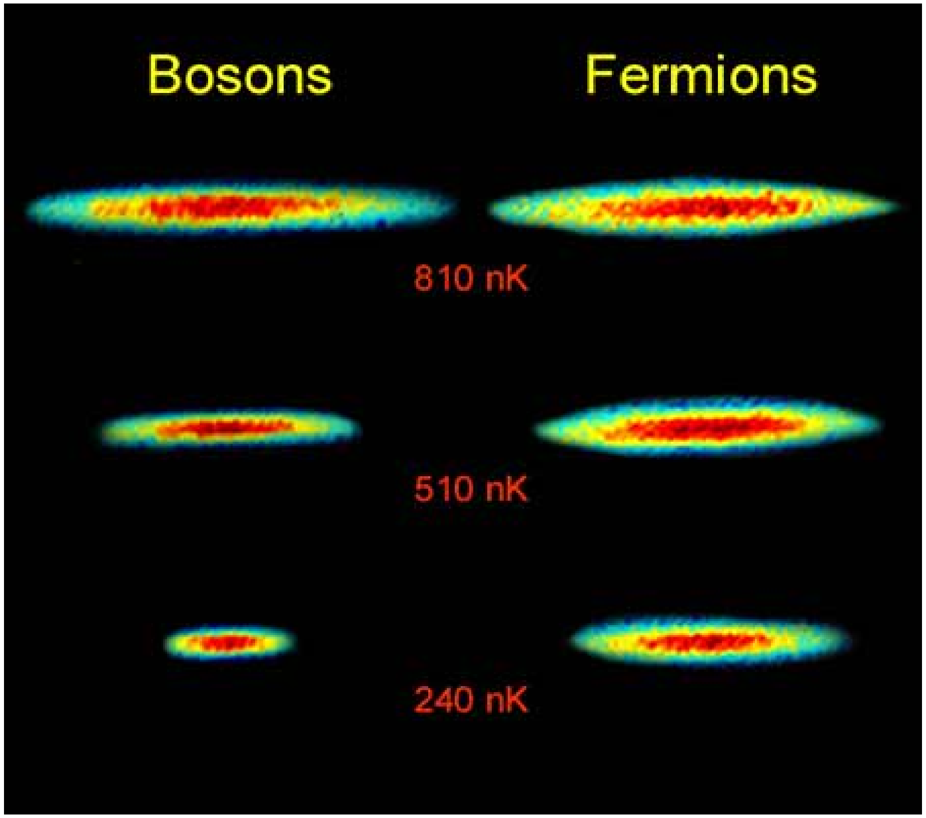
Advanced Quantum Physics

Lecture 4



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Section 1 - Review of Quantum Physics

1.1 Postulates of quantum mechanics, operator methods, time dependence.

1.2 Solutions of Schrodinger's equation.

1.3 Angular momentum and spin, matrix representation.

✦ 1.4 Identical particles.

Identical particles (1)

- Consider a system of identical particles – in classical mechanics we can (in principle) keep track of them – effectively the particles are distinguishable.

- In quantum mechanics when two identical particles interact we cannot distinguish between them – we cannot follow their trajectories since this measurement will disturb the system.

- The Hamiltonian for an N particle system:

$$\hat{H}\left(1,2,..,N\right)=\sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2+v_{ext}(i)\right]+V_{int}(1,2,..,N)$$

- The labels $1,2...$ each represents the internal (e.g.spin) and external (e.g.position) degrees of freedom of the i^{th} particle. $v_{ext}(i)$ is the external potential acting on the i^{th} particle.

- $V_{int}(1,2,..,N)$ represents the mutual interaction between the particles, so for a two-body interaction:

$$V_{int}(1,2,..N)=\frac{1}{2}\sum_{i\neq j}^{N}V_{int}(i,j) \quad \text{Newton III} \quad \Rightarrow V_{int}(i,j)=V_{int}(j,i)$$

Identical particles (2)

- So the N particle Hamiltonian is given by:

$$\hat{H}(1,2,..,N)=\sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\nabla_i^2+v_{ext}(i)\right]+\frac{1}{2}\sum_{i\neq j}^{N}V_{int}(i,j)$$

- This Hamiltonian is invariant under the exchange of particles – effectively a definition of identical or indistinguishable particles.
- If $\hat{P}_{ij}$ is a two particle exchange operator then;

$$\hat{P}_{ij}\psi(1,2,..i,j..N)=\psi(1,2,..j,i..N)$$

hence $\hat{P}_{ij}^2=\hat{I}$, and $\hat{P}_{ij}$ will have eigenvalues of ± 1 (it is both Hermitian and unitary) and represents an observable.

- We can also extend this to an arbitrary particle exchange operator $\hat{P}$ which is made up of a product of pairwise exchanges $\hat{P}_{ij}$.
- Since $\hat{P}^2=\hat{I}$; by the symmetry of the Hamiltonian $\left[\hat{H},\hat{P}\right]=0$.

Identical particles (3)

- Given that $\hat{H}\psi = E\psi$ and since $\left[\hat{H},\hat{P}\right]=0$ we have;

$$\hat{H}\left(\hat{P}\psi\right)=\hat{P}\left(\hat{H}\psi\right)=\hat{P}\left(E\psi\right)=E\left(\hat{P}\psi\right)$$

- So if ψ is an eigenfunction of $\hat{H}$ with eigenvalue E then so is $\hat{P}\psi$.
- This means we can use the eigenvalues of $\hat{P}$ and the energy E to label the eigenstates of the Hamiltonian and that the eigenstates will retain their symmetry properties for all time.
- As we have seen for a pairwise interchange:

$$\hat{P}_{ij}\psi\left(1,2,..i,\,j..N\right)=\pm\psi\left(1,2,..i,\,j..N\right)$$

- The $+$ sign corresponding to a symmetric ψ under particle exchange representing bosons.
- The – sign corresponds to an anti-symmetric ψ under particle exchange representing fermions.
- The spin-statistics theorm of quantum field theory states that particles with integer spin are bosons (obeying Bose-Einstein statistics) and those with half integer spin fermions (obeying Fermi-Dirac statistics).

Identical particles (4)

- If we have a totally anti-symmetric wavefunction: $\psi_A(1,2,..i,j..N)$

$$\hat{P}_{ij}\psi_A(1,2,..i,j..N)=\psi_A(1,2,..j,i..N)=-\psi_A(1,2,..i,j..N)$$

- If we set $i=j$ we find:

$$\psi_A(1,2,..i,i..N)=-\psi_A(1,2,..i,i..N)=0$$

- Given that *i* represents both the spatial and spin degrees of freedom this means that two fermions in the same spin state cannot occupy the same spatial state - the *Pauli Exclusion Principle.*

- This effect leads to the appearance of a repulsion between the particles.

"It is the fact that the electrons cannot all get on top of each other that makes tables and everything else solid"

Richard Feynman

Identical particles (5)

- For N identical non-interacting particles the Hamiltonian is the sum of N identical single particle Hamiltonians: $\hat{H}(1,2,..,N) = \sum_{i=1}^{N} \hat{H}(i)$
- Assume that eigenstates of $\hat{H}(i)$ are given by the solutions to the single particle Schrodinger equation, $\hat{H}(i)\psi_{\alpha_i}(i) = E_{\alpha_i}\psi_{\alpha_i}(i)$ where i labels the particles and α_i the different single particle states.

- We can use these single particle eigenstates to construct the N-particle eigenstates in different ways e.g. If we have:

$$\psi(1,2,...,N) = \psi_{\alpha_1}(1)\psi_{\alpha_2}(2)...\psi_{\alpha_N}(N)$$

then: $$\hat{H}\psi = \sum_{i=1}^{N} \hat{H}(i)\left[\psi_{\alpha_1}(1)\psi_{\alpha_2}(2)...\psi_{\alpha_N}(N)\right]$$

$$= \sum_{i=1}^{N} \psi_{\alpha_1}(1)...\left[\hat{H}(i)\psi_{\alpha_i}(i)\right]...\psi_{\alpha_N}(N)$$

$$= \sum_{i=1}^{N} \psi_{\alpha_1}(1)...\left[E_{\alpha_i}\psi_{\alpha_i}(i)\right]...\psi_{\alpha_N}(N) = \sum_{i=1}^{N} E_{\alpha_i}\psi = E\psi$$

- These states are in general neither symmetric or anti-symmetric and therefore cannot describe real systems of identical particles where there is *significant* overlap of the wavefunctions.

Fermions

- For two fermions the following state is anti-symmetric under particle exchange:

$$\psi_A(1,2)=\frac{1}{\sqrt{2}}\left[\psi_{\alpha_1}(1)\psi_{\alpha_2}(2)-\psi_{\alpha_1}(2)\psi_{\alpha_2}(1)\right]$$

- Swop particles 1 and 2 : $\psi_A \to -\psi_A$
- When $\psi_{\alpha_1}=\psi_{\alpha_2}$ then $\psi_A=0$.

} as required for fermions.

- For N identical fermions we have:

$$\psi_A(1,2\ldots N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\psi_{\alpha_1}(1) & \psi_{\alpha_1}(2) & \ldots. & \psi_{\alpha_1}(N)\\ \psi_{\alpha_2}(1) & \psi_{\alpha_2}(2) & \ldots. & \psi_{\alpha_2}(N)\\ : & : & : & :\\ \psi_{\alpha_N}(1) & \psi_{\alpha_N}(2) & \ldots. & \psi_{\alpha_N}(N)\end{vmatrix}$$

'*Slater determinant*'

- The $\frac{1}{\sqrt{N!}}$ prefactor normalises the overall wavefunction.
- Interchange of two particle coordinates is the same as swopping two columns in the determinant so: $\psi_A \to -\psi_A$
- If two rows are the same (two particles in the same state; $\alpha_i=\alpha_j$) the determinant is zero.

} as required for fermions.

Bosons

- For two bosons the symmetric state for $\alpha_1 \neq \alpha_2$ is:

$$\psi_S(1,2) = \frac{1}{\sqrt{2}}\left[\psi_{\alpha_1}(1)\psi_{\alpha_2}(2) + \psi_{\alpha_1}(2)\psi_{\alpha_2}(1)\right]$$

and for particles 1 and 2 in the same state: $\alpha_1 = \alpha_2$ and we have a normalised wavefunction of:

$$\psi_S(1,2) = \psi_{\alpha_1}(1)\psi_{\alpha_1}(2)$$

- This result suggests that the probability of finding two identical bosons in the same place is enhanced – crucial for the operation of Lasers.

- Hence even for non-interacting bosons there appears to be an attraction between them.

- To construct the symmetric N particle wavefunction for bosons expand the Slater determinant but make all the signs positive.

Exchange forces (1)

- We consider the effect of the symmetrization requirement for identical particles.
- 1D case of two non-interacting identical particles in states $\psi_a\left(x_1\right)$ and $\psi_b\left(x_2\right)$ - the two states being orthonormal.
- For distinguishable particles the overall wavefunction is:

$$\psi\left(x_1, x_2\right) = \psi_a\left(x_1\right)\psi_b\left(x_2\right)$$

- Identical bosons:

$$\psi_S\left(x_1, x_2\right) = \frac{1}{\sqrt{2}}\left[\psi_a\left(x_1\right)\psi_b\left(x_2\right) + \psi_a\left(x_2\right)\psi_b\left(x_1\right)\right]$$

- Identical Fermions:

$$\psi_A\left(x_1, x_2\right) = \frac{1}{\sqrt{2}}\left[\psi_a\left(x_1\right)\psi_b\left(x_2\right) - \psi_a\left(x_2\right)\psi_b\left(x_1\right)\right]$$

- We calculate the expectation value of the square of the particle separation:

$$X_{12} = \left\langle\left(x_1 - x_2\right)^2\right\rangle = \int \psi^*\left(x_1, x_2\right)\left(x_1 - x_2\right)^2 \psi\left(x_1, x_2\right) dx_1 dx_2$$

$$= \left\langle x_1^2\right\rangle + \left\langle x_2^2\right\rangle - 2\left\langle x_1 x_2\right\rangle$$

Exchange forces (2)

- Distinguishable particles: $\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$

$$\langle x_1^2 \rangle = \int \psi^*(x_1, x_2)\, x_1^2 \psi(x_1, x_2)\, dx_1 dx_2$$

$$= \int x_1^2 |\psi_a(x_1)|^2 dx_1 \int |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_a$$

- This is the expectation value of x^2 in the one-particle state ψ_a.
- Similarly: $\langle x_2^2 \rangle = \int |\psi_a(x_1)|^2 dx_1 \int x_2^2 |\psi_b(x_2)|^2 dx_2 = \langle x^2 \rangle_b$

and

$$\langle x_1 x_2 \rangle = \int x_1 |\psi_a(x_1)|^2 dx_1 \int x_2 |\psi_b(x_2)|^2 dx_2 = \langle x \rangle_a \langle x \rangle_b$$

- So we have:

$$X_{12} = \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b$$

- The result would have been the same if particle 1 had been in ψ_b and particle 2 in ψ_a.

Exchange forces (3)

- For indistinguishable particles we have:

$$\psi(x_1,x_2)=\frac{1}{\sqrt{2}}\left[\psi_a(x_1)\psi_b(x_2)\pm\psi_a(x_2)\psi_b(x_1)\right]\begin{cases}+ & \text{bosons}\\ - & \text{fermions}\end{cases}$$

- And so:

$$\left\langle x_1^2\right\rangle=\tfrac{1}{2}\int x_1^2\left|\psi_a(x_1)\right|^2dx_1\int\left|\psi_b(x_2)\right|^2dx_2+\tfrac{1}{2}\int x_1^2\left|\psi_b(x_1)\right|^2dx_1\int\left|\psi_a(x_2)\right|^2dx_2$$

$$\pm\tfrac{1}{2}\int x_1^2\psi_a^*(x_1)\psi_b(x_1)dx_1\int\psi_b^*(x_2)\psi_a(x_2)dx_2$$

$$\pm\tfrac{1}{2}\int x_1^2\psi_b^*(x_1)\psi_a(x_1)dx_1\int\psi_a^*(x_2)\psi_b(x_2)dx_2=\tfrac{1}{2}\left[\left\langle x^2\right\rangle_a+\left\langle x^2\right\rangle_b\pm0\pm0\right]$$

$$=\tfrac{1}{2}\left[\left\langle x^2\right\rangle_a+\left\langle x^2\right\rangle_b\right]$$ because of orthonormality of ψ_a and ψ_b.

- Similarly: $\left\langle x_2^2\right\rangle=\tfrac{1}{2}\left[\left\langle x^2\right\rangle_b+\left\langle x^2\right\rangle_a\right]$

and $\left\langle x_1x_2\right\rangle=\left\langle x_a\right\rangle\left\langle x_b\right\rangle\pm\left|\left\langle x_{ab}\right\rangle\right|^2$ where $\left\langle x_{ab}\right\rangle=\int x\psi_a^*(x)\psi_b(x)dx$

Exchange forces (4)

- In summary we have:

$$X_{12} = \begin{cases} \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b & \text{distinguishable particles} \\ \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b - 2\left|\langle x \rangle_{ab}\right|^2 & \text{bosons} \\ \langle x^2 \rangle_a + \langle x^2 \rangle_b - 2\langle x \rangle_a \langle x \rangle_b + 2\left|\langle x \rangle_{ab}\right|^2 & \text{fermions} \end{cases}$$

- This suggests that identical bosons tend to be closer together and identical fermions further apart than distinguishable particles in the *same pair* of states.

- Note that $\langle x \rangle_{ab}$ vanishes unless the wavefunctions overlap – thus it is reasonable to assume that identical particles with non-overlapping wavefunctions (very far apart) are distinguishable.

- If there is wavefunction overlap the system behaves as if there is a *'exchange force'* of attraction between identical bosons and a force of repulsion between identical fermions.

- A strictly quantum mechanical effect – no classical counterpart.

Composite particles

•Particles comprising several fermions can themselves behave either as a fermion or as a boson.

•Example – H atom consists of two fermions – a proton and an electron.

•Consider the wavefunction for two H atoms close enough to interact and interchange their constituent particles $\psi\left(p_1, e_1, p_2, e_2\right)$.

•Since electrons and protons are both fermions:

$$\psi\left(p_1, e_1, p_2, e_2\right) = -\psi\left(p_2, e_1, p_1, e_2\right) = \psi\left(p_2, e_2, p_1, e_1\right) \Rightarrow$$ composite boson

•So...on exchange of *all* the identical particles in a composite particle:

•Wavefunction symmetry implies a composite boson (e.g. H)

•Wavefunction anti-symmetry implies a composite fermion.

•In general if a particle composes an even number of fermions it is a composite boson, an odd number means it is a composite fermion.

•Composite bosons: ^{4}He,^{7}Li – both undergo Bose Einstein condensation.

•Composite fermions: ^{3}He, ^{6}Li, p (uud quarks), n (udd quarks).

Spin and spatial components of the wavefunction

- Often helpful to consider spin and spatial parts of wavefunction separately - the overall wavefunction is the product of the two.
- Consider a system of two spin $\frac{1}{2}$ particles – fermions so overall wavefunction must be antisymmetric for a single particle exchange.
- The three $S=1$ states are all symmetric under particle exchange

$$\uparrow_1\uparrow_2,\quad \downarrow_1\downarrow_2,\quad \frac{1}{\sqrt{2}}\left(\downarrow_1\uparrow_2+\uparrow_1\downarrow_2\right)$$

- Symmetric spin state $\Rightarrow$ antisymmetric spatial wavefunction for overall antisymmetry
- The $S=0$ state $\frac{1}{\sqrt{2}}\left(\downarrow_1\uparrow_2-\uparrow_1\downarrow_2\right)$ is antisymmetric under particle exchange
- Antisymmetric spin state $\Rightarrow$ symmetric spatial wavefunction for overall antisymmetry

Interacting particles

•If the particles are non-interacting there is no difference between the energies of the symmetric and anti-symmetric spatial wavefunctions. But if the particles interact....consider two electrons:

•The Coulomb repulsion of two electrons means that an anti-symmetric spatial wavefunction – with the electrons on average further apart will have a lower energy than a symmetric spatial wavefunction.

•The energy difference is known as the *exchange interaction*.

•The exchange interaction causes a symmetric spin wavefunction to have lower energy and the electron spins tend to line up.

•The exchange interaction is behind ferromagnetism.

•This interaction is much stronger than the electron spin-spin magnetic dipole interaction (an energy of $0.8eV$ between the 1s2s and 1s2p states in helium as compared to $10^{-2}eV$ for the magnetic interaction).

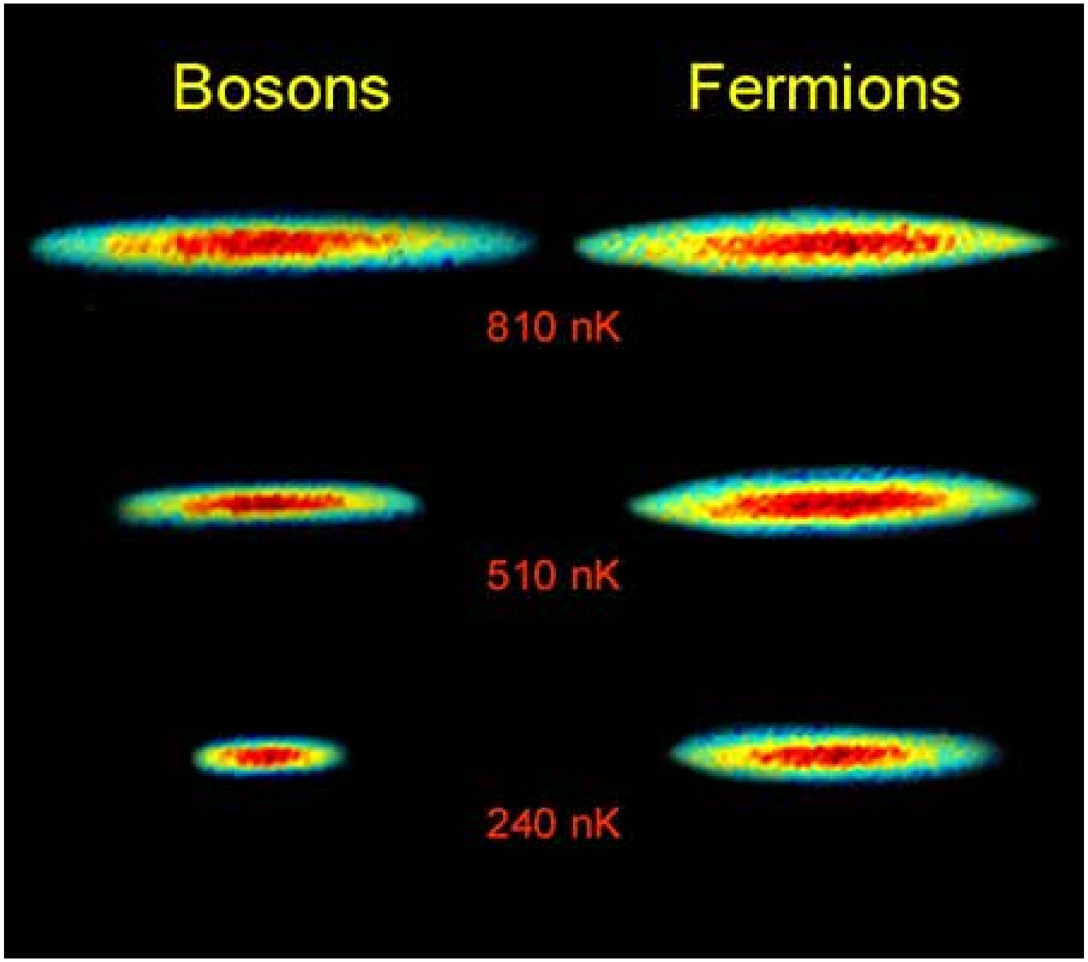
Experiment - bosons and fermions

- In 2001 an experiment was reported which clearly showed the differences between fermions and bosons*****.
- ^{7}Li; a boson (3 protons,3 electrons, 4 neutrons) and ^{6}Li a fermion (3 protons,3 electrons, 3 neutrons) were compared.
- The two types of atoms were first laser cooled to $700\mu K$ and spin polarised optically.
- 3.10^{9} atoms of ^{7}Li and 10^{6} atoms of ^{6}Li were placed in a magnetic trap with a harmonic potential (the atoms have nearly the same μ - same forces).
- 'Evaporative' cooling to a few $100nK$ by microwaves-more energetic atoms given just enough energy to escape.
- ^{6}Li cooled by elastic collisions with ^{7}Li – they avoid other ^{6}Li.
- Optical absorption of both atom 'clouds' measured. Tuned lasers differentiated between the two. CCD camera on microscope took images of cloud of around $5\ \mu m$ diameter.
- Temperature obtained by fitting distribution of atoms to quantum statistics.

***** A G Truscott et al Science **291**, 2570 (2001)

Experiment - bosons and fermions

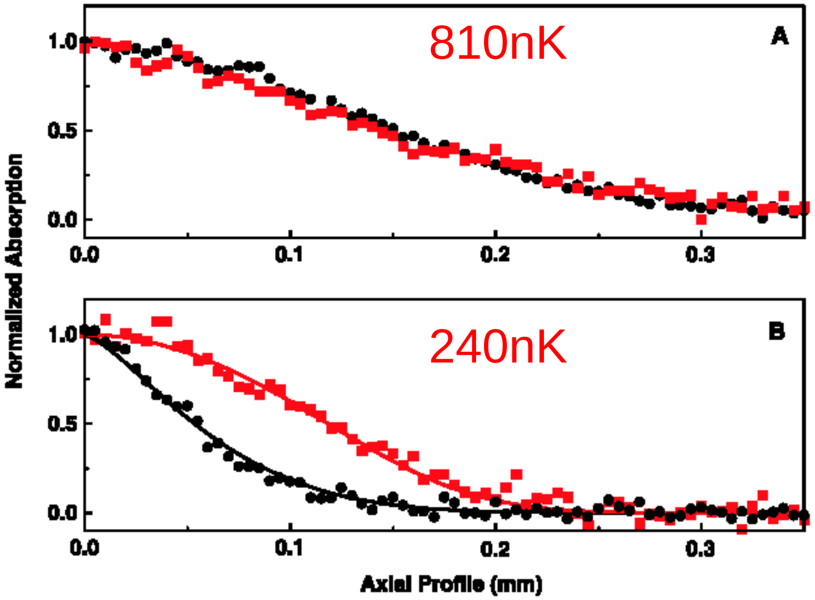
- As the temperature is reduced the boson cloud reduces steadily in size.
- The fermion cloud initially decreases in size but then stops decreasing.
- Explained by the spin polarized fermions being unable to occupy the same spatial states – generating ‘Fermi pressure’.
- Another example of this is the Fermi pressure in white dwarves and neutron stars.



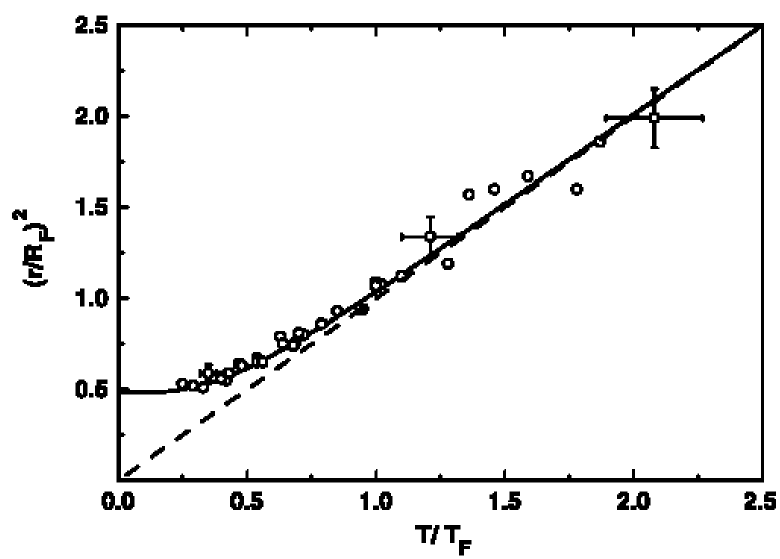
Experiment - bosons and fermions

Distributions with radius of:

- ^{7}Li; boson, black symbols
- ^{6}Li; fermion, red symbols



- A graph of (Radius)^2 of ^{6}Li (fermion) cloud with temperature.
- Behaves classically $\left(kT \propto r^2\right)$ until deviations at the lowest temperatures – solid line is a fit to the distribution for an ideal Fermi gas.



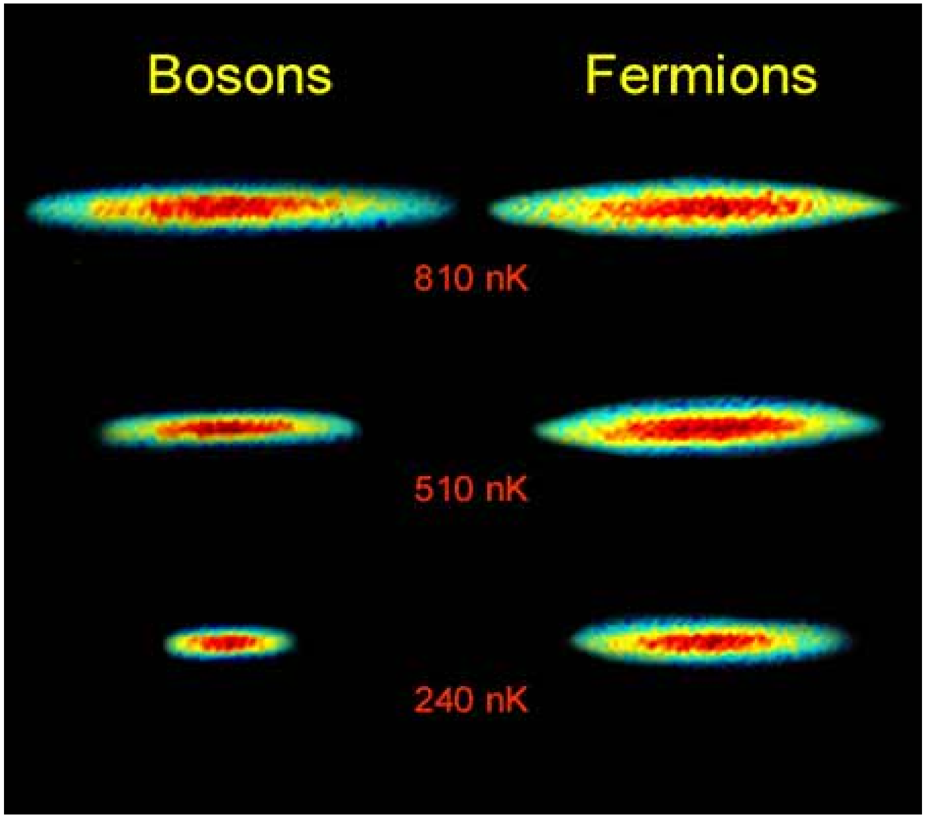
Fermions and bosons are different!!

Lecture 4 - Summary

Identical particles:

- Hamiltonian for system of N particles.
- Particle exchange operator and Pauli Exclusion Principle.
- Wavefunction of fermions – Slater determinant.
- Wavefunction of bosons.
- Exchange forces – calculation of particle separation for distinguishable particles, bosons and fermions.
- Composite particles – an even no. of fermions given a composite boson, an odd number of fermions gives a composite fermion.
- Spin and spatial wavefunction components.
- Exchange interaction for electrons – effect of Coulomb interaction.
- Experimental observation of exchange forces with boson and fermion gases.

Lecture 4



The End!!

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