Theoretical Atom Optics

(as seen on TV)

Lectures for the ACQAO Summer School

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"Bosons like to be in the same state"

"Bose-Einstein Condensation occurs when all the particles go into the same quantum state"

How do we describe atoms?

Classical description of N atoms

– State $\{\mathbf{x}_j, \mathbf{p}_j\}$

- 2 vectors per atom
- 2 N D real numbers

Quantum description of 1 atom

– State

$$\psi(\mathbf{x}) = \sum_{j=1}^{\infty} c_j u_j(\mathbf{x})$$

- ∞ complex numbers

$$|\psi\rangle = \sum_{j=1}^{\infty} c_j |\phi_j\rangle \qquad |\psi\rangle = \int d^D\mathbf{x}\, \psi(\mathbf{x}) |\mathbf{x}\rangle$$

Quantum description of 2 atoms

– State is much more than twice as large

$$|\psi\rangle = \sum_{j_1,j_2} c_{j_1,j_2} |\phi_{j_1}\rangle |\phi_{j_2}\rangle \qquad |\psi\rangle = \iint d^D\mathbf{x}_1 d^D\mathbf{x}_2\, \psi(\mathbf{x}_1,\mathbf{x}_2) |\mathbf{x}_1\rangle |\mathbf{x}_2\rangle$$

$$c_{j_1,j_2} \neq c_{j_1} d_{j_2} \qquad \psi(\mathbf{x}_1,\mathbf{x}_2) \neq \psi(\mathbf{x}_1)\,\phi(\mathbf{x}_2)$$

(unless the state is separable)

Quantum description of N atoms?

$$|\psi\rangle = \sum_{j_1,\ldots,j_N} c_{j_1,\ldots,j_N} |\phi_{j_1}\rangle |\phi_{j_2}\rangle \cdots |\phi_{j_N}\rangle$$

Warm-up Exercises

1. If $\left|\phi_j\right\rangle = \int d^D\mathbf{x}\; u_j(\mathbf{x})\left|\mathbf{x}\right\rangle$, what is $\left|\mathbf{x}\right\rangle$ in terms of $\left|\phi_j\right\rangle$?

2. For what modes $u_j(\mathbf{x})$ is this transformation the identity?

3. Write down a general quantum state for N atoms in the continuous variable (position space) basis.

Indistinguishability

The states we just defined are a little *too* general, as we haven't included some restrictions.

e.g. Swapping any two fundamental particles should not change the physics. In other words, the labels we put on the state are arbitrary.

Define a switching operator $\hat{P}_{12}\,\psi(\mathbf{x}_1,\mathbf{x}_2) \equiv \psi(\mathbf{x}_2,\mathbf{x}_1)$

$$\hat{P}_{12}\,\psi(\mathbf{x}_1,\mathbf{x}_2) = \underbrace{\psi(\mathbf{x}_2,\mathbf{x}_1) = e^{i\theta}\psi(\mathbf{x}_1,\mathbf{x}_2)}_{\text{indistinguishability of particles}}$$

Consequences of indistinguishability

Switching two particles twice must be the identity:

$$\left(\hat{P}_{12}\right)^2 \psi(\mathbf{x}_1,\mathbf{x}_2) = \psi(\mathbf{x}_1,\mathbf{x}_2) = e^{i2\theta}\psi(\mathbf{x}_1,\mathbf{x}_2)$$

$$\therefore \quad e^{i2\theta} = 1$$

We have two and only two choices:

$$\underbrace{\psi(\mathbf{x}_1,\mathbf{x}_2) = \psi(\mathbf{x}_2,\mathbf{x}_1)}_{\text{Symmetric wavefunctions}}$$

Symmetric wavefunctions

Bosons

$$\underbrace{\psi(\mathbf{x}_1,\mathbf{x}_2) = -\psi(\mathbf{x}_2,\mathbf{x}_1)}_{\text{Anti-symmetric wavefunctions}}$$

Anti-symmetric wavefunctions

Fermions

“Fermions don’t like to be in the same state”

Fermions have anti-symmetric wavefunctions:

$$|\psi\rangle = \sum_{j_1,\dots,j_N} c_{j_1,\dots,j_N} |\phi_{j_1}\rangle|\phi_{j_2}\rangle\cdots|\phi_{j_N}\rangle$$

Where $c_{j_1,\dots,j_k,\dots,j_l,\dots,j_N} = -c_{j_1,\dots,j_l,\dots,j_k,\dots,j_N}$

Now what if $j_k = j_l$ for any two indices?

(i.e. any two particles are in the same state)

$$c_{j_1,\dots,j_N} = -c_{j_1,\dots,j_N} = 0$$

“Bosons like to be in the same state”

Bosons have symmetric wavefunctions:

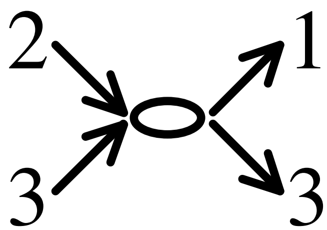
$$|\psi\rangle = \sum_{j_1,\ldots,j_N} c_{j_1,\ldots,j_N} |\phi_{j_1}\rangle |\phi_{j_2}\rangle \cdots |\phi_{j_N}\rangle$$

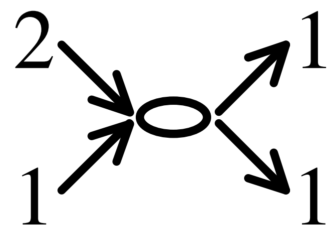
Where $c_{j_1,\ldots,j_k,\ldots,j_l,\ldots,j_N} = c_{j_1,\ldots,j_l,\ldots,j_k,\ldots,j_N}$

1. Bosons *can* be in the same state.
2. There is an enormous redundancy in this description whenever more than one particle is in the same state.

Bose enhancement
Pauli blocking

Consider two atoms (a and b) undergoing a change of state from 2 to 1:



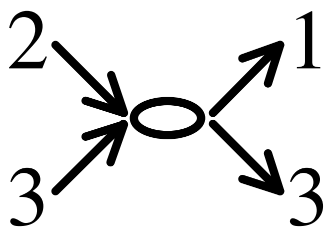


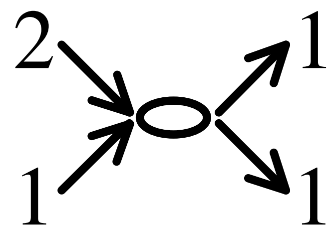
Hamiltonian $\hat{H} = U\left(|1_a\rangle\langle 2_a| + |2_a\rangle\langle 1_a| + |1_b\rangle\langle 2_b| + |2_b\rangle\langle 1_b|\right)$

Initial States:

$$\frac{1}{\sqrt{2}}\left(|2_a\rangle|3_b\rangle \pm |3_a\rangle|2_b\rangle\right) \qquad \frac{1}{\sqrt{2}}\left(|2_a\rangle|1_b\rangle \pm |1_a\rangle|2_b\rangle\right)$$

Bose enhancement
Pauli blocking





$$\hat{H} = U\left(|1_a\rangle\langle 2_a| + |2_a\rangle\langle 1_a| + |1_b\rangle\langle 2_b| + |2_b\rangle\langle 1_b|\right)$$

$$\hat{H}|\psi_{init}\rangle = \hat{H}\frac{1}{\sqrt{2}}\left(|2_a\rangle|3_b\rangle \pm |3_a\rangle|2_b\rangle\right)$$

$$= U\frac{1}{\sqrt{2}}\left(|1_a\rangle|3_b\rangle \pm |3_a\rangle|1_b\rangle\right)$$

$$\hat{H}|\psi_{init}\rangle = \hat{H}\frac{1}{\sqrt{2}}\left(|2_a\rangle|1_b\rangle \pm |1_a\rangle|2_b\rangle\right)$$

$$= U\frac{1}{\sqrt{2}}\begin{pmatrix}|1_a\rangle|1_b\rangle \pm |1_a\rangle|1_b\rangle \\ +|2_a\rangle|2_b\rangle \pm |2_a\rangle|2_b\rangle\end{pmatrix}$$

Transition rate: $\left|\langle\psi_{final}|\hat{H}|\psi_{init}\rangle\right|^2$

$|U|^2$

$2\,|U|^2$ Bose enhancement

0 Pauli blocking

Bose enhancement for N bosons

Suppose we start with N particles in state 1 and one in state 2?

$$\hat{H} = U \sum_x \left(|1_x\rangle\langle 2_x| + |2_x\rangle\langle 1_x| \right)$$

$$|\psi_{init}\rangle = \frac{1}{\sqrt{N+1}} \left(|2_{x_1}\rangle |1_{x_2}\rangle \cdots |1_{x_{N+1}}\rangle + |1_{x_1}\rangle |2_{x_2}\rangle \cdots |1_{x_{N+1}}\rangle + \cdots + |1_{x_1}\rangle \cdots |1_{x_N}\rangle |2_{x_{N+1}}\rangle \right)$$

$$\hat{H}|\psi_{init}\rangle = U \frac{1}{\sqrt{N+1}} \left((N+1) |1_{x_1}\rangle |1_{x_2}\rangle \cdots |1_{x_{N+1}}\rangle + |2_{x_1}\rangle |2_{x_2}\rangle |1_{x_3}\rangle \cdots |1_{x_{N+1}}\rangle + \cdots \right)$$

$$\left| \langle \psi_{final} | \hat{H} | \psi_{init} \rangle \right|^2 = (N+1)\, |U|^2$$

all other combinations with two atoms in state 2

Bose enhancement: Transition into a state already containing N bosons is enhanced by a factor of (N+1)

Occupation number notation

(Only showing detail for Bosons)

$$c_{3,1,1,2,4,2,1,3,\cdots} = c_{\underbrace{1,1,1,\cdots,}_{n_1}\underbrace{2,2,2,\cdots}_{n_2}}$$

We can simplify things dramatically by collecting all the states with identical coefficients:

$$\sum_{j_1,\ldots,j_N} c_{j_1,\ldots,j_N} \left|\phi_{j_1}\right\rangle \left|\phi_{j_2}\right\rangle \cdots \left|\phi_{j_N}\right\rangle = \sum_{n_1,n_2,n_3,\cdots} \bar{c}_{n_1,n_2,n_3,\cdots} \left|n_1,n_2,n_3,\cdots\right\rangle$$

$$\left|n_1,n_2,n_3,\cdots\right\rangle = \frac{1}{N}\Big(\underbrace{|1\rangle\cdots|1\rangle}_{n_1}\underbrace{|2\rangle\cdots|2\rangle}_{n_2}\cdots \quad + |2\rangle\underbrace{|1\rangle\cdots|1\rangle}_{n_1}\underbrace{|2\rangle\cdots|2\rangle}_{n_2-1}\cdots \quad + \cdots\Big)$$

normalisation coefficient

all other permutations of the states distributed amongst the atoms

Occupation number notation

Examples: $$\frac{1}{\sqrt{2}}\left(|2\rangle|1\rangle + |1\rangle|2\rangle\right) = |1,1,0,0,\cdots\rangle$$

$$|1\rangle|1\rangle = |2,0,0,0,\cdots\rangle$$

$$\frac{1}{\sqrt{6}}\begin{pmatrix} |1\rangle|2\rangle|3\rangle + |1\rangle|3\rangle|2\rangle + |2\rangle|1\rangle|3\rangle \\ +|3\rangle|1\rangle|2\rangle + |2\rangle|3\rangle|1\rangle + |3\rangle|2\rangle|1\rangle \end{pmatrix} = |1,1,1,0,\cdots\rangle$$

All the symmetry of the states is built into this notation. This means that writing them down becomes enormously simpler.

Second Quantisation

The new notation is very clean, but to use it we will have to translate the Hamiltonian so that it deals easily with them. To this end, we introduce annihilation and creation operators

$$\hat{b}_j \quad \text{and} \quad \hat{b}_j^\dagger$$

They are fully defined by their commutation relations.

$$\left[\hat{b}_j, \hat{b}_k^\dagger\right] = 1 \qquad \left[\hat{b}_j, \hat{b}_k\right] = \left[\hat{b}_j^\dagger, \hat{b}_k^\dagger\right] = 0$$

$$\hat{b}_j \left| n_1, n_2, \cdots, n_j, \cdots \right\rangle = \sqrt{n_j} \left| n_1, n_2, \cdots, n_j - 1, \cdots \right\rangle$$

$$\hat{b}_j^\dagger \left| n_1, n_2, \cdots, n_j, \cdots \right\rangle = \sqrt{n_j + 1} \left| n_1, n_2, \cdots, n_j + 1, \cdots \right\rangle$$

As their names suggest, they remove/create a particle in state j

Second Quantisation

$$\hat{b}_j^{\dagger}\hat{b}_j \left| n_1, n_2, \cdots \right\rangle = n_j \left| n_1, n_2, \cdots \right\rangle$$

$\hat{n}_k \equiv \hat{b}_k^{\dagger}\hat{b}_k$ is often called the number operator

These operators may be familiar from the analysis of harmonic oscillators. It is a coincidence that systems of bosons have the same underlying structure as sets of coupled harmonic oscillators. (But it does go some way to explaining our strange fascination for harmonic oscillators)

These annihilation and creation operators form a complete set of operators for systems of bosons, and they operate simply on number states, but we still have to find the Hamiltonian in terms of these operators.

Second Quantised Hamiltonian

A general translation could be quite onerous. Fortunately, most Hamiltonians can be written in the form

$$\hat{H} = \sum_{x} \hat{T}_x + \sum_{\substack{x,y \\ x \neq y}} \hat{V}_{x\,y}$$

This has terms acting on single particles and pairwise interactions. This form enforces the indistinguishability of the particles.

In a particular basis for the single particle states:

$$\hat{H} = \sum_{x} \sum_{j\,k} T_{j\,k} \left| j_x \right\rangle \left\langle k_x \right| + \sum_{\substack{x,y \\ x \neq y}} \sum_{j\,k\,l\,m} V_{j\,k\,l\,m} \left| j_x \right\rangle \left| k_y \right\rangle \left\langle l_x \right| \left\langle m_y \right|$$

Second Quantised Hamiltonian

We change the order of the summation

$$\hat{H} = \sum_{jk} T_{jk} \left(\sum_{x} \left| j_x \right\rangle \left\langle k_x \right| \right) + \sum_{jklm} V_{jklm} \left(\sum_{\substack{x,y \\ x \neq y}} \left| j_x \right\rangle \left| k_y \right\rangle \left\langle l_x \right| \left\langle m_y \right| \right)$$

A straightforward calculation with far too many indices shows that the operators in brackets are very simple in our new notation:

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

So, we pick a basis and can easily write the Hamiltonian in "second quantised" form.

Exercises

1. Is there any state in first-quantized form that cannot be written in the occupation number notation?

2. Is there any state in the occupation number notation that cannot be written in the first quantized notation?

3. The occupation number states are normalised by definition. Show that they are orthogonal.

4. Repeat the demonstration of Bose enhancement using a second quantised Hamiltonian and number states.

Fixed number of atoms?

With our new notation, we have slipped in the possibility of including states with different numbers of atoms.

$$\left|1,1\right\rangle + i\left|1,0\right\rangle$$

This can be useful concept for systems interacting with an environment and exchanging particles.

Note that for a closed system, the Hamiltonian usually conserves the number of particles:

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