Temperature and stochasticity in PDE model numerics for Bose Einstein condensates

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The Gross-Pitaevskii equation (GPE)

Simplest "one particle" approximation : Gross-Pitaevskii equation (i.e. cubic NLS with confinement potential)

$$i\hbar\frac{\partial}{\partial t}\psi(\mathrm{x},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{ext}}(\mathrm{x},t) + g|\psi(\mathrm{x},t)|^2\right)\psi(\mathrm{x},t)$$

V_{ext} = time dependent confining potential : anisotropic ("cigar shape" BEC)

coupling constant: g $= N \cdot \frac{4\pi\hbar^2 a_s}{m}$
(Note : g is somewhat a modeling parameter,
g positive or negative : "defocussing" or "focussing" NLS !)

normalization: $\|\psi(\cdot,t)\| = \int |\psi(\mathrm{x},t)|^2 d\mathrm{x} = 1$

$\psi(\mathrm{x},t=0) = \psi_I$ = Ground state for $V_{\mathrm{ext}}(t=0)$ parabolic

"Hartree Condensate ansatz" for N-body problem

GPE is the simplest "one particle" approximation of
the "N particle Schrödinger equation with contact interaction"

"Bosons" : class of quantum particles,
many particle wavefunction is symmetrized.
Example : photons, phonons, atoms

"Condensate" : N bosons occupy the same quantum state

$$\Psi(x_1, ..., x_N) = \prod_{1 \leq i \leq N} \psi(x_i)$$

Note : This is sometimes called "Hartree ansatz",
indeed it is a special case of the general Hartree ansatz, where the one particle wavefunctions $\psi_j(x_i)$ are different.

The extended Gross-Pitaevskii equation (eGPE)
Simulation of dipolar Bose-Einstein condensates

Extended Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = (GPE)\,\psi(x,t) + \Big[\Phi(x,t) + \gamma_{qf}|\psi(x,t)|^3 - \frac{i\hbar L_3}{2}|\psi(x,t)|^4\Big]\psi(x,t)$$

with

$$\Phi(x,t) = \frac{\mu_0\mu^2}{4\pi}\int U(x-x')|\psi(x',t)|^2\,dx'$$

describing dipole-dipole interactions

$\gamma_{qf}|\psi(x,t)|^3$ is the Lee-Huang-Yang beyond mean-field correction to include the effect of quantum fluctuations

$\frac{i\hbar L_3}{2}|\psi(x,t)|^4$ models three-body loss processes

Extended Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = (GPE)\,\psi(x,t) + \Big[\Phi(x,t) + \gamma_{qf}|\psi(x,t)|^3 - \frac{i\hbar L_3}{2}|\psi(x,t)|^4\Big]\psi(x,t)$$

Numerical solution

Time-splitting spectral method (split-step Fourier method) [Weizhu Bao, Shi Jin, P. Markowich 2002]

The dipolar interaction potential $\Phi(x,t)$ can be evaluated with spectral accuracy using the *fast convolution with free-space Green's functions approach* [F. Vico, L. Greengard, M. Ferrando 2016]

Extended Gross-Pitaevskii equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = (GPE)\,\psi(x,t) + \Big[\Phi(x,t) + \gamma_{qf}|\psi(x,t)|^3 - \frac{\imath\hbar L_3}{2}|\psi(x,t)|^4\Big]\psi(x,t)$$

Optimal control problem

Find time-evolution of the s-wave scattering length a_s and the trap frequencies ω_ρ and ω_z such that

$$\mathcal{J}(\psi(T)) = \big(N_0 - |\langle\psi_d, \psi(T)\rangle|\big)^2$$

is minimized

desired state ψ_d, final time T, number of atoms N_0

Numerical solution

Parameterize the control inputs a_s, ω_ρ and ω_z by means of B-spline functions

$$u(c,t) = \sum_{k=1}^{K} c_k N_{k,p}(t),$$

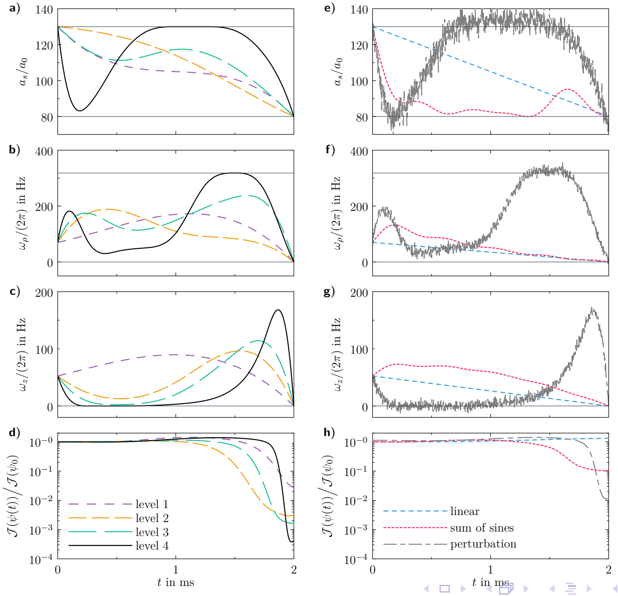
where $N_{k,p}$ denotes the kth B-spline basis function of polynomial order p

Solve a finite dimensional optimization problem, i.e., determine an optimal coefficient vector c collecting the B-spline coefficients of all control inputs

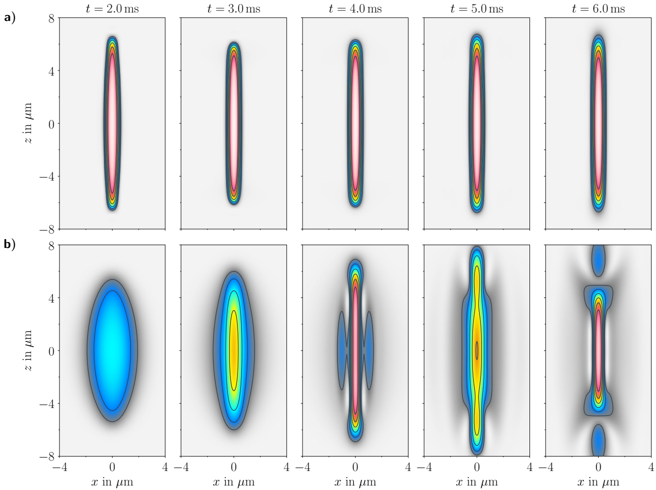
Speed up the solution process by employing a multilevel (hierarchical) basis approach, i.e., solve a sequence of optimization tasks with ever increasing complexity

J.-F. Mennemann, T. Langen, L. Exl, and N.J. Mauser, "Optimal control of the self-bound dipolar droplet formation process", *Comput. Phys. Commun.* 244, 205 (2019))

The extended Gross-Pitaevskii equation
Simulation of dipolar Bose-Einstein condensates



Time-evolution of the density after final time T



Top row: optimized control inputs, bottom row: linear control inputs

Experiment: Matter-wave interference in a double well

Analogous to the double-slit experiment for photons (light),
but now for atoms (rubidium) of a Bose-Einstein condensate (BEC)

- Creation of BEC at extremely low temperatures ($\sim 10\,\mathrm{nK}$), sophisticated cooling techniques necessary
- BEC confined in a trap: harmonic potential well, realized with combination of static and radio-frequency (RF) magnetic fields, numerical simulation starts here
- Splitting the condensate: splitting single well $\rightarrow$ double well by slowly changing parameters of RF-currents
- Free expansion: Sudden switch off of the external potential, recombine BEC clouds in time-of-flight expansion
- Measurement of interference pattern, ... *(show movie of experiment)*

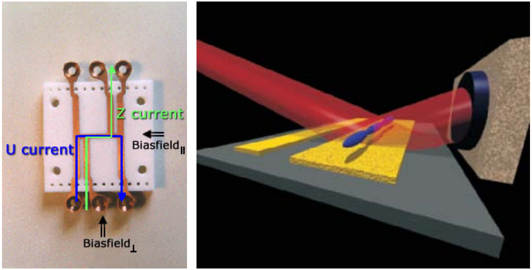


Figure: Left: Photograph of the macroscopic wire structures mounted underneath the atom chip. Right: Simulation of the experimental set-up. A Bose-Einstein condensate (blue) is created and trapped by a current-carrying wire (gold) mounted on the silicon surface of the atom chip (grey). The laser beam (red) from a CCD camera indicates the imaging assembly. Allocated by the AtomChip Group.

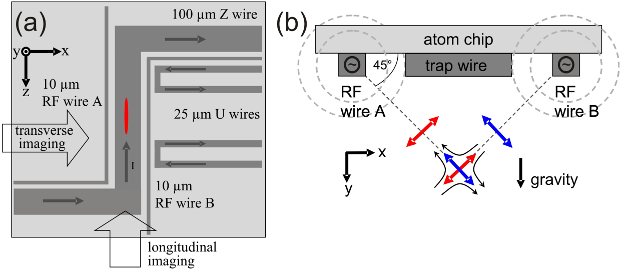
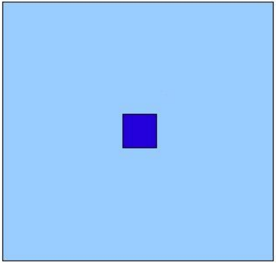


Figure: Schematic of the three-wire rf trap (a) top view, (b) side view from the longitudinal direction. Allocated by the AtomChip Group.

Rescaling of Domain

Free flight phase:

- Fast expansion of condensate $\Rightarrow$ expansion of computational domain

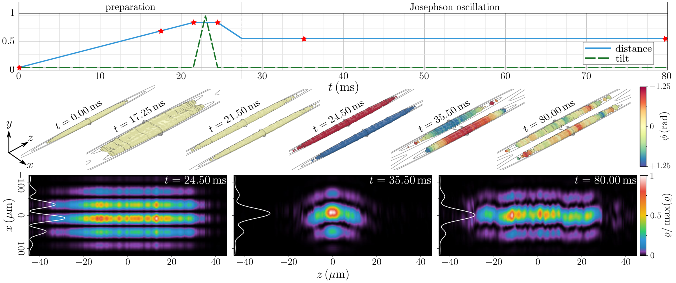


- Density low $\Rightarrow$ dynamics of condensate may be modelled by the free (linear) Schrödinger equation ($g = 0$)
- Kinetic step implemented with "pruned" FFTs

Simulation of a BEC at finite temperature

Numerical verification of the main experimental findings in a recent experiment:

M. Pigneur, T. Berrada, M. Bonneau, T. Schumm, E. Demler, and J. Schmiedmayer, "Relaxation to a Phase-locked Equilibrium State in a One-dimensional Bosonic Josephson Junction", *Phys. Rev. Lett.* 120, 173601 (2018).



Top: external parameters, center: density and phase, bottom: time of flight

GPE beyond zero temperature : "stochastic GPE"

Gross-Pitaevskii Equation with "stochasticity" :

A) "stochastic GPE" (SGPE)

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = (GPE)\,\psi(x,t) + \Omega(x,t) + iV_{absorb}(x,t)\psi(x,t)$$

where $\Omega(x,t)$ = white noise in x and t,

and possibly this comes with an "absorbing potential" $iV_{absorb}(x,t)$:

Note : in more than 1-d the "wave-function" ψ is not in L^2 but rather a "rough path".

GPE beyond zero temperature : "Truncated Wigner Approach"

Gross-Pitaevskii Equation with "stochasticity":

B) "GPE with random initial data"

$$i\hbar\frac{\partial}{\partial t}\psi(\mathrm{x}, t) = (GPE)\,\psi(\mathrm{x}, t)$$

,

with initial data a probability distribution for the amplitude A and/or phase ϕ

$\psi(x, t = 0) = A(x, t)exp(i\phi(x, t,))$

Take a "realization A_k, ϕ_k of the random distribution of $A(x, t = 0)$ and/or $\phi(x, t = 0)$
and compute the deterministic evolution.
Then "average" over a sufficiently large "sample" $(k = O(500))$.

Simulation of a BEC at finite temperature
GPE = "mean field" = "Classical fields" simulation

Solve the Gross-Pitaevskii equation (GPE)

$$i\hbar \frac{\partial}{\partial t}\psi(\boldsymbol{r}, t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}, t) + \frac{4\pi\hbar^2 a_s}{m}|\psi(\boldsymbol{r}, t)|^2\right]\psi(\boldsymbol{r}, t),$$
$$\psi(\cdot, 0) = \psi_0(\boldsymbol{r})$$

many times using a different initial condition $\psi_0(\boldsymbol{r})$ in each single run.

The initial condition of every single run is prepared in a two-stage process:

- First, compute a ground state solution $\psi_0(\boldsymbol{r})$ of the GPE using imaginary time propagation. Take into account atom number fluctuations by normalizing $\psi_0(\boldsymbol{r})$ to a desired atom number N from a given distribution $\mathcal{N}(\bar{N}, \sigma_N^2)$.
- Second, imprint thermal noise to $\psi_0(\boldsymbol{r})$ by means of a suitable thermal noise sampling process.

Different methods are available to imprint thermal noise to $\psi_0(\boldsymbol{r})$:

- The Metropolis-Hastings algorithm

Pjotrs Grišins and Igor E. Mazets, "Metropolis-Hastings thermal state sampling for numerical simulations of Bose-Einstein condensates", *Computer Physics Communications* 185 (2014).

- The stochastic Gross-Pitaevskii equation

P. B. Blakie, A. Bradley, M. Davis, R. Ballagh, and C. Gardiner, "Dynamics and statistical mechanics of ultra-cold Bose gases using c-field techniques", *Adv. Phys.* 57, 363 (2008).

The second approach turned out to be more efficient in our application.

Simulation of a BEC at finite temperature
SGPE simulation

Propagate the zero temperature ground state solution $\psi_0(\boldsymbol{r})$ using the stochastic Gross-Pitaevskii equation (SGPE)

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) &= (1-i\gamma)\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r},0) \\
&\qquad + g|\psi(x,t)|^2 - \mu\Big]\psi(\boldsymbol{r},t) + \eta(\boldsymbol{r},t), \\
\psi(x,0) &= \psi_0(\boldsymbol{r})
\end{aligned}
$$

until a new quasi-stationary thermal state is reached.

μ: chemical potential of the eigenvalue problem at zero temperature
γ: positive, freely tunable parameter to improve the speed of convergence
η: complex, Gaussian, white noise process with correlations

$$\langle \eta^*(\boldsymbol{r},t)\,\eta(\boldsymbol{r}',t')\rangle = 2\hbar\gamma k_{\mathrm{B}} T\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')$$

T: temperature

Simulation of a BEC at finite temperature
SGPE simulation

Propagate the zero temperature ground state solution $\psi_0(\boldsymbol{r})$ using the stochastic Gross-Pitaevskii equation (SGPE)

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = (1 - i\gamma)\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r},0) + g|\psi(\boldsymbol{r},t)|^2 - \mu\Big]\psi(\boldsymbol{r},t) + \eta(\boldsymbol{r},t),$$

$$\psi(\boldsymbol{r},0) = \psi_0(\boldsymbol{r})$$

until a new quasi-stationary thermal state is reached.

The numerical propagation of the SGPE is based on:

- a second-order accurate operator splitting
- spatial derivatives are approximated by means of the Fourier spectral collocation method
- the thermal noise term η is assumed to be constant for the duration of every time step

Simulation of a BEC at finite temperature
SGPE simulation

Propagate the zero temperature ground state solution $\psi_0(\boldsymbol{r})$ using the stochastic Gross-Pitaevskii equation (SGPE)

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = (1-i\gamma)\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r},0) + g|\psi(\boldsymbol{r},t)|^2 - \mu\Big]\psi(\boldsymbol{r},t) + \eta(\boldsymbol{r},t),$$

$$\psi(\boldsymbol{r},0) = \psi_0(\boldsymbol{r})$$

until a new quasi-stationary thermal state is reached.

Normalize the wave function after each time step to preserve the exact atom number distribution already included in the first stage of the algorithm.

Problem:
For strongly elongated condensates (typically realized in atom chip experiments) the above outlined thermal state sampling process may results in unrealistic excitations along the tightly confined transverse directions (x and y) of the trap.

Two possible solutions:

1st solution: Projected stochastic GPE: project the wave function onto a few of the lowest energy single particle eigenstates of the harmonic trap after every time step.

For strongly elongated condensates (typically realized in atom chip experiments) the above outlined thermal state sampling process may results in unrealistic excitations along the tightly confined transverse directions (x and y) of the trap.

Two possible solutions:

2nd solution: Use a modified (quasi one-dimensional) thermal noise term

$$\eta(\boldsymbol{r}) = \lambda(z)\psi^{\perp}(x, y, z), \;\; \psi^{\perp}(\boldsymbol{r}) = \psi(\boldsymbol{r})/\sqrt{\rho(z)}$$

with

$$\rho(z) = \int\int |\psi(x, y, z)|^2 \, dxdy$$

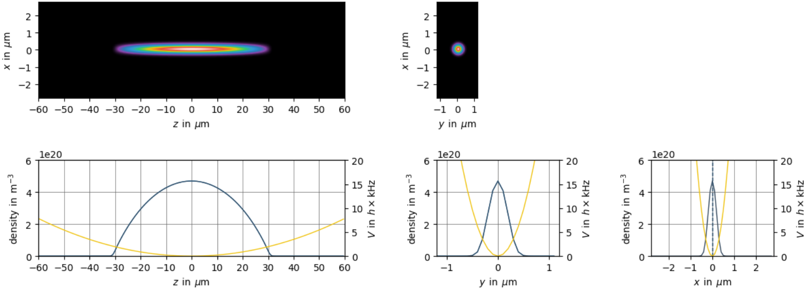
and one-dimensional Gaussian white noise λ with zero mean and variance

$$\langle \lambda^*(z, t)\, \lambda(z', t')\rangle = 2\hbar\gamma k_{\mathrm{B}} T \delta(z - z')\delta(t - t').$$

Simulation of a BEC at finite temperature
GPE simulation

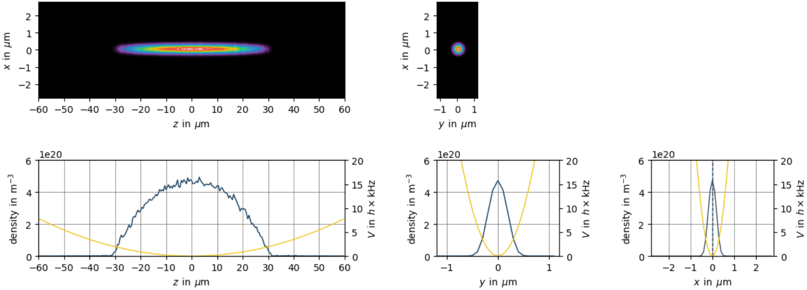
Prepared initial states using different temperatures:

$T = 0\,\mathrm{nK}$



Prepared initial states using different temperatures:

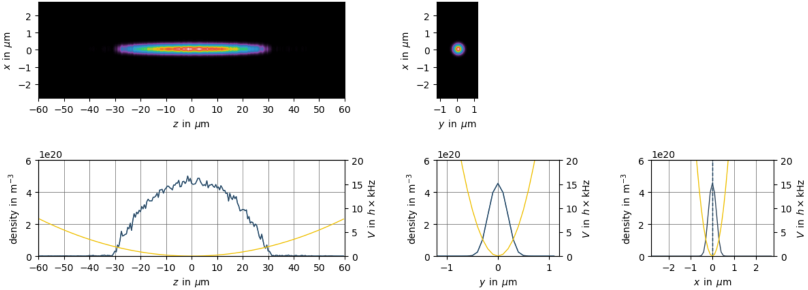
$T = 5\,\mathrm{nK}$



Simulation of a BEC at finite temperature
GPE simulation

Prepared initial states using different temperatures:

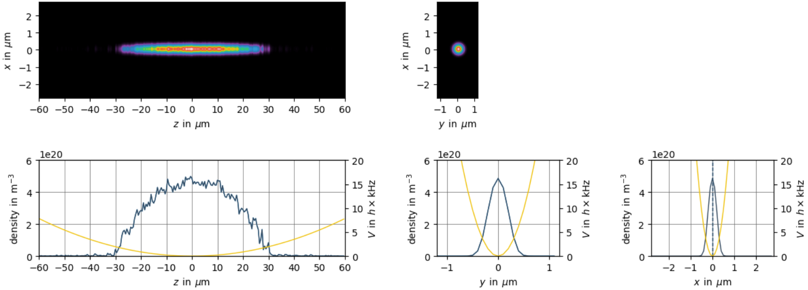
$T = 10\,\mathrm{nK}$



Simulation of a BEC at finite temperature
GPE simulation

Prepared initial states using different temperatures:

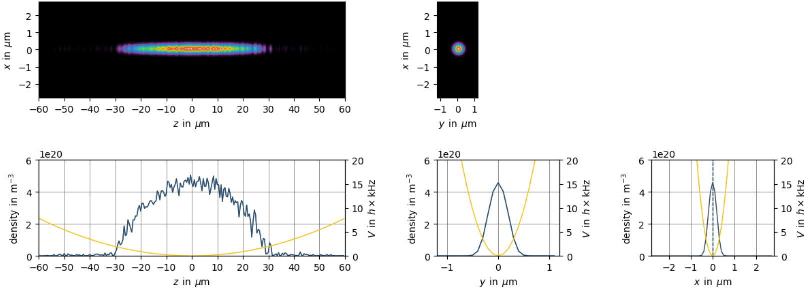
$T = 20\,\mathrm{nK}$



Simulation of a BEC at finite temperature
GPE simulation

Prepared initial states using different temperatures:

$T = 40\,\mathrm{nK}$



The temperature of the condensate may be estimated using the g_1 auto correlation function

$$g_1(\delta_z) = \mathrm{Re}\left[\frac{\psi_z^*(0)\psi_z(\delta_z)}{|\psi_z(0)\psi_z(\delta_z)|}\right], \quad \delta_z \geq 0,$$

where ψ_z denotes the restriction of the wave function to the line along the longitudinal direction at the center of the trap.

For a system in thermal equilibrium we
expect (approximate Bose-Einstein statistics by Rayleigh-Jeans)

$$g_1(\delta_z) = e^{-\delta_z/\lambda_T}$$

with the thermal coherence length

$$\lambda_T = \frac{2\hbar^2 \bar{n}}{m k_B T}$$

and the mean density of the condensate $\bar{n}$.