Theoretical Atom Optics

(Didn't we just learn this?)

Lectures for the ACQAO Summer School

Joe Hope

61252780, room 103

joseph.hope@anu.edu.au

"Double lectures are always better with a short break"

How do we describe atoms?

Complete description of multiple bosonic atoms

- Each single particle state $\left|\phi_j\right\rangle$, has a quantum mode with the structure of a harmonic oscillator
- Hilbert space is the outer product of all those states

$$\left|\psi\right\rangle = \sum_{n_1,n_2,n_3,\cdots} f_{n_1,n_2,n_3,\cdots} \left|n_1,n_2,n_3,\cdots\right\rangle$$

Typical Hamiltonian:

$$\hat{H} = \sum_{jk} T_{jk}\, \hat{b}_j^\dagger \hat{b}_k + \sum_{jklm} V_{jklm}\, \hat{b}_j^\dagger \hat{b}_k^\dagger \hat{b}_l \hat{b}_m$$

So what *is* a BEC?

According to John:

– "Macroscopic occupation of a single quantum state"

Aren't all collections of atoms in *some* quantum state?

– Yes, but not necessarily with a large number in some single particle basis

$$|\psi\rangle = \sum_{n_1, n_2, n_3, \cdots} f_{n_1, n_2, n_3, \cdots} |n_1, n_2, n_3, \cdots\rangle$$

– Cooling a collection of particles approaches BEC

So what *is* a BEC?

Definition of BEC can be controversial:

– Originally defined only for particles in free space

Does cooling reach the ground state?

simplest form: $\hat{H} = \sum_j E_j \hat{b}_j^\dagger \hat{b}_j$

A BEC is made by reaching:

– The ground state of the Hamiltonian *for a given average number of atoms*

The Ground State

The ground state of $\hat{H} = \sum_j E_j \, \hat{n}_j$

- Has all the atoms in the lowest energy state E_0.
- There are still many possibilities

$$\left|\psi_{BEC}\right\rangle = \left|N,0,0,0,\cdots\right\rangle$$

$$\left|\psi_{BEC}\right\rangle = \sum_n c_n \left|n,0,0,0,\cdots\right\rangle \qquad \left(\sum_n \left|c_n\right|^2 = N\right)$$

This includes number states, coherent states, squeezed states, states that spell "Joe is great", …

Changing basis

The states on the last slide would be difficult to describe if the Hamiltonian was $\hat{H} = \sum_{jk} T_{jk}\, \hat{b}_j^\dagger \hat{b}_k$

Can we transform that to $\hat{H} = \sum_{j} E_j\, \hat{a}_j^\dagger \hat{a}_j$?

Go back to the original Hamiltonian and change the basis defining the number states:

$$\hat{H}_{\text{single particle}} = \hat{T} = \sum_{jk} T_{jk} \left| u_j \right\rangle \left\langle u_k \right| \qquad = \sum_{jk} \tilde{T}_{jk} \left| v_j \right\rangle \left\langle v_k \right|$$

$$T_{jk} = \left\langle u_j \middle| \hat{T} \middle| u_k \right\rangle \qquad \tilde{T}_{jk} = \left\langle v_j \middle| \hat{T} \middle| v_k \right\rangle$$

Changing basis via first quantisation

A transformation between states: $\left|v_k\right\rangle = \sum_j A_{kj}\left|u_j\right\rangle$

$$\tilde{T}_{jk} = \left(\sum_l A^*_{jl}\left\langle u_l\right|\right)\hat{T}\left(\sum_m A_{km}\left|u_m\right\rangle\right)$$

$$= \sum_{lm} A^*_{jl} A_{km} T_{lm}$$

Introduce new annihilation operators $\hat{c}_k$ associated with $\left|v_k\right\rangle$:

$$\hat{H}_{\text{single particle}} = \sum_{jk} T_{jk}\left|u_j\right\rangle\left\langle u_k\right| = \sum_{jk} \tilde{T}_{jk}\left|v_j\right\rangle\left\langle v_k\right|$$

$$\hat{H}_{\text{many particles}} = \sum_{jk} T_{jk}\hat{b}^\dagger_j \hat{b}_k = \sum_{jk} \tilde{T}_{jk}\hat{c}^\dagger_j \hat{c}_k$$

Changing basis in second quantisation

A transformation between operators: $\hat{c}_k = \sum_j A^*_{jk} \hat{b}_j$

$$\hat{H}_{\text{many particles}} = \sum_{jk} T_{jk} \hat{b}^\dagger_j \hat{b}_k = \sum_{jk} \tilde{T}_{jk} \hat{c}^\dagger_j \hat{c}_k$$

This is exactly the same transformation.

Both versions change the single particle basis by a linear transformation

How do we transform into the position basis?

$$|x\rangle = \sum_j u^*_j(x) |u_j\rangle \qquad |u_k\rangle = \int dx\; u_k(x) |x\rangle$$

The field operator

Introduce the operator: $\hat{\psi}(x) = \sum_j u_j(x)\hat{b}_j$

Note the continuous index: $\hat{b}_j = \int d\mathbf{x}\, u_j^*(\mathbf{x})\hat{\psi}(\mathbf{x})$

$$\hat{H} = \int d\mathbf{x} \int d\mathbf{x}'\, \hat{\psi}^\dagger(\mathbf{x}) T(\mathbf{x},\mathbf{x}')\hat{\psi}(\mathbf{x}')$$

$$+ \int d\mathbf{x} \int d\mathbf{x}' \int d\mathbf{x}'' \int d\mathbf{x}'''\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}') V(\mathbf{x},\mathbf{x}',\mathbf{x}'',\mathbf{x}''')\hat{\psi}(\mathbf{x}'')\hat{\psi}(\mathbf{x}''')$$

In position space many of these indices are typically not needed:

$$\hat{H} = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\hat{\psi}(\mathbf{x})$$

$$+ \int d\mathbf{x} \int d\mathbf{x}'\, \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}') V(\mathbf{x},\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})$$

Exercises

$$\hat{H} = \int d\mathbf{x}\, \hat{\psi}^{\dagger}(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right) \hat{\psi}(\mathbf{x})$$

$$+ \int d\mathbf{x} \int d\mathbf{x}' \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}^{\dagger}(\mathbf{x}') V(\mathbf{x},\mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x})$$

1. Show that $\left[\hat{\psi}(\mathbf{x}), \hat{\psi}^{\dagger}(\mathbf{x}') \right] = \delta(\mathbf{x} - \mathbf{x}') \quad \Rightarrow \quad \left[\hat{b}_j, b_k^{\dagger} \right] = \delta_{jk}$

2. Find the Heisenberg equation of motion for the field operator

3. What is the interpretation of $\left\langle \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}(\mathbf{x}) \right\rangle$?

Exercises

$$\hat{H} = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right) \hat{\psi}(\mathbf{x})$$

$$+ \int d\mathbf{x} \int d\mathbf{x}' \hat{\psi}^\dagger(\mathbf{x}) \hat{\psi}^\dagger(\mathbf{x}') V(\mathbf{x},\mathbf{x}') \hat{\psi}(\mathbf{x}') \hat{\psi}(\mathbf{x})$$

4. Write the down the single particle momentum eigenstates

5. Find the momentum space field operator in terms of $\hat{\psi}(\mathbf{x})$

6. Find the Hamiltonian in terms of those operators

Multiple (non-spatial) states

Our single particle states might include non-spatial degrees of freedom, such as spin, or the electronic states of atoms:

$$\text{e.g.} \qquad |\psi\rangle = \sum_{s,j} c_{s,j} |s, u_j\rangle$$

$$\hat{H} = \sum_{s_1,s_2,j_1,j_2} T_{s_1,j_1,s_2,j_2}\, \hat{b}^\dagger_{s_1,j_1} \hat{b}_{s_2,j_2} + \sum_{\substack{s_1,s_2,j_1,j_2 \\ s_3,s_4,j_3,j_4}} V_{\substack{s_1,s_2,j_1,j_2 \\ s_3,s_4,j_3,j_4}}\, \hat{b}^\dagger_{s_1,j_1} \hat{b}^\dagger_{s_2,j_2} \hat{b}_{s_3,j_3} \hat{b}_{s_4,j_4}$$

$$\hat{H} = \sum_{s_1,s_2} \int d\mathbf{x}\, \hat{\psi}^\dagger_{s_1}(\mathbf{x}) \left(-\delta_{s_1,s_2} \frac{\hbar^2}{2m} \nabla^2 + V_{s_1,s_2}(\mathbf{x}) \right) \hat{\psi}_{s_2}(\mathbf{x})$$

$$+ \sum_{s_1,s_2,s_3,s_4} \int d\mathbf{x} \int d\mathbf{x}'\, \hat{\psi}^\dagger_{s_1}(\mathbf{x}) \hat{\psi}^\dagger_{s_2}(\mathbf{x}') V_{s_1,s_2,s_3,s_4}(\mathbf{x},\mathbf{x}') \hat{\psi}_{s_3}(\mathbf{x}') \hat{\psi}_{s_4}(\mathbf{x})$$

Contact Potential

At low temperatures, the particles don't have the energy to probe the details of the interparticle interactions, so we can make a powerful approximation:

$$V(x,x') = U\,\delta(x - x') \qquad U = \frac{4\pi\hbar^2 a}{m}$$

scattering length

$$\hat{H} = \int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\hat{\psi}(\mathbf{x}) + U\int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x})$$

Observables

1. We know the Hamiltonian for a large number of bosons.

2. We can transform basis to make it as simple as possible.

3. The equation of motion for $\hat{\psi}(\mathbf{x})$ is familiar:

$$i\hbar\frac{\partial\hat{\psi}(\mathbf{x})}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+U\hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x})\right)\hat{\psi}(\mathbf{x})$$

All observables can be written in terms of the field operators

Calculating observable quantities

All interesting quantities are expectation values of the field operators: e.g. $\left\langle \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\right\rangle$ $\quad \left\langle \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})\right\rangle$

$$i\hbar \frac{\partial \left\langle \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x}')\right\rangle}{\partial t} = -\frac{\hbar^2}{2m}\left(\left\langle \hat{\psi}^\dagger(\mathbf{x})\nabla^2\hat{\psi}(\mathbf{x}')\right\rangle - \left\langle \left(\nabla^2\hat{\psi}^\dagger(\mathbf{x})\right)\hat{\psi}(\mathbf{x}')\right\rangle\right)$$
$$+U\left(\left\langle \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}')\right\rangle - \left\langle \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x}')\right\rangle\right)$$

These rarely form closed sets of equations, so we need to know about the actual fields.

…So Now What?

With the nonlinear term, exact results are rare.
What about numerical results?

1. Assume the field is one dimensional
2. Assume there is only relevant electronic level
3. Put the field on a grid of 100 points in that dimension

How many complex numbers describe the state? A. ∞

4. What if there are at most 100 atoms? A. $\approx (100)^{100}$

Tomorrow

Now we know the underlying theory:

We need ways to do actual calculations!