

Lesson 6 - Quantum Many-Body Systems

Unit 6.1 Identical particles, bosons and fermions

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Identical quantum particles (I)

The generalized coordinate $x = (\mathbf{r}, \sigma)$ of a particle which takes into account the spatial coordinate \mathbf{r} but also the intrinsic spin σ pertaining to the particle. For instance, a spin $1/2$ particle has $\sigma = -1/2, 1/2 = \downarrow, \uparrow$. By using the Dirac notation the corresponding single-particle state is

$$|x\rangle = |\mathbf{r} \sigma\rangle. \quad (1)$$

We now consider N identical particles; for instance particles with the same mass and electric charge. The many-body wavefunction of the system is given by

$$\Psi(x_1, x_2, \dots, x_N) = \Psi(\mathbf{r}_1, \sigma_1, \mathbf{r}_2, \sigma_2, \dots, \mathbf{r}_N, \sigma_N), \quad (2)$$

According to quantum mechanics identical particles are indistinguishable. As a consequence, it must be

$$|\Psi(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_N)|^2 = |\Psi(x_1, x_2, \dots, x_j, \dots, x_i, \dots, x_N)|^2, \quad (3)$$

which means that the probability of finding the particles must be independent on the exchange of two generalized coordinates x_i and x_j .

Identical quantum particles (II)

Experiments suggests that there are only two kind of identical particles which satisfy Eq. (3): bosons and fermions.

For N identical bosons one has

$$\Psi(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_N) = \Psi(x_1, x_2, \dots, x_j, \dots, x_i, \dots, x_N), \quad (4)$$

i.e. the many-body wavefunction is symmetric with respect to the exchange of two coordinates x_i and x_j .

For N identical fermions one has instead

$$\Psi(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_N) = -\Psi(x_1, x_2, \dots, x_j, \dots, x_i, \dots, x_N), \quad (5)$$

i.e. the many-body wavefunction is anti-symmetric with respect to the exchange of two coordinates x_i and x_j .

An immediate consequence of the anti-symmetry of the fermionic many-body wavefunction is the *Pauli Principle*: if $x_i = x_j$ then the many-body wavefunction is zero. In other words: the probability of finding two fermionic particles with the same generalized coordinates is zero.

Identical quantum particles (III)

A remarkable experimental fact, which is often called *spin-statistics theorem* because can be deduced from other postulates of relativistic quantum field theory, is the following:

identical particles with integer spin are bosons while identical particles with semi-integer spin are fermions. For instance, photons are bosons with spin 1 while electrons are fermions with spin $1/2$.

Notice that for a composed particle it is the total spin which determines the statistics. For example, the total spin (sum of nuclear and electronic spins) of ${}^4\text{He}$ atom is 0 and consequently this atom is a boson, while the total spin of ${}^3\text{He}$ atom is $1/2$ and consequently this atom is a fermion.

Non-interacting identical particles (I)

The quantum Hamiltonian of N identical non-interacting particles is given by

$$\hat{H}_0 = \sum_{i=1}^N \hat{h}(x_i), \quad (6)$$

where $\hat{h}(x)$ is the single-particle Hamiltonian. Usually the single-particle Hamiltonian is given by

$$\hat{h}(x) = -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}), \quad (7)$$

with $U(\mathbf{r})$ the external confining potential. In general the single-particle Hamiltonian \hat{h} satisfies the eigenvalue equation

$$\hat{h}(x) \phi_n(x) = \epsilon_n \phi_n(x), \quad (8)$$

where ϵ_n are the single-particle eigenenergies and $\phi_n(x)$ the single-particle eigenfunctions, with $n = 1, 2, \dots$

Non-interacting identical particles (II)

The many-body wavefunction $\Psi(x_1, x_2, \dots, x_N)$ of the system can be written in terms of the single-particle wavefunctions $\phi_n(x)$ but one must take into account the spin-statistics of the identical particles. For N bosons the simplest many-body wave function reads

$$\Psi(x_1, x_2, \dots, x_N) = \phi_1(x_1) \phi_1(x_2) \dots \phi_1(x_N), \quad (9)$$

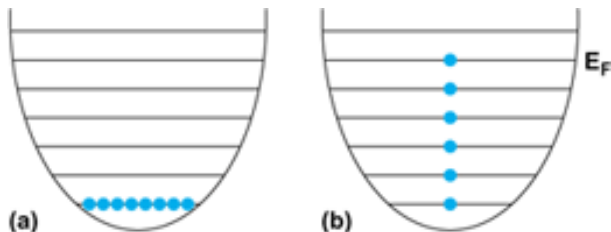
which corresponds to the configuration where all the particles are in the lowest-energy single-particle state $\phi_1(x)$. This is indeed a pure Bose-Einstein condensate.

For N fermions the simplest many-body wave function is instead very different, and it is given by

$$\Psi(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{pmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_N) \\ \dots & \dots & \dots & \dots \\ \phi_N(x_1) & \phi_N(x_2) & \dots & \phi_N(x_N) \end{pmatrix} \quad (10)$$

that is the so-called Slater determinant of the $N \times N$ matrix obtained with the N lowest-energy single particle wavefunctions $\phi_n(x)$, with $n = 1, 2, \dots, N$, calculated in the N possible generalized coordinates x_i , with $i = 1, 2, \dots, N$.

Non-interacting identical particles (III)



For non-interacting identical particles the Hamiltonian (6) is separable and the total energy associated to the bosonic many-body wavefunction (9) is simply

$$E = N \epsilon_1 , \quad (11)$$

while for the fermionic many-body wavefunction (10) the total energy (in the absence of degenerate single-particle energy levels) reads

$$E = \epsilon_1 + \epsilon_2 + \dots + \epsilon_N , \quad (12)$$

which is surely higher than the bosonic one. The highest occupied single-particle energy level is called Fermi energy, and it is indicated as ϵ_F (or, as in the figure, E_F); in our case it is obviously $\epsilon_F = \epsilon_N$.