Quantics Tensor Train for solving Gross-Pitaevskii equation

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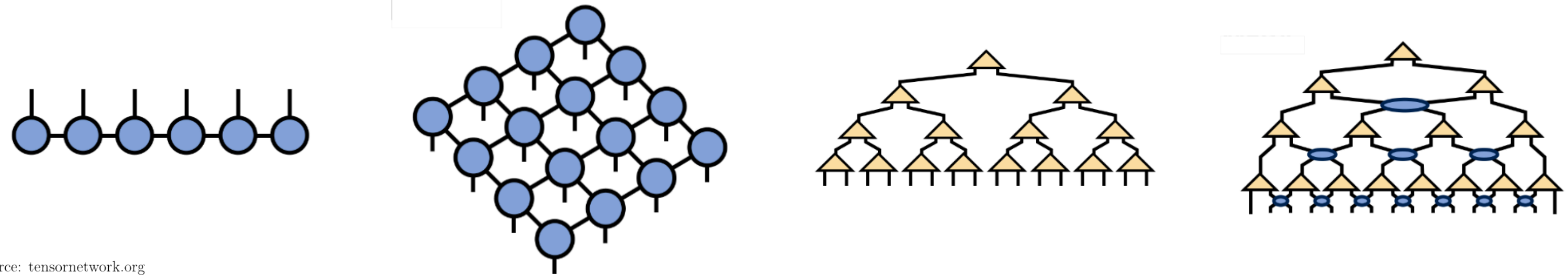
Tensor Networks

Tensor networks were introduced to efficiently represent tensors with exponentially many parameters by expressing them as a network contraction of smaller tensors.



source: tensornetwork.org

They were developed in the context of many-body quantum physics to simulate strongly correlated systems. However, over time their utility has proven to extenst beyond quantum mechanics.

Quantics Tensor Trains

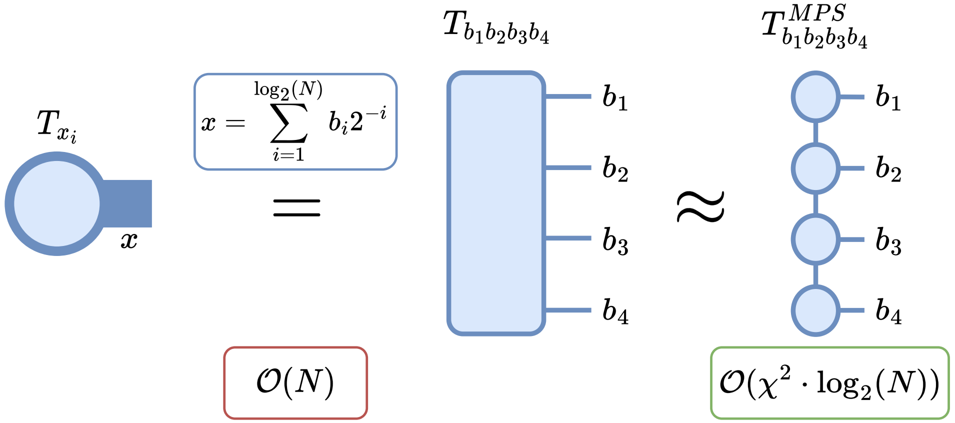
Quantic Tensor Trains (QTT) or Matrix Product States (MPS) are one dimensional tensor networks that:

- The efficient representation ground state of one-dimensional gapped Hamiltonians, solutions of DMRG.
- Represents strongly correlated one-dimensional many-body systems and Markov chains.

In reccent years, it has been shown that they are also able to compress a wide set of analytical *one-dimensional* functions.

Quantics Tensor Trains

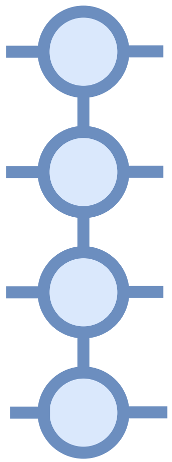
To encode an analytical function $f(x) : [a, b) \rightarrow \mathbb{R}$ we first discretize your domain $x_i \in \Lambda$ and we try to compress $T_{x_i} = f\left(\{x_i\}_{x_i \in \Lambda}\right)$.



The ability to compress the MPS is dictated by the **bond dimension** (χ), which will determine whether the compression is efficient.

Quantics Tensor Trains

To represent operators that act onto QTTs, there is a generalization of the MPS, the matrix product operator (MPO).



If we have an MPS with bond dimension χ and an MPO with bond dimension k, then the MPO-MPS contraction scales as

$$\mathcal{O}\left(4\log_2\left(N_{grid}\right)\left(\chi^2 k^2 + \chi^3 k\right)\right)$$

Gross-Pitaevskii Equation

The Gross-Pitaevskii equation is a nonlinear Schrödinger equation that describes dilute Bose gases. It is widely used to model Bose Einstain condensates (BEC).

Gross-Pitaevskii Equation

The simplest Gross-Pitaevskii equation (GPE) includes a BEC interacting with an external potential, and it follows

$$i\hbar\partial_t\psi(x,t) = \left(\hat{H}_0 + gN\,|\psi(x,t)|^2\right)\psi(x,t)$$

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The GPE can be generalized to different physical scenarios

- **Long-range interactions:** We assume the mean-field approximation of a two-body interacion, which follows the convolution

$$V_{LR}(x) = \int dx'\,|\psi(x',t)|^2\,W(|x-x'|)$$

Gross-Pitaevskii Equation

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The GPE can be generalized to different physical scenarios

- **Different BEC species:** The GPE equation can track the evolution of M different BEC species, this equation sometimes is called coupled GPE

$$i\hbar\partial_t\psi_{i(x,t)} = \left(\hat{H}_0 + \sum_{j=0}^{M} g_{ij}\sqrt{N_i N_j}\,|\psi_{j(x,t)}|^2\right)\psi_{i(x,t)} + \sum_{j\neq i}\lambda_{ij}\psi_j(x)$$

Gross-Pitaevskii Equation

To simulate the GPE with QTT we need the following elements

1. **Represent the linear differential equation**
    1. Initial wave-function ($\psi_0(x)$)
    2. Linear Hamilonian (H_0): Kinetic and local potential terms

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2. **Represent the non-linear term $g|\psi(x)|$**
3. **Represent the long-range interaction**
4. **Represent different BEC species**
   1. Generalize the linear Hamiltonian
   2. Generalize the non-linear term
   3. Create the tunneling term $\lambda_{ij}\psi_j(x)$

QTT Toolbox

Load analytical functions into MPS

To load an analytical function $f(x) : \mathbb{R} \to \mathbb{R}$ into a MPS there are several methods.

1. Brute force: $\mathcal{O}\left(N_{grid}\right)$ evaluations
2. Tensor Cross Interpolation: $\mathcal{O}\left(\log_2\left(N_{grid}\right)\right)$ evaluations
3. Chebyshev Interpolation: $\mathcal{O}\left(\log_2\left(N_{grid}\right)\right)$ evaluations

The wavefunction can be loaded into an MPS with any of these methods, the same happens with the local potential which can be then updated to a MPO through Kroenecker δ's.

Translation operators

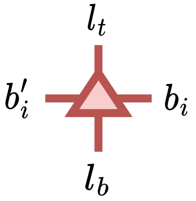
The translation operator of a function

$$\mathcal{T}_a(f(x)) = \int dx' \delta(x' - (x-a)) = f(x-a)$$

can be implemented through the *ripple carry algorithm* and corresponds to an MPO of bond dimension $(\chi = 2)$.

$a = \sum_i a_i 2^{-i}$

$\boxed{\mathcal{T}^{(a_i=0)}_{l_t,b_i,b'_i,l_b}}$



$\mathcal{T}^{(a_i=0)}_{0,0,0,0} = 1$

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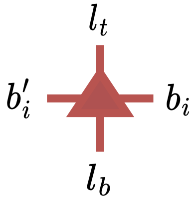

$\mathcal{T}^{(a_i=1)}_{0,0,1,0} = 1$

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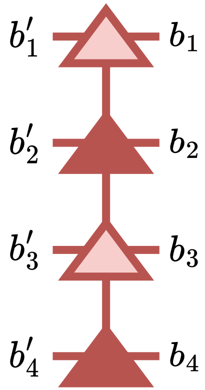


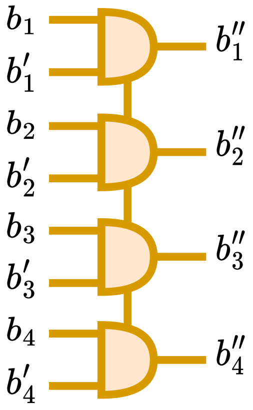
$\mathcal{T}_a = \delta(y - (x-a))$

Convolution operators

The convolution operator transforms a function

$$\mathcal{C}(f(x)) = \int dx' \delta(x' - (x-y)) = f(x-y)$$

can be implemented through the *ripple carry algorithm* and corresponds to a generalized MPO (with 3 external legs) of bond dimension $(\chi = 2)$.



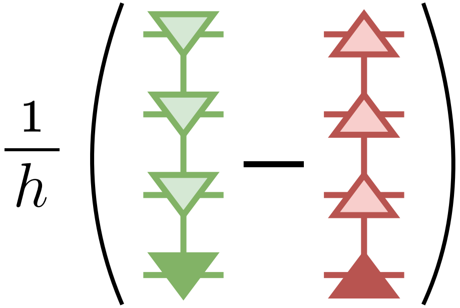
$\mathcal{C} = \delta(x' - (y+x))$

Differential operator

We can create approximate the differential operator through central finite differences,

$$f'(x) = \frac{f(x+h) - f(x-h)}{h}$$

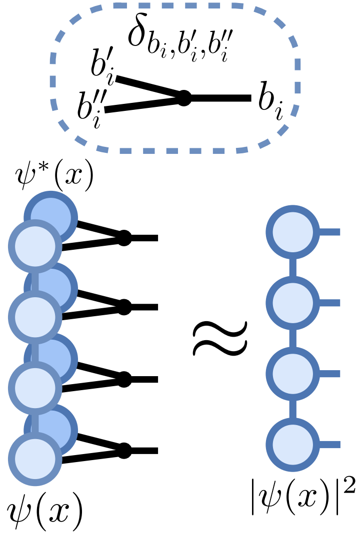
This expression can be constructed with the translation operators and δ-functions.



Non-linearlity

The difference between the Schrödinger equation and the GPE are the non-linear interactions, the terms $|\psi(x)|^2$. The term can be created upgrading one $\psi(x)$ to an MPO (with Kroenecker δ's) and then perform MPO-MPS contraction.

This operation is often the bottle-neck of the simulations. It scales as $\mathcal{O}(8\log_2(N_{grid})\chi^4)$. There are other possible options like TCI or the paper "Tensor Train multiplication" by A. A. Michailidis et al. (2024).



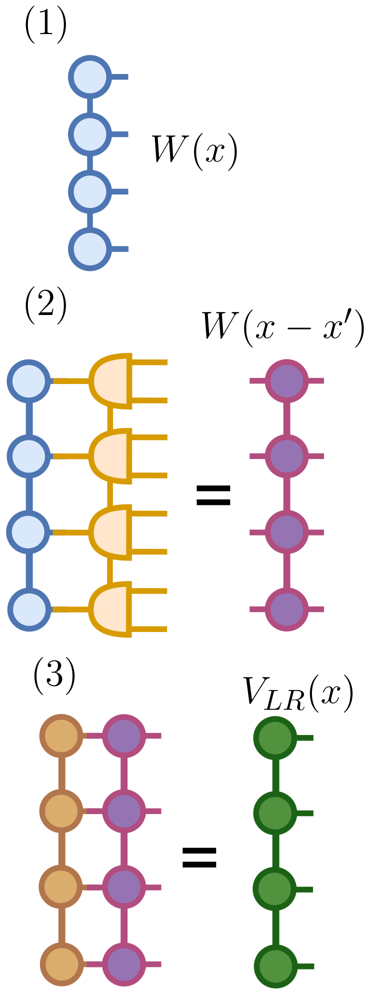
Long-Range Potential

To create a long-range potential of the form

$$V_{LR}(x) = \int dx' W(x-x')|\psi(x')|^2$$

The long-range potential can be created with 3 steps,

1. Load the potential shape $W(x)$.
2. Use the convolution operator to create $W(x-x')$.
3. Perform the MPO-MPS contraction with $|\psi(x)|^2$ to create $V_{LR}(x)$.

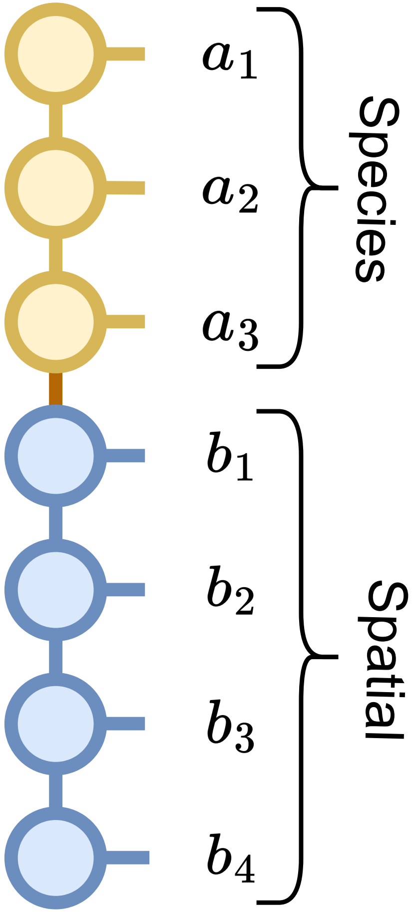


Multiple BEC species

To solve the multiple species Gross-Pitaevskii we encode the different species in the sites of the Tensor Train. If we have M species and $a \in \{1, \ldots, M\}$. Writing

$$a = \sum_{j=0}^{\log_2(M)} a_i 2^i$$

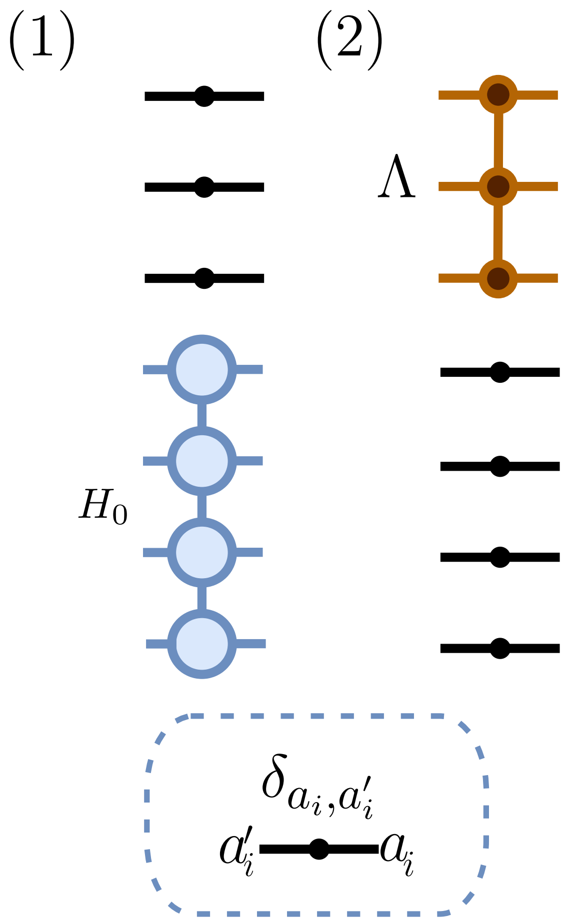
The MPS can be separated in a part involving the different BEC species and another that takes into account the different degrees of freedom.



Multiple BEC species

Now, we need to adequate all the terms in the cGPE to work in this set-up.

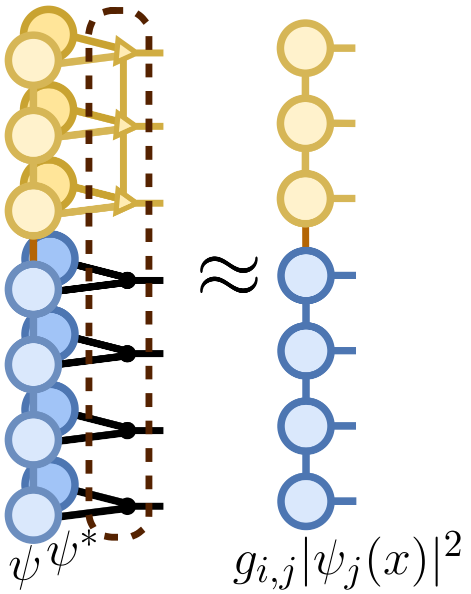
1. **Local Hamiltonian:** all species act individually therefore, there are no correlations between species and spatial degrees of freedom.
2. **Tunneling term:** There is only mixing of different species, there is no action in space. Therefore we only need to turn the tunneling matrix (λ_{ij}) to the MPO, Λ.

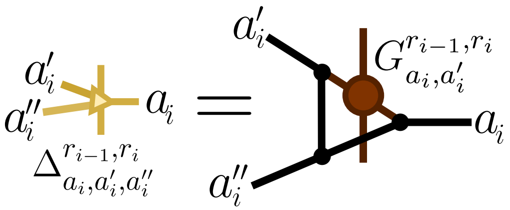


Multiple BEC species

The last term that we need to adapt is the interaction term. On the spatial sites we need to introduce the Kroenecker δ's while the species part we need to turn the interaction matrix (g_{ij}) into an MPO (G).

These elements allow us to create the generalized MPO to compute the non-linear interaction term.





Ground State

The ground state of the GPE is found through imaginary time evolution,

$$\psi_{gs}(x) = \lim_{\tau \to \infty} \frac{\exp\left(-\tau \hat{H}_{GP}\right)|\psi_0\rangle}{\sqrt{\langle\psi_0|\exp\left(-\tau \hat{H}_{GP}\right)|\psi_0\rangle}}$$

which can be found iteratively by

$$\tilde{\psi}_n = \psi_{n-1} - d\tau \hat{H}_{GP}\psi_{n-1}; \psi_n = \frac{\tilde{\psi}_n}{\sqrt{\int dx \ |\tilde{\psi}_n|^2}}$$

We evolve it until energy convergence:

$$E = \int dx \left(\psi_n^* \hat{H}_{GP}\psi_n - \frac{1}{2} g N \ |\psi_n|^4\right)$$

Time Evolution

The Runge-Kutta 4 (RK4) is a method to solve any initial value problem

$$\partial_t \psi = f(\psi, t); \psi(x, 0) = \psi_0(x)$$

$$f(\psi, t) = -i\left(-\frac{1}{2}\partial_{xx} + V + gN|\psi(x)|^2\right)\psi(x)$$

The RK4 solver finds $\psi(t + dt)$ as a function of $\psi(t)$ by solving

$$\psi(t + dt) = \psi(t) + \tfrac{dt}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = f(\psi(t), t); \quad k_2 = f\left(\psi(t) + \tfrac{dt}{2} \cdot k_1, t + \tfrac{dt}{2}\right)$$

$$k_3 = f\left(\psi(t) + \tfrac{dt}{2} \cdot k_2, t + \tfrac{dt}{2}\right); \quad k_4 = f(\psi(t) + dt \cdot k_3, t + dt)$$

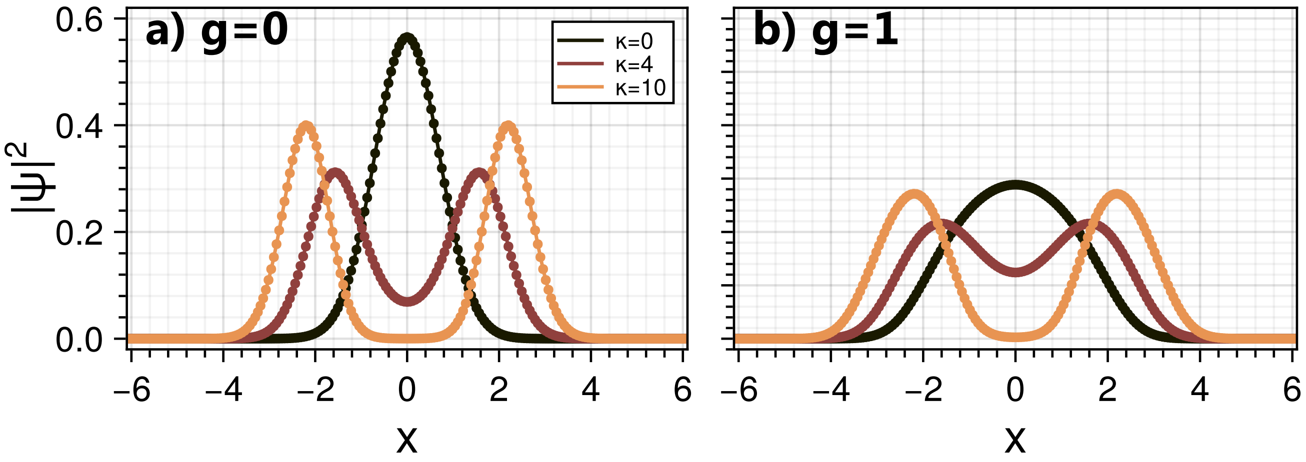
Applications

Double-well potential ground state

We describe the ground state of bosons in an harmonic trap experiencing a Gaussian barrier at the center $x = 0$.

$$\hat{H}_0 = -\frac{1}{2}\partial_{xx} + \frac{1}{2}x^2 + \kappa \exp(-x^2)$$

$\psi_0(x)$ is the Thomas-Fermi distribution.



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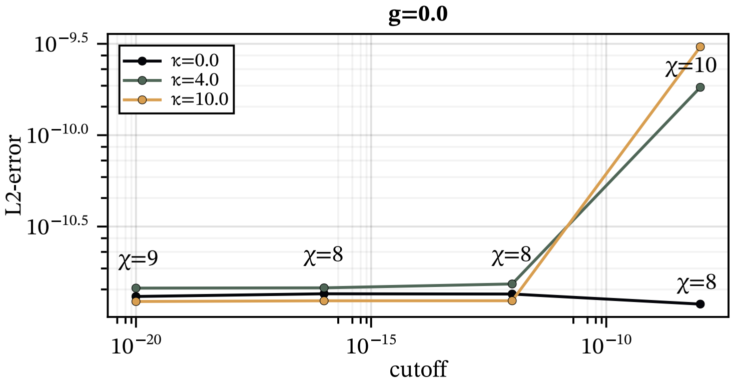
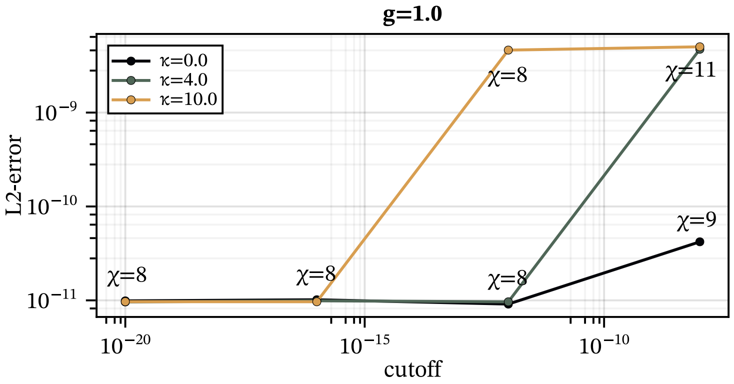




Long-range potential

Long-range interactions induced by Ryberg-dressed interactions on the ground state of a BEC. The induced interactions follow

$$W(r) = \beta \frac{C_6}{R_B^6 + r^6}$$

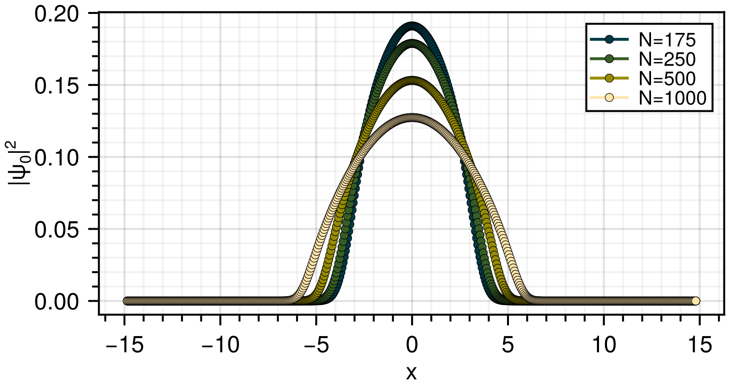
If the radius of the BEC is smaller than the blockade radius, the Rydberg-dressed interaction result in a non-linear potential

$$V_{LR} = \int dx \; |\psi(x)|^2 \; W(x - x')$$

Long-range potential

To measure the effect of the long-range interactions the proposed set-up

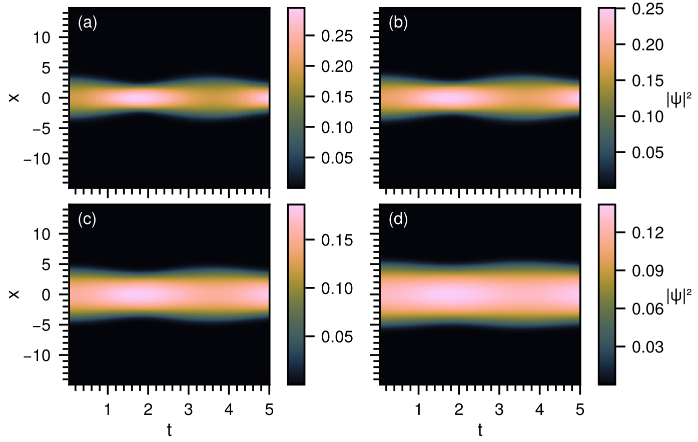
1. Prepare the ground state in an harmonic trap with lasers turned on.

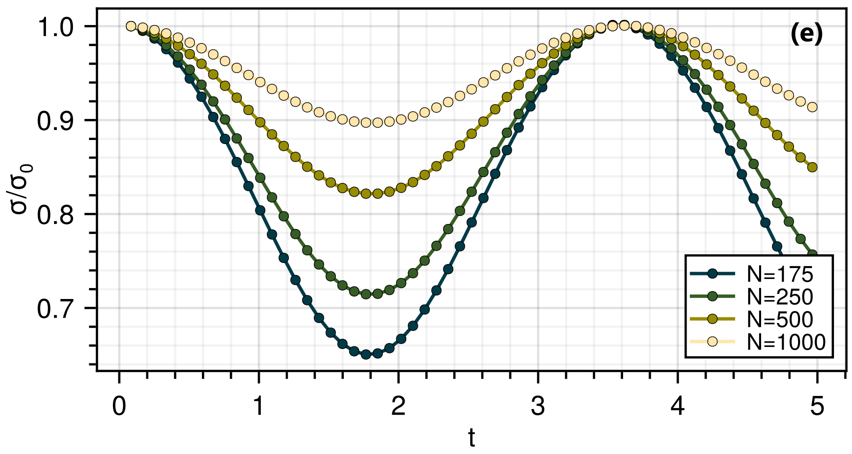


2. The lasers are switched-off and the system evolves under the Gross-Pitaevskii equation.

Long-range potential

After the quench, the wavefunction begins breathing oscillations whose frequency depends on β and the amplitude on gN. The breathing oscillations can be measured by computing evolution of the standard devitaion $\frac{\sigma(t)}{\sigma(0)}$.





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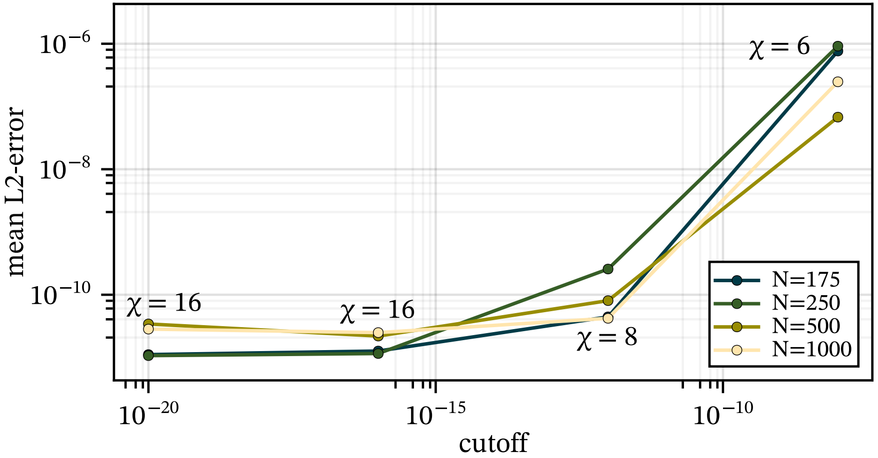
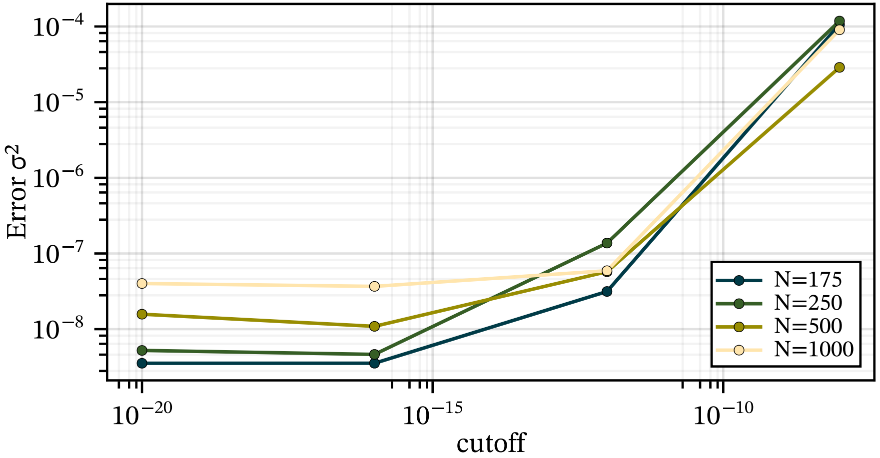




Multiple species

In this case, we look at the real time evolution of the coupled Gross-Pitaevskii equation.

$$i\hbar\partial_t\psi_{i(x,t)} = \left(\hat{H}_0 + \sum_{j=0}^{M} g_{ij}\sqrt{N_i N_j}\,\left|\psi_{j(x,t)}\right|^2\right)\psi_{i(x,t)} + \sum_{j\neq i}\lambda\psi_j(x)$$

In this study $g_{ii} = 1$ and $g_{ij} = g$ otherwise. The initial wave-function is

$$\psi_{0j} = \frac{1}{2}\,\text{sech}\left(x - \mu_j\right)e^{i\frac{p_{0j}}{4}x}$$

Multiple species

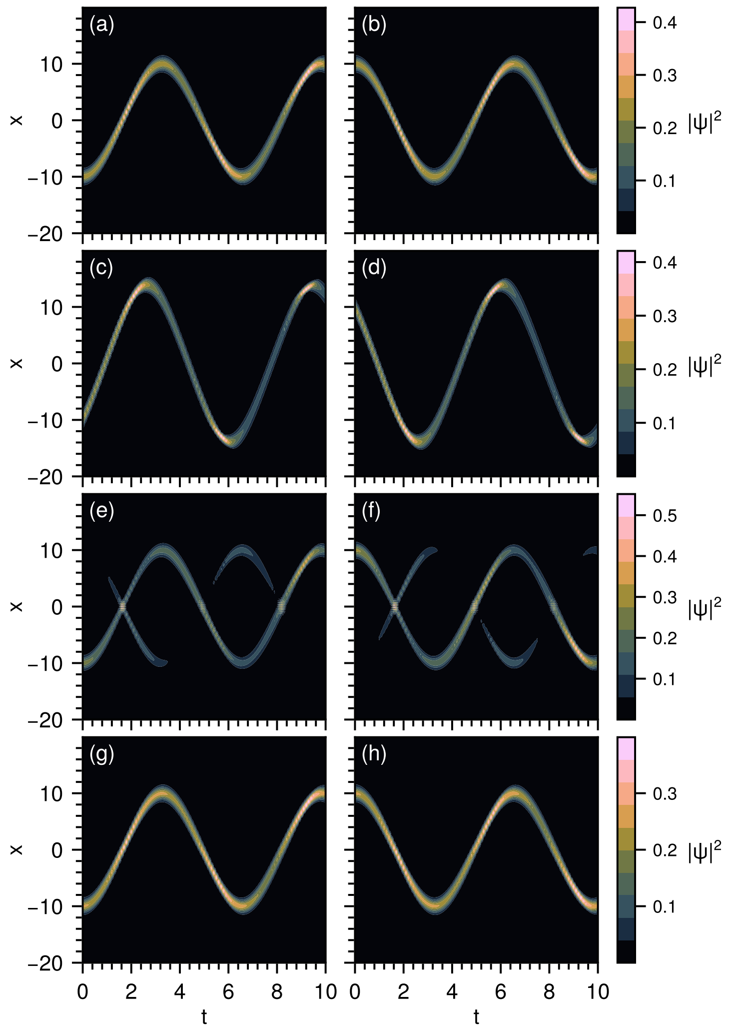
Results for different coupled GPE. Left and right panels correspond to different species.

(a-b) Non-interacting GPE.

(c-d) Non-interacting $p_0 \neq 0$

(e-f) Tunneling between species

(g-h) Non-linear interaction between species.



Thanks for your attention!

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Long-range errors