Fragmentation, resonances and vortices in rotated Bose-Einstein condensates

A study beyond mean-field and Gross-Pitaevskii theory

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Critical Stability
Santos, São Paulo
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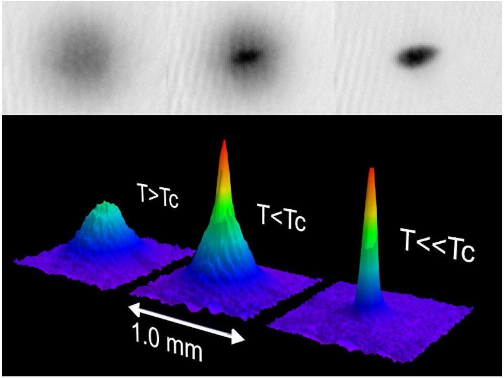
Who we are

- Formerly in Heidelberg (A. Lode, O. Alon. A. Streltsov, K. Sakmann, L. Cederbaum, MCT)
- Now in São Carlos, BR (MCT, V. Bagnato, T. Wells, S. Weiner) and Basel, CH (A. Lode)
- São Carlos: IFSC and CePOF
- Mainly experimental work but also theory sub-group growing

The task Solve the Schrödinger equation for a $T = 0$ bosonic trapped gas



Fundamental and governing equation

The task Solve the Schrödinger equation for a $T = 0$ bosonic trapped gas

The task Solve the many-body Schrödinger equation for a $T = 0$ bosonic trapped gas

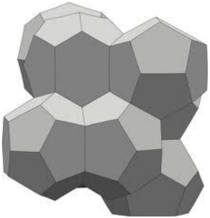
The methods

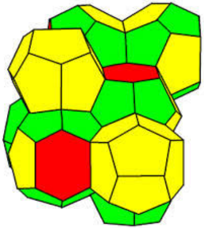
An old variational problem

Kelvin 1887: Given some volume $\mathcal{V}$ how can a partition it in blocks of the same volume v such that the total area of inter-surface of the blocks is minimal?

Kelvin conjecture: The optimal surface is the 14-face block (tetradecahedron)

Waire-Phelan 1993: If you use two different building blocks you get a better answer! With an alternating irregular dodecahedron and a tetrakaidecahedron the total area is reduced by 0.3%.





Many-body Schrödinger equation

$$\hat{H}\Psi = E\Psi$$

Key-method: variational approach!

Define an action

$$\mathcal{S} = \int L dt$$

and find conditions where this is minimized

$$\frac{\delta S}{\delta \mathcal{U}} = 0 \Rightarrow \text{conditions},$$

with respect to some variational parameter $\mathcal{U}$.

Many-body Schrödinger equation

$$\hat{H}\Psi = E\Psi$$

where $\Psi = \Psi(r_1, r_2, \ldots r_N)$ and $\hat{H} = \sum_i [\hat{T}_i + \hat{V}_i] + \sum_{i,j} \hat{W}_{ij}$.
General analytic solution is hard ($\simeq$imposible) to obtain.
Historically, various approaches developed in the context of nuclear physics, electronic structure, quantum chemistry (atomic and molecular clusters). One maps the n-body problem to a single- (or few-) body problem (Hartree).
Define

$$\rho(r, r') = N \int \Psi^*(r, r_2, r_3, \ldots, r_N)\Psi(r', r_2, r_3, \ldots, r_N) dr_2 dr_3 \ldots dr_N$$

as the single-particle reduced density matrix, to 'extract' as much information possible from the N-body function. Based on ρ are the definitions of a condensed (also coherent), fragmented or normal

The Gross-Pitaevskii (GP) approximation

- Most commonly: The Gross-Pitaevskii (GP) Ansatz, a Mean-Field (MF) approach with only one orbital.
- One writes $\Phi \sim \phi^{\otimes N}$, where $\phi \equiv \phi(r)$ is the orbital (single-particle state) that describes the state of the gas and is determined through

  the GP equation: $(\hat{T} + \hat{V} + \lambda|\phi|^2)\phi = \mu\phi$.
- Thus, MB problem = 1B (nonlinear) problem! $\rightarrow$ The simplest and most limited approach!

Multi-orbital approach

- GP works fine in certain circumstances (i.e., large N). BUT there is a lot beyond it (for instance fragmentation, fluctuations, correlations etc)
- Relax the restriction of 100% occupancy of a single ϕ; Multi-orbital MF, here Best-Mean-Field (BMF)[1]:

→ $\{\phi_i\}_{i=1}^{M}$:

$$\Phi = \hat{\mathcal{S}} \prod_{i}^{N} \phi_1(r_1) \ldots \phi_1(r_{n_1}) \phi_2(r_{n_1+1}) \ldots \phi_2(r_{n_1+n_2}) \ldots \phi_M(r_N)$$

or

$$\Phi = |n_1, n_2, \ldots, n_M\rangle, \qquad \sum_i n_i = N$$

✓ Appication: fragmentation influences the collapse of an attractive gas[2]

[1] L. S. Cederbaum and A. I. Streltsov, Best-Mean-Field for condensates, Phys. Lett. A **3**18, 564 (2003).

[2] L.S. Cederbaum, O.E. Alon, A. I. Streltsov, Fragmented Metastable States Exist in an Attractive Bose-Einstein Condensate for Atom Numbers Well above the Critical Number of the Gross-Pitaevskii Theory, Phys. Rev. Lett., **100**, 040402 , (2008).

Many-body: Multi-configurational Hartree for Bosons

→ Configuration Interaction Expansion ('exact diagonalization')

→ From the general ansatz

$$|\Psi\rangle = \sum_i C_i |\Phi_i\rangle$$

calculate and minimize action ⇒ derive system of equations[3] [4] to determine both the set of orbitals $\{\phi_i\}_{i=1}^{M}$ and the expansion coefficients $\{C_i\}_{i=1}^{N_p}$.

- Size of configuration space $N_p = \binom{N+M-1}{N}$. For instance, if $M = 3$ then $N_p \sim N^2$, while if $M = 4$ then $N_p \sim N^3$.

[3] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A **7**3, 063626, (2006).

[4] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. A **7**7, 033613, (2008).

Many-body: Multi Configurational Hartree for Bosons

- E.o.m.:

$$i\dot{\phi}_j = \hat{P}\left[\hat{h}\phi_j + \lambda_0 \sum_{k,s,q,l}^{M} \{\rho\}_{jk}^{-1} \rho_{ksql} \phi_s^* \phi_l \phi_q\right]$$

$$\mathcal{H}(t)\mathbf{C}(t) = i\frac{\partial \mathbf{C}(t)}{\partial t}$$

Many-body: Multi-configurational Hartree for Bosons

Beyond mean-field theory:

- ✓ Capable of describing fragmentation, correlations and fluctuations of the ground and excited states and transitions between coherent-to-fragmented
- ✓ Applied to various scenarios, such as Mott Insulator-to-Superfluid transition, BJJ, splitting the condensate, solitons and fragmentons, tunneling to open space and predicted new phenomena
- In ED (or CI) the basis is fixed. In MCTDHB it is time-adaptive
- How to solve it? Purelly numerical: latest application R-MCTDHB (2013)
- and a very user-friendly interface, named Guantum

Summarize

Mean-field vs Many-body

$$|\Phi\rangle \sim \prod \phi_i(r_j) = \text{product state}$$

vs

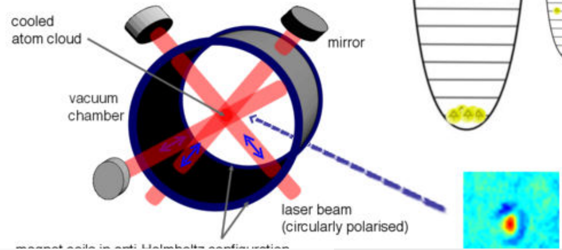
$$|\Psi\rangle = \sum_i C_i |\Phi_i\rangle = \text{superposition state}$$

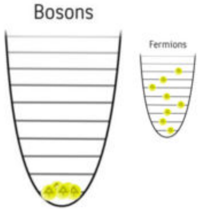
Applications

Trapped BECs as laboratories for many-body physics

- Dilute gas of spinless bosons
- External trap (1-body potential), interparticle interaction (2-body potential) and
- dimensionality can be changed in the lab
- Hence, the Hamiltonian is known and can be manipulated!

Big variety of physics manifests in BECs: from many-body correlated states to pure classical effect owing to its fluid nature

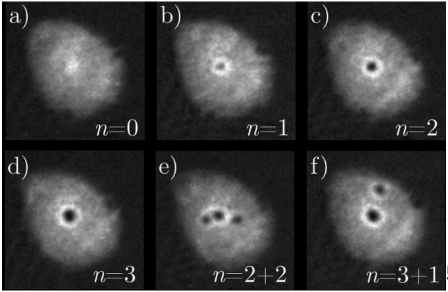




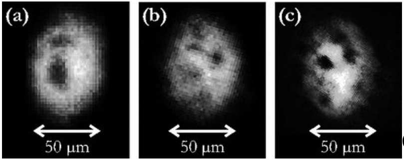
vortices in water

vortices in air

vortices in BECs



[5]



[6]

[5] Stirring in a torus, NIST, 2013

[6] Oscillating trap, São Carlos, 2009

Vortices and phantom vortices

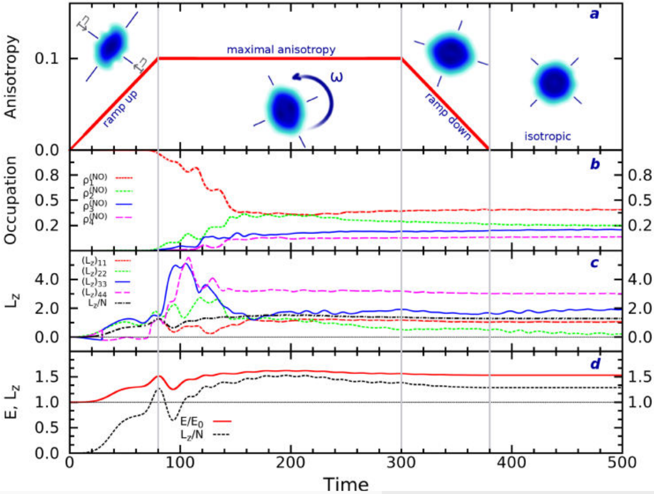
- In GP theory, one system↔one orbital. So if there is ~~angular momentum~~ vorticity in the system this is carried by this one orbital.
- However, if there are more modes participating in the MB state of the system, AM and vorticity can be exchanged. With MCTDHB we want to investigate how!
- Fragmentation + vorticity ⇒ sub-vortices

Vortices and phantom vortices

- Vortex nucleation is a transient process, that involves ‘pouring’ of energy and AM.
- GP predicts more vortices and faster nucleation than MB.
- The system fragments while steering/rotating is on and ‘relaxes’ into few orbitals once it is off.
- Vortices can be nucleated in orbitals and thus not be seen in the density but
- in the correlation function!

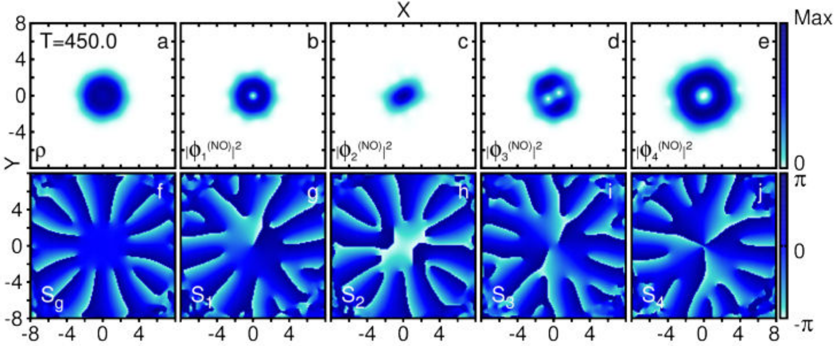
Rotating anisotropy

MCTDHB(4): Rotating anisotropy $\epsilon_{max} = \omega_x/\omega_y = 0.9$, $g = 17.4$, $N = 100$, $\Omega = 0.78$



Rotating anisotropy[7]

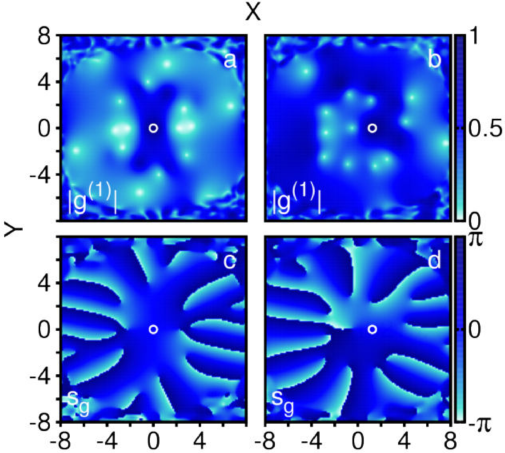
Phantom vortices in the orbitals



[7] Angular momentum in interacting many-body systems hides in phantom vortices, S. Weiner, M.C.T., L.S. Cederbaum and A.U.J. Lode, *submitted*, arXiv:1409.7670.

Rotating anisotropy[8]

Phantom vortices in the correlation function

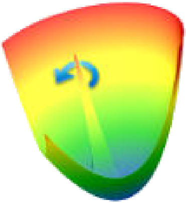


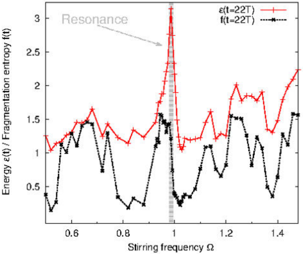
[8] Angular momentum in interacting many-body systems hides in phantom vortices, S. Weiner, M.C.T., L.S. Cederbaum and A.U.J. Lode, *submitted*, arXiv:1409.7670.

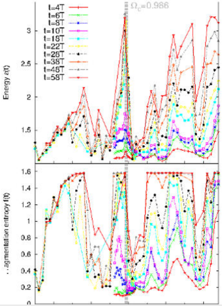
Stirred 2D gas

Numerical experiment: stir a Bose gas with a Gaussian thread, at various frequencies Ω and find out what happens after some time τ in the:

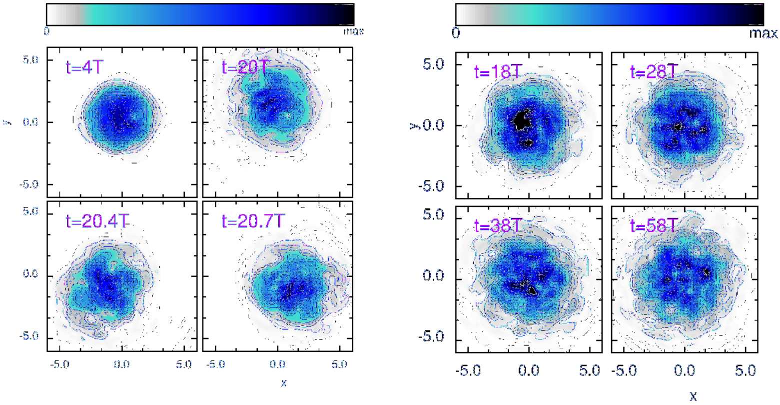
1- energy
2- fragmentation
3- bulk of the gas (excitations)







$\Omega = 0.986, \quad \Omega = 1.24$[9]

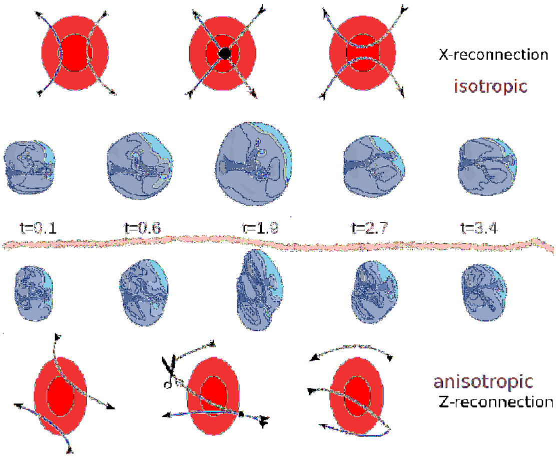


Occupation number quickly increase to $n_1 = n_2 = n_3 = N/3$.

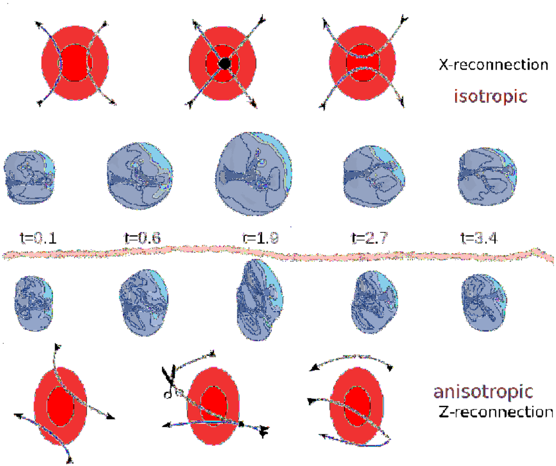
[9] MCT and A.U.J. Lode, arXiv:1410.0414

Quantum Vortex reconnections

Transient, out of equilibrium process; topology-changing mechanism that plays a role in turbulence



X-reconnection vs Z-reconnections[10]



[10] T. Wells, A.U.J. Lode, V.S. Bagnato and M.C. Tsatsos, arXiv:1410.2859

The Package

Guantum and Recursive MCTDHB

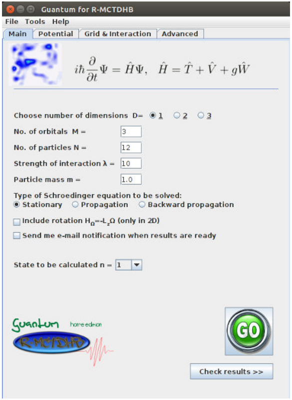
Powerful package that:

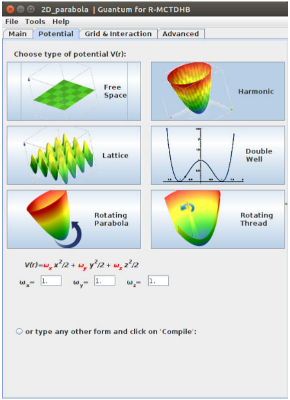
- is the latest numerical implementation to solve the MCTDHB equations of motion
- is accessible to anyone and user friendly (command-line level or graphical with *Guantum*)
- trivially sets up calculations for any trap geometry and no. of dim, various numerical integrators
- calculates 1st order densities of fragments and plots images and videos of their time evolution
- calculates 2nd and higher order correlations

Visit ultracold.org!!!

http://ultracold.org

Guantum


Guantum for R-MCTDHB
File Tools Help
Main Potential Grid & Interaction Advanced
$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \quad \hat{H} = \hat{T} + \hat{V} + g\hat{W}$
Choose number of dimensions D= 1 2 3
No. of orbitals M = 3
No. of particles N = 12
Strength of interaction λ = 10
Particle mass m = 1.0
Type of Schroedinger equation to be solved:
Stationary Propagation Backward propagation
Include rotation H_Ω=-$L_z\Omega$ (only in 2D)
Send me e-mail notification when results are ready
State to be calculated n = 1
GO
Check results >>


2D_parabola | Guantum for R-MCTDHB
File Tools Help
Main Potential Grid & Interaction Advanced
Choose type of potential V(r):
Free Space
Harmonic
Lattice
Double Well
Rotating Parabola
Rotating Thread
$V(r)=\omega_x x^2/2 + \omega_y y^2/2 + \omega_z z^2/2$
ω_x= 1. ω_y= 1. ω_z= 1.
or type any other form and click on 'Compile':

Summarize

Outlook

- Fragmentation and loss of coherence appear in rotating systems
- Vortices are possibly nucleated through fragmentation (stirred gas)
- Quantum turbulent can be better understood under this perspective; QVR as the fundamental mechanism
- R-MCTDHB easy to install / play around; visit ultracold.org!
- See our youtube channel: Quantum Cinema!

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Long- and short-term visits available!