kind in Anderson classification.

Atom Interferometry with Bose-Einstein Condensates in a Double-Well Potential

Heavy Solitons in a Fermionic Superfluid

Quantized Superfluid Vortex Rings in the Unitary Fermi Gas
Let us consider for simplicity a BEC.

*The ground state of a fermionic superfluid is a BEC of Cooper pairs.*

**Off-diagonal long-range order:**

\[ \rho(\vec{r}_1, \vec{r}_2) = \langle \psi^\dagger(\vec{r}_2)\psi(\vec{r}_1) \rangle \Rightarrow n_0 \psi^*(\vec{r}_2)\psi(\vec{r}_1) \quad \text{when} \quad |\vec{r}_1 - \vec{r}_2| \to \infty \]

where \( n_0 = O(N) \) has a macroscopic value

\( \psi(\vec{r}_1) \) is an eigenvector of \( \rho(\vec{r}_1, \vec{r}_2) \)

The rest of the eigenvalues of the density matrix are typically \( O(1) \ll O(N) \)

A fragmented condensate is defined as a state for which there are more than one eigenvalues of the density matrix with macroscopic values.
The wave function at $T=0$ is given by

$$a^\dagger = \int d^3 r \psi^\dagger (\vec{r}) \varphi(\vec{r})$$

$$|\Psi(N)\rangle \propto \int_0^{2\pi} d\alpha \ e^{i\alpha N} e^{i\alpha a^\dagger} |0\rangle$$

$$\langle \Psi(N+1)|\psi^\dagger (\vec{r})|\Psi(N)\rangle = e^{i\alpha} \varphi(\vec{r})$$

$\alpha$ and $N$ are canonical variables which are subject to the Heisenberg uncertainty relation.

In a macroscopic system the phase becomes a classical variable and any experiment can be interpreted as if this phase is a constant, even though the particle number if well defined!
Consider now two initially isolated BEC clouds, therefore strictly speaking a fragmented condensate. In BEC the density and the complex order parameter are described by the same field, the wave function.

\[
    i\hbar \partial_t \psi_k(\vec{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi_k(\vec{r}, t) + V_k(\vec{r})\psi_k(\vec{r}, t) + g\left|\psi_k(\vec{r}, t)\right|^2 \psi_k(\vec{r}, t)
\]

\[
    \psi_k(\vec{r}, t) = \phi_k(\vec{r})\exp\left(-i\frac{\mu_k t}{\hbar}\right), \quad \int d^3r \left|\psi_k(\vec{r}, t)\right|^2 = N_k, \quad k = 1, 2
\]

Now send the two clouds towards each other. The wave function before coming into contact (initial condition) is

\[
    \Psi(\vec{r}, t) = \psi_1(\vec{r}, t) + \exp(i\alpha)\psi_2(\vec{r}, t), \text{ where } \alpha \text{ is in principle arbitrary}
\]

\[
    \psi_k(\vec{r}, t) = \phi_k(\vec{r} - \vec{r}_k - \vec{u}_k t)\exp\left(i\frac{m\vec{u}_k \cdot \vec{r}}{\hbar} - i\frac{\mu_k t}{\hbar} - i\frac{m\vec{u}_k^2}{2\hbar}\right), \quad k = 1, 2
\]

\[
    V_k(\vec{r}) \Rightarrow V_k(\vec{r} - \vec{r}_k - \vec{u}_k t)
\]
At all times this combined wave function satisfies the Gross-Pitaevskii equation

\[ \Psi(\vec{r}, t) = \psi_1(\vec{r}, t) + \exp(i\alpha)\psi_2(\vec{r}, t), \] where \( \alpha \) is in principle arbitrary

\[ \psi_k(\vec{r}, t) = \varphi_k(\vec{r} - \vec{r}_k - \vec{u}_k t) \exp \left( i \frac{m\vec{u}_k \cdot \vec{r}}{\hbar} - i \frac{\mu_k t}{\hbar} - i \frac{m\vec{u}_k^2}{2\hbar} \right), \quad k = 1, 2 \]

\[ V_k(\vec{r}) \Rightarrow V_k(\vec{r} - \vec{r}_k - \vec{u}_k t) \]

At all times this combined wave function satisfies the Gross-Pitaevskii equation

\[ i\hbar \partial_t \Psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \Delta \Psi(\vec{r}, t) + \sum_{k=1}^{2} V_k(\vec{r} - \vec{r}_k - \vec{u}_k t) \Psi(\vec{r}, t) + g|\Psi(\vec{r}, t)|^2 \Psi(\vec{r}, t) \]

If \( g=0 \) the equation is linear and each component of the wave function satisfies independently the equation:

\[ i\hbar \partial_t \psi_k(\vec{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi_k(\vec{r}, t) + \left[ V_1(\vec{r} - \vec{r}_1 - \vec{u}_1 t) + V_2(\vec{r} - \vec{r}_2 - \vec{u}_2 t) \right] \psi_k(\vec{r}, t), \quad k = 1, 2 \]
Phase Locking and Macroscopic Entanglement

$\alpha = 0$  $\alpha = \pi$

$g = 0$  

$g = 0.5$  

$g = 1$

$N_1 = 120, \ N_2 = 80$
Let us look now at realistic nuclear fermion condensates, at the collisions of superfluid nuclei and induced fission, and see if phase locking emerges in fermion condensates too.
Two $^{120}$Sn collision at $E_{cm} = 360$MeV

\[ \alpha = 0, \quad g = -233 \text{ MeV} \cdot \text{fm}^3 \]
Two $^{120}$Sn collision at $E_{cm} = 360\text{MeV}$

$\text{density (fm}^{-3}\text{)}$

$\text{pairing gap (MeV)}$

$\text{pairing phase}$

$\Delta \phi = \pi$

t = 0.0 (fm/c)

$^{120}\text{Sn} + ^{120}\text{Sn}, \quad E_{CM} = 360\text{ MeV}, \quad \alpha = \pi, \quad g = -233\text{ MeV} \cdot \text{fm}^3$
Two $^{120}\text{Sn}$ ($g=-2000$ MeV) collision at $E_{cm} = 360$ MeV

$^{120}\text{Sn} + ^{120}\text{Sn}, \; E_{CM} = 360$ MeV, \; $\alpha = 0$, \; $g = -2000$ MeV $\cdot$ fm$^3$
Two $^{120}$Sn ($g=-2000$ MeV) collision at $E_{cm} = 360$ MeV

$\rho$ (density (fm$^{-3}$))

$\Delta \phi = \pi$

$\Delta \phi = \pi$

$\alpha = \pi$

$g = -2000$ MeV·fm$^3$

$\rho$ (pairing gap (MeV))

$\Delta \phi = \pi$

$\Delta \phi = \pi$

$\alpha = \pi$

$g = -2000$ MeV·fm$^3$
$^{240}$Pu fission

$^{240}$Pu fission in the normal pairing gap

$^{240}$Pu fission in a larger pairing gap

Normal pairing strength
Saddle-to-scission 14,000 fm/c

Enhanced pairing strength
Saddle-to-scission 1,400 fm/c !!!
Consider only two bosons

\[ \Psi(\vec{r}_1, \vec{r}_2, t) = \left[ \psi_1(\vec{r}_1, t) + \exp(i\alpha)\psi_2(\vec{r}_1, t) \right] \left[ \psi_1(\vec{r}_2, t) + \exp(i\alpha)\psi_2(\vec{r}_2, t) \right] \]

\[ = \psi_1(\vec{r}_1, t)\psi_1(\vec{r}_2, t) + \exp(i\alpha)\left[ \psi_1(\vec{r}_1, t)\psi_2(\vec{r}_2, t) + \psi_1(\vec{r}_2, t)\psi_2(\vec{r}_1, t) \right] + \exp(2i\alpha)\psi_2(\vec{r}_1, t)\psi_2(\vec{r}_1, t) \]

Consequently, the un-projected initial wave function is a superposition of three different physical initial conditions.

Using Bloch-Messiah theorem for two fermion clouds

\[ \left| \Psi(\tau, \alpha) \right| = \prod_k \left[ u_k + e^{i\tau} e^{i\alpha} v_k a_k^\dagger a_k^\dagger \right] \prod_l \left[ u_l + e^{i\tau} e^{-i\alpha} v_l a_l^\dagger a_l^\dagger \right] \]

\[ \left| \mathcal{N}_1 + \mathcal{N}_2, \mathcal{N}_1 - \mathcal{N}_2 \right| \propto \frac{1}{(2\pi)^2} \int_0^{2\pi} d\tau e^{-2i\tau(N_1+N_2)} \int_0^{2\pi} d\beta e^{-2i\alpha(N_1-N_2)} \left| \Psi(\tau, \alpha) \right| \]
Second Set of Conclusions

A new mechanism can emerge, the phase locking and macroscopic entanglement, and it should be accurately accounted for.

If the interaction responsible for superfluidity exceeds a critical value the phases of two colliding condensates get locked very fast upon contact and the entire system becomes macroscopically entangled!

If phase locking does not take place a projection of particle number difference between the two colliding condensates is required in order to extract meaningful observables!
• No need to introduce and to guess the number and character of collective variables. The number of excited shape degrees of freedom is large and it increases during the evolution. This makes treatments like GCM, based on a fix number of collective coordinates quite doubtful.

• No need to evaluate the rather ill-defined potential energy surface. (A bit about this later.) Not clear how to choose the collective coordinates, how to choose the constraints, how to choose their number, and whether to require the nucleus to be cold or not.

• No need to determine the rather ill-defined inertia tensor. Several prescriptions are used in literature.

• There is no need to invoke (or not) adiabaticity, since as a matter of fact the dynamical evolution is not close to equilibrium, at either zero or at a finite temperature. The evolution is truly a non-equilibrium one.

• One-body dissipation, the window and wall dissipation mechanisms are automatically incorporated into the theoretical framework.

• No modeling (except for the energy density functional, which so far is tested in completely unrelated conditions and which has a relative accuracy of \( \approx 10^{-3} \) or better).

• All shapes are allowed and the nucleus chooses dynamically the path in the shape space, the forces acting on nucleons are determined by the nucleon distributions and velocities, and the nuclear system naturally and smoothly evolves into separated fission fragments.

• There is no need to introduce such unnatural quantum mechanical concepts as “rupture” and there is no worry about how to define the scission configuration.

• One can extract difficult to gain otherwise information: angular momentum distribution and excitation energies of the fission fragments, ....