BEC's & QMC:

Simulating Systems of Ultracold Atomic Gases

Joel C. Corbo

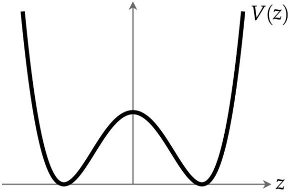
UC Berkeley

May 7, 2013

What do I Do?

Theoretical and computational work on:

- A dilute atomic gas . . .
- that is ultracold ($T \leq 10^{-7}$ K) . . .
- in a double well potential . . .
- with variable repulsive interactions.



Some important TLA's (Three-Letter Acronyms):

- BEC = Bose-Einstein Condensate
- QMC = Quantum Monte Carlo

What is a Bose-Einstein Condensate?

A *Bose-Einstein condensate* (BEC) is a state of matter formed when a gas of bosons* is cooled to temperatures close to absolute zero, which causes a large fraction of the bosons to occupy the system's ground state* and exhibit quantum effects on a macroscopic scale*.

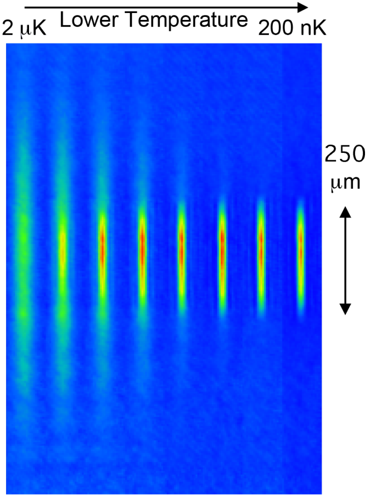
BEC's were first observed in 1995.

*Jargon alert!

Experimental Data: Forming a BEC

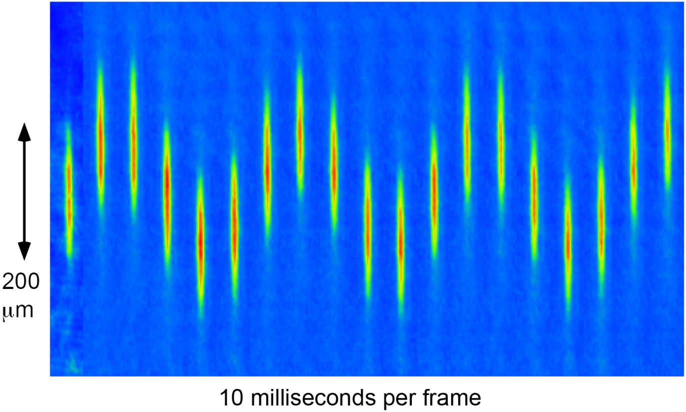
Experimental setup:

- Sodium atoms
- 10^{14} atoms/cm^3 $\approx 10^{-9}$ g/cm^3 (compare: 1 g/cm^3 for solid sodium at STP)
- Magnetic trapping creates a harmonic oscillator potential ($V \propto x^2$)



D.S. Durfee and W. Ketterle. Optics Express **2**, 299-313 (1998)

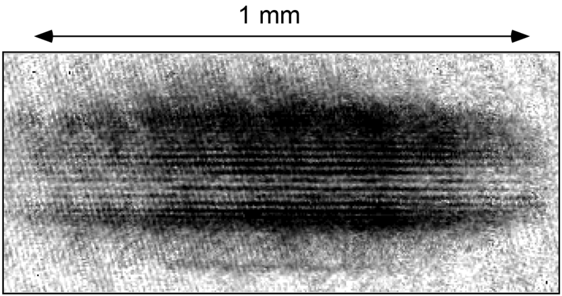
Experimental Data: Oscillating BEC



Oscillations excited by moving trap center periodically

D.S. Durfee and W. Ketterle. Optics Express **2**, 299-313 (1998)

Experimental Data: Two Interfering BEC's

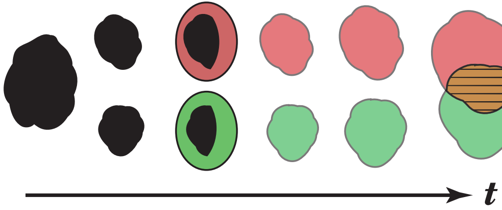


Merger of two BEC's after release from a trap

D.S. Durfee and W. Ketterle. Optics Express **2**, 299-313 (1998)

How are BEC's Useful?

Interference of BEC's useful for *atom interferometry*:



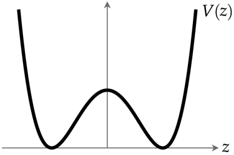
This effect can be used to very precisely measure gravity (oil exploration, cargo inspection) and rotation (gyroscopes, variation in Earth's rotation).

Precision goes like $N^{-1/2}$ for N-particle BEC. If the BEC is "number squeezed", precision increases to N^{-1}.

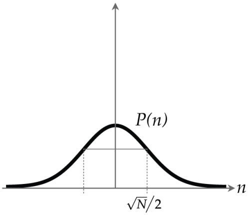
Number Squeezing

Suppose we have an N-particle BEC in a double well. Define:

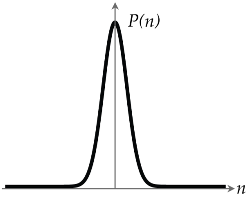
$$n = \frac{1}{2}(n_L - n_R)$$



In a *number-squeezed* BEC, repulsive interactions reduce the uncertainty in n.



Weak interaction



Strong interaction

What is a Boson?

All particles in nature are either *fermions* or *bosons*.

- **Fermion**: Particles that *cannot* share the same quantum state (electrons, quarks, neutrinos, etc.)
- **Boson**: Particles that *can* share the same quantum state (photons, gluons, W, Z, etc.)

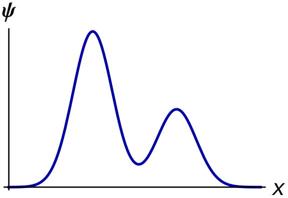
Composite particles (like atoms) can also be bosons or fermions. Atoms used to make BEC's include isotopes of Li, Na, K, Rb, and Cs.

What is a Quantum State?

In quantum mechanics, the state of a system of N particles is completely described by the *wavefunction* $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$

- $|\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2$ = probability density for finding particles at $\mathbf{r}_1, \ldots, \mathbf{r}_N$
- Normalization: $\int_{-\infty}^{\infty} |\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \, \mathrm{d}x = 1$

Ex. 1: A particle in 1D



Ex. 2: $2p_z$ orbital in H

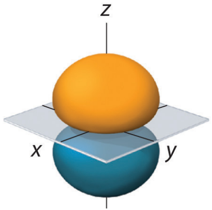


Illustration from *General Chemistry: Principles, Patterns, and Applications* by Bruce Averill and Patricia Eldredge.

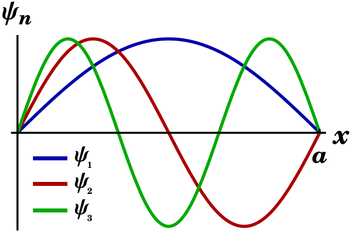
Energy Eigenstates

Energy eigenstate: Special states with definite energy, found by solving *Schrödinger equation*

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}_1, \ldots, \mathbf{r}_N)\right)\psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E_n\psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

Example: particle in a 1D "tube"

- $V(x) = 0$ for $0 < x < a$
  $V(x) = \infty$ otherwise
- $\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$
- $E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2$



A BEC is in the the *ground state* (lowest energy eigenstate).

Three More Quantum Facts

1. Energy eigenstates form a complete set of functions (just like Taylor or Fourier series):

$$\psi(\mathbf{r}) = \sum_{i=1}^{\infty} c_n \psi_n(\mathbf{r}).$$

2. Can write Schrödinger equation as $\hat{H}\psi_n = E_n\psi_n$ ($\hat{H}$ is called the *Hamiltonian*). Then:

$$f(\hat{H})\psi_n = f(E_n)\psi_n.$$

3. The average value of a quantity A is given by:

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^*(x) A(x) \psi(x) \, \mathrm{d}x.$$

Computing the Ground State, Part 1

Guess a trial wavefunction ψ_T. Then:

$$\psi_T(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \sum_{i=1}^{\infty} c_n \psi_n(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N),$$

and

$$e^{-\beta \hat{H}} \psi_T = e^{-\beta \hat{H}} \sum_{i=1}^{\infty} c_n \psi_n = \sum_{i=1}^{\infty} e^{-\beta \hat{H}} c_n \psi_n = \sum_{i=1}^{\infty} e^{-\beta E_n} c_n \psi_n.$$

So, $e^{-\beta \hat{H}} \psi_T \to \psi_1$ (the ground state!) as $\beta \to \infty^\dagger$. Yay!

But, can only write $e^{-\beta \hat{H}}$ in terms of position for $\beta \ll 1$. Oh, no!

---

†As written, $e^{-\beta \hat{H}} \psi_T \to 0$, because I am ignoring a detail (normalization).

Computing the Ground State, Part 2

Solution: write $e^{-\beta\hat{H}} = (e^{-\epsilon\hat{H}})^M$, for $\epsilon \ll 1$ and M large enough to approximate the ground state.

Then[‡]:

$$\begin{aligned}
\langle A\rangle &= \int \psi_g^*(R)A(R)\psi_g(R)\,\mathrm{d}R \\
&\approx \int (e^{-\epsilon\hat{H}})^M\psi_T^*(R)A(R)(e^{-\epsilon\hat{H}})^M\psi_T(R)\,\mathrm{d}R \\
&= \int \psi_T^*(R_0)G(R_0,R_1)\cdots G(R_{M-1},R_M)A(R_M) \\
&\qquad \times G(R_M,R_{M+1})\cdots G(R_{2M-1},R_{2M})\psi_T(R_{2M})\,\mathrm{d}R_0\cdots\mathrm{d}R_{2M},
\end{aligned}$$

where $R = \{\mathrm{r}_1,\ldots,\mathrm{r}_N\}$. This is a $3NM$-dimensional integral!

[‡] I'm skipping **a lot** of steps here.

What is Quantum Monte Carlo?

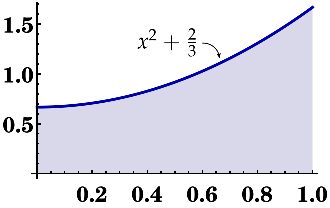
Quantum Monte Carlo (QMC) is a large collection of computer algorithms that simulate (many-body) quantum systems using statistical Monte Carlo integration methods.

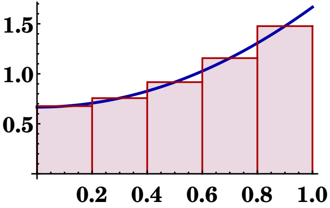
Numerical Integration, with Boxes

Suppose we want to compute $I = \int_0^1 (x^2 + \frac{2}{3})\, \mathrm{d}x$.§

Use "box integration": divide domain into k intervals and add areas of resulting boxes.

For this integral, $I - I_{box} = \frac{1}{12} k^{-2}$.





§Hint: $I = 1$.

The Curse of Dimensionality

Suppose our integral has d dimensions, with k intervals in each. Then the number of function evaluations is k^d.

Recall: we want to compute an integral in $3NM$ dimensions.

Feasible?

- For me, $N \sim 10$ and $M \sim 1000 \rightarrow d \sim 10^4$
- Number of function evaluations: k^{10^4}
- For $k = 2$ and a 1 GHz CPU, $t \sim 10^{3000} \times$ age of universe!

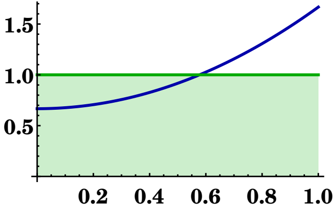
We need a better method!

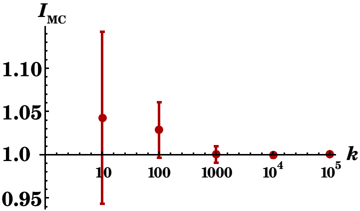
Monte Carlo Integration

Monte Carlo integration is a method for computing the definite integral of a function via statistical sampling.

Recall that $\int_a^b f(x)\,\mathrm{d}x = \langle f \rangle\,(b-a)$.

Estimate $\langle f \rangle \approx \frac{1}{k}\sum_{i=1}^{k} f(x_k)$ with k random points $\{x_1, \ldots, x_k\}$





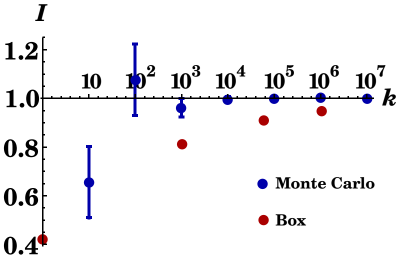
Error $\propto k^{-1/2}$

BOX VS. MONTE CARLO FOR "LARGE" d

Choose $d = 10$ and $f(x_1, \ldots, x_{10}) = (x_1^2 + \frac{2}{3}) \cdots (x_{10}^2 + \frac{2}{3})$[¶]

Errors:

- For MC: $\propto k^{-1/2}$
- For boxes: $\propto k^{-0.1}$



Monte Carlo makes quantum many-body problems solvable in practice!

¶ I is still 1.

Summary

- Overview of BEC, uses for interferometry
- Analytical techniques for expressing the ground state of a many-body quantum system
- Computational techniques (QMC) for computing the ground state

Thanks!

Solving the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}_1, \ldots, \mathbf{r}_N)\right)\psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E_n\psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

Two cases:

- $V = \sum_{i=1}^{N} V_1(\mathbf{r}_i)$ (no particle interactions):
  Each particle in the single-particle ground state $\psi_g(\mathbf{r})$:

  $$\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \psi_g(\mathbf{r}_1)\psi_g(\mathbf{r}_2)\cdots\psi_g(\mathbf{r}_N).$$

- $V = \sum_{i=1}^{N} V_1(\mathbf{r}_i) + \sum_{i<j}^{N} V_2(\mathbf{r}_i, \mathbf{r}_j)$ (two-particle interactions):
  Cannot compute ground state analytically!