Quantum Statistics

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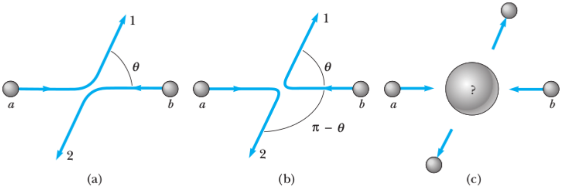
Scattering of Two Identical Particles

- Consider the scattering of two indentical particles (let us say electrons) in their center of mass frame

$$e(\vec{p}) + e(-\vec{p}) \to e(\vec{p}') + e(-\vec{p}').$$

There are two possibilities to get the same final state



- As it was claimed in the last class, if one can follow each particle unambiguously, then the total cross section for the scattering is $\sigma_{\rm tot} = \sigma_a + \sigma_b$.

Scattering of Two Identical Particles

- This is equivalent to assuming that the two identical particles can traced from their initial positions and are distinguishable (the same assumption we made while deriving the Maxwell-Boltzmann distribution).
- Such an assumption is not valid in quantum mechanics. If that assumption is true, it means that we should be able follow the electrons as their distance of approach becomes arbitrarily small.
- To be able to locate the electrons to such precision (using the Heisenberg microscope concept) we need to use a probe with a high momentum, which will completely disturb the state of electrons that was prepared.
- The only assumption, consistent with quantum mechanics, is that it is not possible to trace the electrons once they approach close together.

Scattering of Two Identical Particles

- Another way to state it is the following: Initially, when the electrons are far apart, we can write separate wave functions for them $\psi_1(\vec{r_1})$ and $\psi_2(\vec{r_2})$. The total wave function describing the two electrons is simply a product of the two wave functions.
- But when the electons are close together, the total wave function is no longer a product of two individual wave functions. It is some complicated function $\psi_{12}(\vec{r_1}, \vec{r_2})$.
- However, we do know that the final electrons come out an angle θ with respect to the initial electrons. And this can be achieved by two possibilities shown in the figure.
- Hence the combined wave function must include the wave function of the process shown in figure (a) and the wave function of the process shown in figure (b).
- And the probability of scattering, given in terms of scattering cross section, is proportional to the square of this combined wave function.

Electrons in a Helium Atom

- Let us now consider a somewhat different two electron problem: How to describe the two electrons in the Helium atom?
- We say that one electron has position vector $\vec{r}_1$ and the other electron has position vector $\vec{r}_2$. Strictly speaking we do not which electron is at $\vec{r}_1$ and which electron is at $\vec{r}_2$.
- The time independent Schroedinger's equation is

$$\left[-\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{2e^2}{4\pi\epsilon_0 r_1} - \frac{2e^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{r_{12}}\right]\psi(\vec{r}_1, \vec{r}_2) = E\psi(\vec{r}_1, \vec{r}_2),$$

  where ∇_1 denotes derivates with respect to coordinates $\vec{r}_1$, ∇_2 the derivatives with respect to coordinates $\vec{r}_2$ and $r_{12} = |\vec{r}_1 - \vec{r}_2|$.
- The wave function, of course, depends on both the coordinates $\vec{r}_1$ and $\vec{r}_2$.

Electrons in a Helium Atom

- We can not distinguish between the two electrons. Hence the probability of finding one electron at $\vec{r}_1$ and the other at $\vec{r}_2$ is given equally well by $|\psi(\vec{r}_1, \vec{r}_2)|^2$ or by $|\psi(\vec{r}_2, \vec{r}_1)|^2$.
- But this probability is a well-defined probability. Hence the wave function must satisfy the condition

$$|\psi(\vec{r}_1, \vec{r}_2)|^2 = |\psi(\vec{r}_2, \vec{r}_1)|^2.$$

  That is, the probabilities exhibit exchange symmetry.
- This symmetry immediately implies

$$\psi(\vec{r}_1, \vec{r}_2) = \pm\psi(\vec{r}_2, \vec{r}_1),$$

  that is, the wave function should be even or odd under the particle exchange.

Spin Statistics Theorem

- A very important theorem in quantum theory, called the Spin-Statistics theorem, proves the following statement:
  - For integer spin particles, the wave function must be even under exchange. Such particles are called bosons because they obey Bose-Einstein statistics. Examples are photons (spin-1) and the recently discovered Higgs boson (spin-0).
  - For half odd integer spin particles, the wave function must be odd under the exchange. Such particles are called fermions because they obey Fermi-Dirac statistics. Examples are electrons, protons and neutrinos (all have spin-1/2).
- This theorem is based on some very simple assumptions that the quantum theory should be relativistically invariant and it should be local. That is, two particles can interact only if they are very close together. There is no "action at a distance".

Pauli's Exclusion Principle

- A simple consequence of Spin-Statistics theorem is that $\psi(\vec{r}_1, \vec{r}_1) = 0$, for two fermions. That is, two electrons can't be found at the "same point".
- We can actually generalize this statement. An electron is described a four quantum numbers in an atom. The generalised form of the above statement is No two electrons can have all the quantum numbers same.
- This is called Pauli's exclusion principle. It was first enunciated by Pauli, who later proved the Spin-Statistics theorem.
- The different electronic configurations we see in different atoms are the consequences of Pauli's exclusion principle. Without it, all the electrons will be in the lowest possible energy state and there will be no Chemistry and no life!
- Moreover, a number of properties of solids also can be understood based on Pauli's exclusion principle. That is one of the topics we will study later.

Two Particle Wave function

- Let us consider the form of possible two particle wave functions. We will make two assumptions:
  1. Each particle is bound within the same potential. The eigenvalue problem of the potential is solved and eigenstates are labelled ϕ_1, ϕ_2, ...
  2. The two particles do not interact with each other.
- We denote the position coordinate of particle 1 by $\vec{r}_1$ and that of particle 2 by $\vec{r}_2$. If particle 1 is in the state ϕ_1, we denote the corresponding wave function as $\phi_1(\vec{r}_1)$.
- Let us assume that one particle is state ϕ_1 and the other particle is in state ϕ_2.
- If the two particles are distinguishable (this can be due to different mass or different spin or some other property), then there are two possible wave functions $\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)$ and $\phi_2(\vec{r}_1)\phi_1(\vec{r}_2)$.

Two Particle Wave function

- If both particles are in state ϕ_1, then the wave function will be $\phi_1(\vec{r}_1)\phi_1(\vec{r}_2)$ and the probability of finding both particles in ϕ_1 is $|\phi_1(\vec{r}_1)\phi_1(\vec{r}_2)|^2$.
- Now let us assume that the two particles are identical bosons. They are indistinguishable. Then, the wave function of the two particles must be necessarily symmetric under the exchange $\vec{r}_1 \leftrightarrow \vec{r}_2$. Therefore, the two particle wave function must be

$$\psi_{\text{boson}} = \frac{1}{\sqrt{2}} \left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) + \phi_2(\vec{r}_1)\phi_1(\vec{r}_2)\right],$$

  where the factor $1/\sqrt{2}$ is added for normalization.
- If both bosons in the state ϕ_1, then the wave function becomes $\sqrt{2}\phi_1(\vec{r}_1)\phi_1(\vec{r}_2)$ and the corresponding probability of finding the two bosons in the same state ϕ_1 is $2|\phi_1(\vec{r}_1)\phi_1(\vec{r}_2)|^2$.

Two Particle Wave function

- We have this amazing result: If the two particles are identical bosons, then the probability for finding them in the same quantum state is twice that of the probability of finding two distinguishable particles in the same state.
- This is purely a consequence of applying the exchange symmetry to two particle wave functions.
- One can say that, for identical bosons, the natural tendency is to be in the same quantum state.
- Extending this logic, Einstein predicted that, at very low temperatures, all the identical bosons will be in the same quantum state. This phenomenon is called Bose-Einstein Condensation (BEC).
- Eventhough prediction was made in 1926, BEC was realised in a lab only in 1995 (with rubidium atoms) because one needed nano-Kelvin temperatures to quell the thermal motion of the atoms.

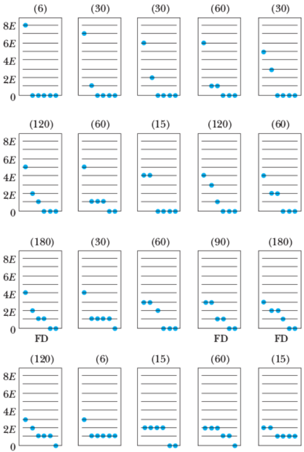
Two Particle Wave function

- If the two identical particles are fermions, the two particle wave function will be
$$\psi_{\text{fermion}} = \frac{1}{\sqrt{2}} \left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_2(\vec{r}_1)\phi_1(\vec{r}_2) \right],$$
which vanishes if the two particles are to be in the same state ϕ_1.
- Just as we derived Maxwell-Boltzmann distribution for large number of distinguishable particles, we can derive Bose-Einstein distribution for a large number of identical bosons and Fermi-Dirac distribution for a large number of identical fermions.
- In the case of Bose-Einstein distribution, there is no restriction on the number of particles in an energy state. However, because of the symmetry under the exchange, the probability for a particle to have a lower energy is larger.
- In the case of Fermi-Dirac distribution, a maximum of two particles can be placed in an energy state. Because of this restriction, the probability of a particle to have lower energy is smaller.

Six Identical Bosons with Total Energy 8E

- Let us consider the old problem of six particles to be distributed in different energy states of energy 0, E, 2E,... with total energy 8E. But now we consider these particles to be identical bosons.
- It was mentioned that there are 20 different arrangements of particles all of which have energy 8E.
- Previously we assumed that the particles are distinguishable and computed a number of microstates for each arrangement of particles in different energy levels.
- These computations were based on looking at the number of different permutations one can make among these distinguishable particles.
- But here all particles are identical. If we make a permutation among them, the permuted state is the same as the original state.
- Therefore, for six bosons with energy 8E, there are only 20 microstates and each of them occurs with the same probability.

Six Identical Bosons with Total Energy 8E



Six Identical Bosons with Total Energy 8E

- The average number of particles in each energy state is given by

$$\bar{n}_{\mathrm{nE}} = \left[n_{\mathrm{nE}}(1) + n_{\mathrm{nE}}(2) + ... + n_{\mathrm{nE}}(20) \right] / 20,$$

  where $n_{\mathrm{nE}}(j)$ is the number of particles in the nE state for the jth arrangement.

- The probability of finding a particle in the state nE is then simply given by

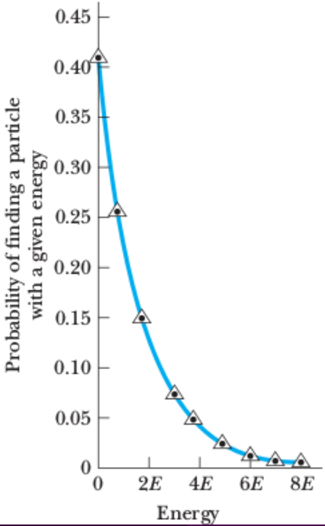
$$\mathrm{p(nE)} = \frac{\bar{n}_{\mathrm{nE}}}{6}.$$

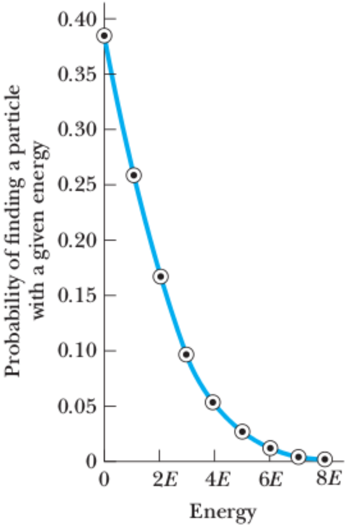
  This way we calculate p(0), p(E), ..., p(8E) and plot them vs E.

- We find that $\mathrm{p}(0)_{\mathrm{BE}} > \mathrm{p}(0)_{\mathrm{MB}}$.

Six Identical Bosons with Total Energy 8E

p(E) vs E plots for bosons and distinguishable particles:





Six Identical Fermions with Total Energy 8E

- Now we repeat the exercise for six identical fermions. For fermions, we have the restriction that a given energy state can not contain more than two fermions.
- Pauli's exclusion principle says that a given quantum state can not contain more than one fermion.
- But almost all the fermions we know have spin-$1/2$. For such fermions, the quantum state of spin has two possibilities: spin up or spin down.
- It does not matter in which direction you are taking the projection of spin. There are only two possible spin projections: spin up or spin down.
- With the additional freedom provided by spin, it is possible to put two (but no more than two) fermions in a given energy state.

Six Identical Fermions with Total Energy 8E

- With this restriction of maximum two particles per energy state, let us count how many different arrangements of six identical fermions we have with energy 8E.
- It turns out that there are only three such arrangements all of which are equally likely.
- As in the case of bosons, we define the average number of particles in each energy state as

$$\bar{n}_{\mathrm{nE}} = \left[n_{\mathrm{nE}}(1) + n_{\mathrm{nE}}(2) + n_{\mathrm{nE}}(3)\right]/3,$$

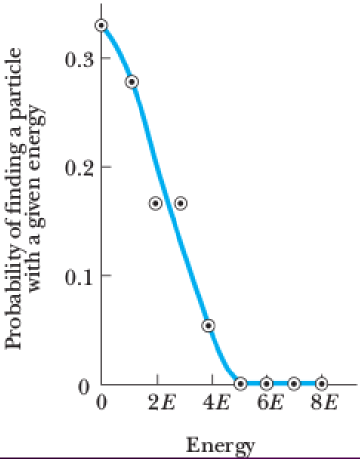
and

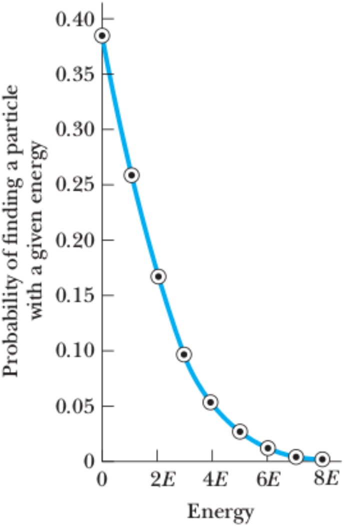
$$\mathrm{p(nE)} = \frac{\bar{n}_{\mathrm{nE}}}{6}.$$

- After computing p(0), p(E), ..., p(8E), we plot them versus E.
- We find that $\mathrm{p(0)_{FD}} < \mathrm{p(0)_{MB}}$.

Six Identical Fermions with Total Energy 8E

p(E) vs E plots for fermions and distinguishable particles:





Bose-Einstein and Fermi-Dirac Distributions

- The quantum energy distributions for large collections of bosons and fermions can be derived by maximising the number of ways of distributing a fixed number of these quantum particles among the allowed energy states subject to the condition fixed total energy.
- We get the following distributions:

$$
\begin{aligned}
f_{\mathrm{BE}}(E) &= \frac{1}{B\exp(E/kT) - 1} \\
f_{\mathrm{FD}}(E) &= \frac{1}{H\exp(E/kT) + 1}.
\end{aligned}
$$

- The constant B and H are determined by the conditions

$$
\begin{aligned}
\left(\frac{N}{V}\right)_{\mathrm{bosons}} &= \int_0^\infty g(E) f_{\mathrm{BE}}(E) dE \\
\left(\frac{N}{V}\right)_{\mathrm{fermions}} &= \int_0^\infty g(E) f_{\mathrm{FD}}(E) dE,
\end{aligned}
$$

where $g(E)$ is the density of states per unit volume, as defined earlier.

Comparison of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac distributions as functions of energy