



# Bose-Einstein Condensation (BEC)

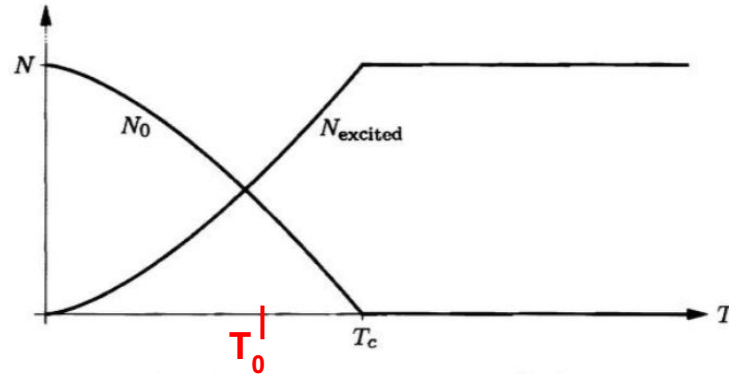
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# Outline

- Introduction: Bose Einstein Condensate
  - What is Bose-Einstein Condensation?
  - Experimental Evidence
- Code Goals & Design
- Mean Field Approach: GPE Equation
- Stochastic Approach: Metropolis-like algorithm
- Conclusions

# What is Bose-Einstein Condensation?

- Accumulation of atoms in ground state below a critical temperature ( $T_c$ ), forming a “condensate”
- $T_c$  is higher than the “freeze-out temperature” ( $T_0$ ), or the temperature at which only the ground state is accessible)



**Figure 7.32.** Number of atoms in the ground state ( $N_0$ ) and in excited states, for an ideal Bose gas in a three-dimensional box. Below  $T_c$  the number of atoms in excited states is proportional to  $T^{3/2}$ .

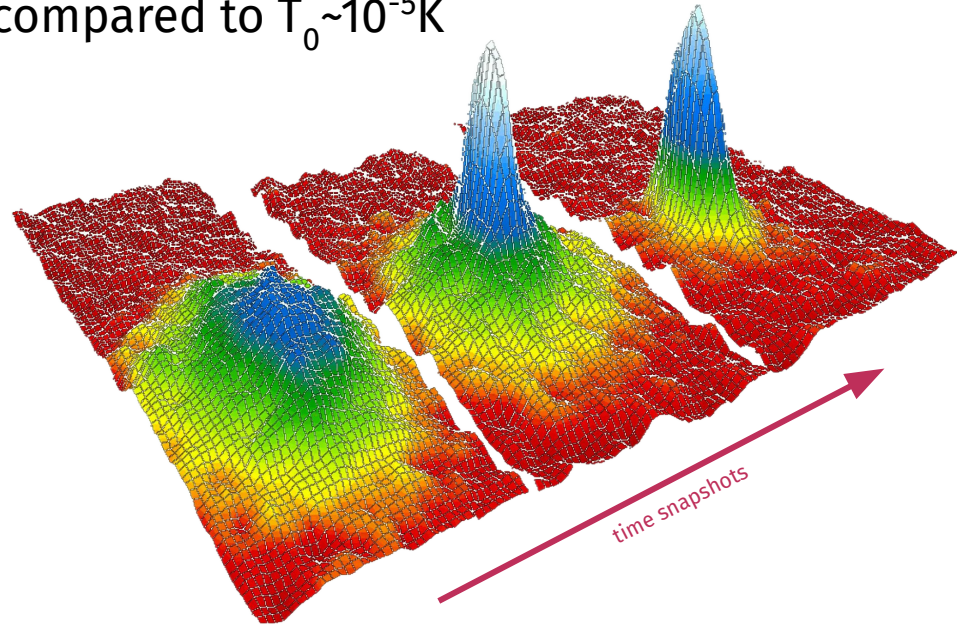
# Experimental Evidence

First observation in 1995 with laser-trapped Rubidium atoms

Condensation occurred at  $T_c \sim 10^{-7} \text{K}$ , compared to  $T_0 \sim 10^{-5} \text{K}$

The atoms condense from less dense red, yellow and green areas into very dense blue to white areas.

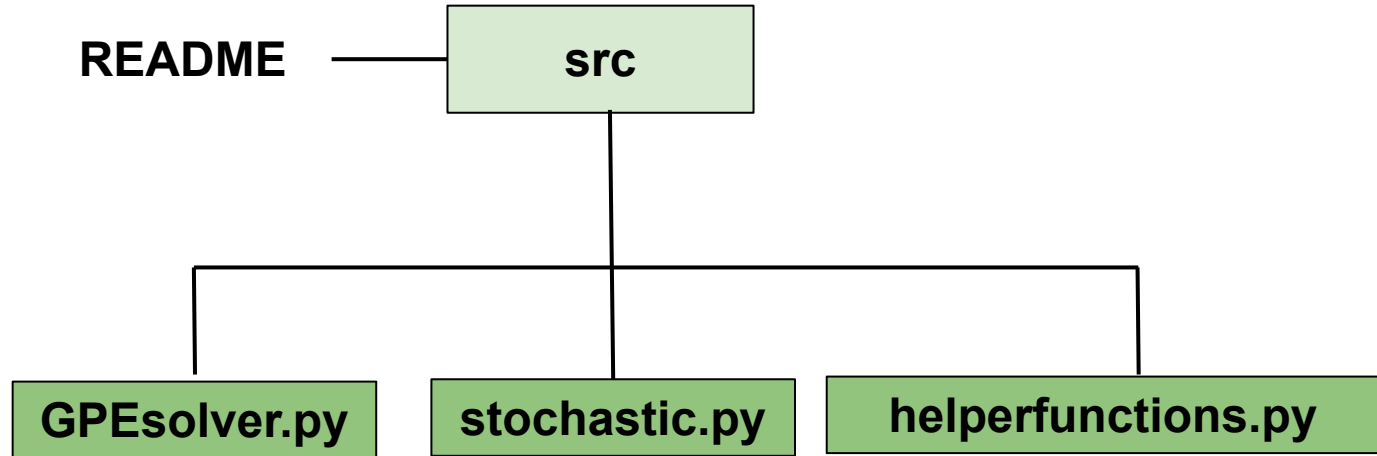
Individual atoms condense into a "superatom" behaving as a single entity.



[https://titan.physx.u-szeged.hu/~dpiroska/atmolfiz/bose\\_einstein\\_condensation.html](https://titan.physx.u-szeged.hu/~dpiroska/atmolfiz/bose_einstein_condensation.html)

# Code Goals & Design

1. Numerically solve the Schrödinger Equation for the BEC Hamiltonian to model behavior of a condensate
2. Stochastically model behavior of condensate when perturbations to system are applied



# Mean Field Approach: Gross-Pitaevskii Equation (GPE)

The Hamiltonian can be quite difficult to compute exactly



$$\hat{H} = \sum_{i=1}^N \left( \frac{\mathbf{p}_i^2}{2m} + V_{\text{ext}}(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N V(|\mathbf{r}_i - \mathbf{r}_j|)$$

We can do “smart” approximations:

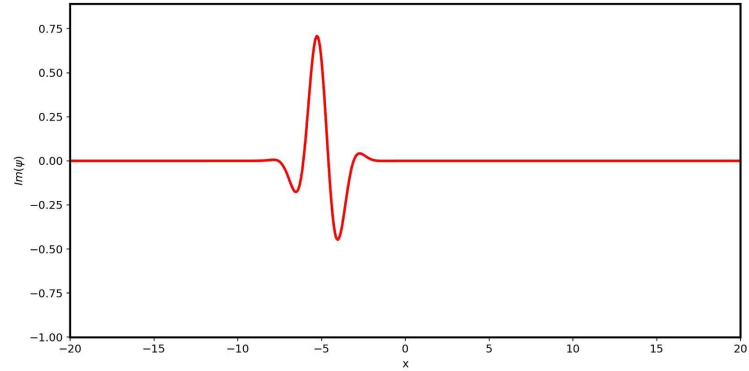
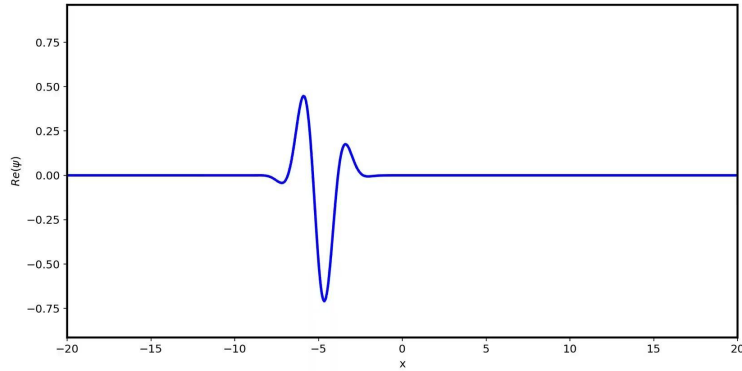
Description by a global wave function

Gross-Pitaevskii Equation (GPE)

$$-i\hbar \frac{\partial \Psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V + g|\Psi|^2 \right) \Psi$$

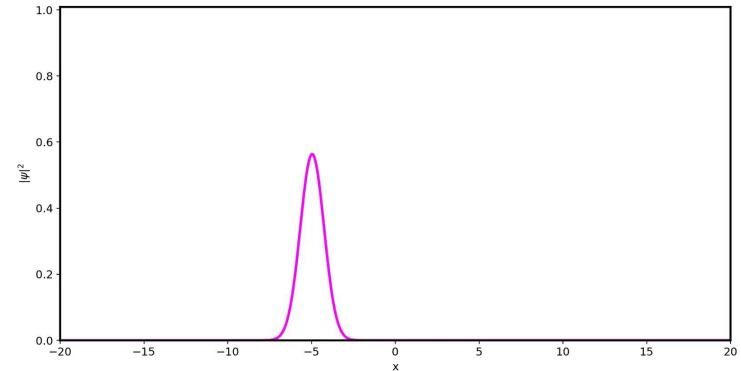
non-linear SE!

# Wave Function Animation



## Parameters:

- Gaussian Wave Packet
- Harmonic Trap
- Crank-Nicolson scheme

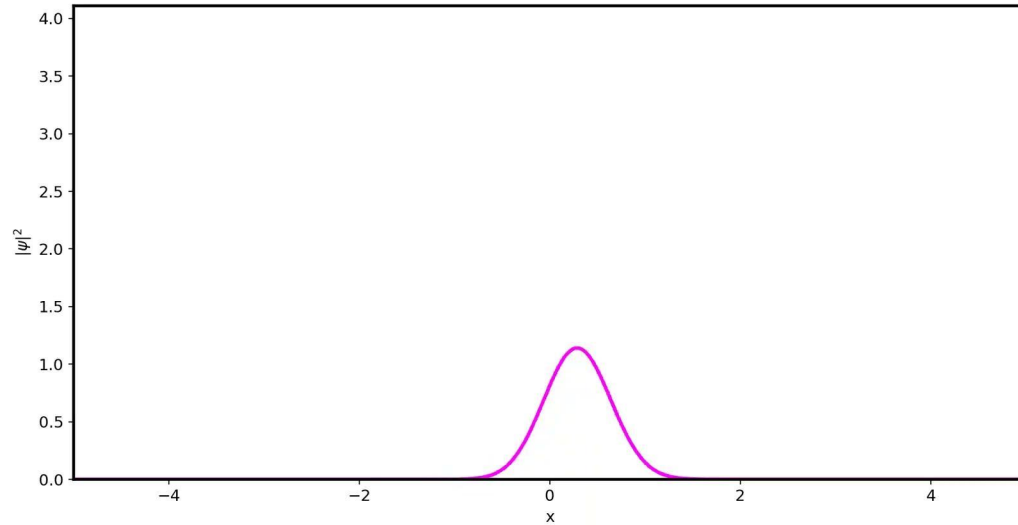


# Stochastic Method: Metropolis-Hastings for BEC

1. Choose initial wave function (ground state)
2. Calculate “reduced entropy” (quantity that involves the BEC Hamiltonian and the number operator)
3. Apply a density perturbation and a number perturbation to the wave function
4. Re-calculate the “reduced entropy”
5. Accept or reject the new wave function based on the probabilities of the wave function to be in the old and new states



# Evolution of Wave Function with Perturbations



Probability density gradually  
localizes!

## Remaining Questions

- Why does the probability density shift away from 0?
- Can we tune parameters to represent experimental conditions?

# Conclusions

- We're able to solve the GPE Equation for a simple potential.
- We implemented a stochastic approach.
- We animated our results.
- Results are encouraging from a qualitative perspective.

## Future Work?

- Solve GPE with other potentials and initial conditions and compare result
- Vary parameters for stochastic approach
- Compare results with paper

# References

1. Schroeder, D. V. (2000). *An Introduction to Thermal Physics*. Addison Wesley Longman.
2. Grišins, P., Mazets, I. (2014). Metropolis–Hastings thermal state sampling for numerical simulations of Bose–Einstein condensates. *Computer Physics Communications*, 185(7), 1926-1931.
3. Rogel-Salazar, Jesus. "The gross–pitaevskii equation and bose–einstein condensates." *European Journal of Physics* 34, no. 2 (2013): 247.
4. Bao, W. and Cai, Y., 2012. Mathematical theory and numerical methods for Bose-Einstein condensation. *arXiv preprint arXiv:1212.5341*.