Multiparticle systems: indistinguishability and consequences

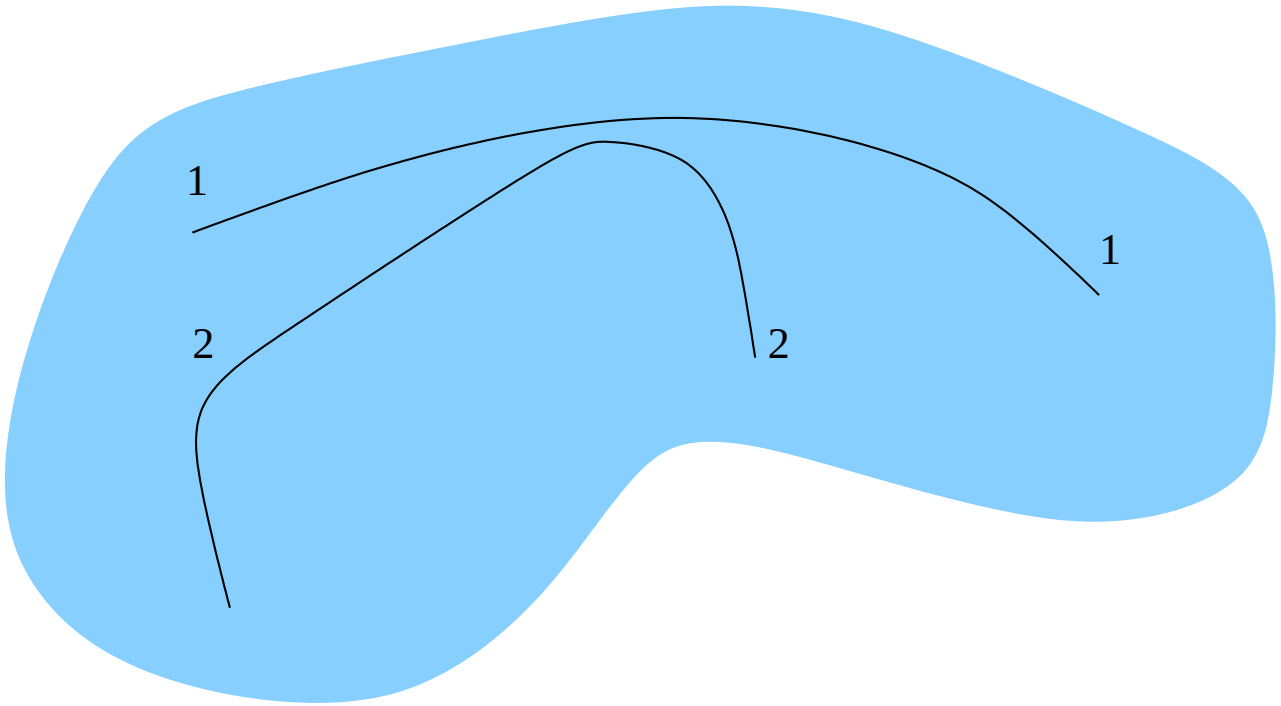
Sourendu Gupta

TIFR Graduate School

Quantum Mechanics 1
October 3, 2008

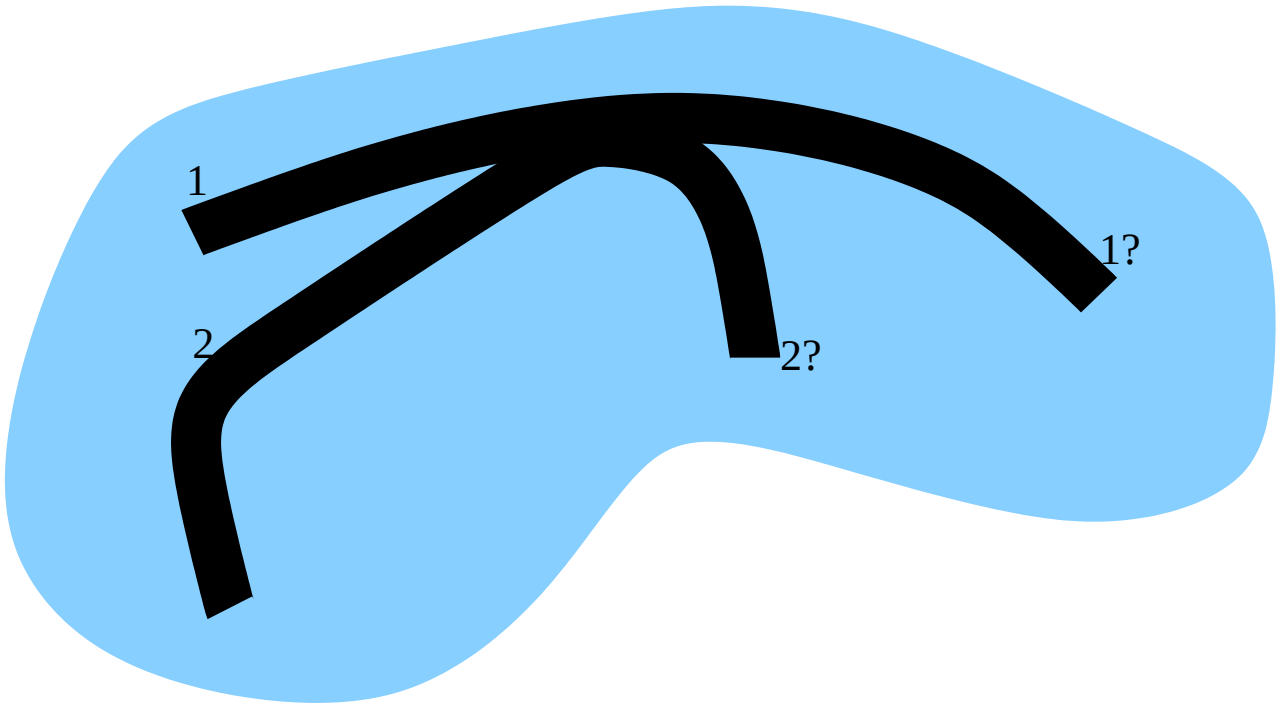
Outline

Classical identical particles



Evolution of identical (non-interacting) particles is unproblematic in classical mechanics. Two particles distinguished by their initial conditions: trajectories forever distinguishable, even if all intrinsic properties are the same. Possible since phase space trajectories do not cross. Classical identical particles can be "painted" to distinguish them.

Quantum identical particles



If two particles cannot be distinguished by **intrinsic** properties, then quantum evolution (even of non-interacting particles) is problematic: unique labelling of initial states not possible in general. There is no quantum "paint".

Two particle states

Take two single particle states $|\lambda_1\rangle$, $|\lambda_2\rangle$, where λ_i are a complete set of eigenvalues. A typical two particle state is $|\lambda_1;\lambda_2\rangle = |\lambda_1\rangle \otimes |\lambda_2\rangle$. Define an interchange operator P, such that

$$P|\lambda_1;\lambda_2\rangle = |\lambda_2;\lambda_1\rangle,$$

i.e., P creates a different outer product $|\lambda_2\rangle \otimes |\lambda_1\rangle$. However, the two particles being identical, the vector space with this basis is the same as the vector space in the other basis. Therefore P must be an unitary matrix, and its eigenvalues must be pure phases, $\exp(i\alpha)$. However, $P^2|\lambda_1;\lambda_2\rangle = |\lambda_1;\lambda_2\rangle$, *i.e.*, $P^2 = 1$, so $\exp(i\alpha) = \pm 1$.
When $P = 1$, the particles are called **bosons**; when $P = -1$ they are called **fermions**. This is an intrinsic property, *i.e.*, all quantum states of many fermions have the same sign under permutations (and similarly for bosons). In the relativistic theory one can prove that all bosons have integer spin and all fermions have half integer spin.

N-particle states and wavefunctions

By extension of the previous argument, any quantum state of N identical particles picks up a definite sign under interchange of any two particles. Using the permutation operators P_α, one may write

$$|\lambda_1;\lambda_2;\cdots\lambda_N\rangle_{B,F} = \frac{1}{\sqrt{N!}}\sum_\alpha (\pm 1)^\alpha P_\alpha |\lambda_1;\lambda_2;\cdots\lambda_N\rangle,$$

where $(-1)^\alpha$ is -1 only if the permutation interchanges an odd number of pairs of fermions. Wavefunctions for non-interacting N-particle systems are

$$\begin{aligned}
\Psi_B^{\lambda_1,\lambda_2,\cdots\lambda_N}(r_1,r_2,\cdots,r_N) &= \frac{1}{N!}\sum_P\prod_{i=1}^N \psi^{\lambda_i}(r_{P(i)}),\\
\Psi_F^{\lambda_1,\lambda_2,\cdots\lambda_N}(r_1,r_2,\cdots,r_N) &= \frac{1}{\sqrt{N!}}\begin{vmatrix}\psi^{\lambda_1}(r_1) & \psi^{\lambda_2}(r_2) & \cdots & \psi^{\lambda_N}(r_N)\\ \psi^{\lambda_1}(r_2) & \psi^{\lambda_2}(r_3) & \cdots & \psi^{\lambda_N}(r_1)\\ \vdots & \vdots & \cdots & \vdots\\ \psi^{\lambda_1}(r_N) & \psi^{\lambda_2}(r_1) & \cdots & \psi^{\lambda_N}(r_{N-1})\end{vmatrix}.
\end{aligned}$$

Some consequences

- The multi-fermion wavefunction (also called a Slater determinant) vanishes whenever two of the single particle quantum states are identical, *i.e.*, when $\lambda_i = \lambda_j$. This means that two fermions cannot be in the same state. This is called **Pauli's exclusion principle**.
- For two particle states, one may create projection operators

$$S = \frac{1}{\sqrt{2}}(1+P) \qquad \text{and} \qquad A = \frac{1}{\sqrt{2}}(1-P),$$

  which project out the symmetric and antisymmetric states respectively. Here $S + A = 1$. For higher number of particles the S and A projectors shown before do not sum to unity.
- Even when particles are interacting, *i.e.*, when the multi-particle state cannot be written as tensor products of two single particle states, the interchange of **all** quantum numbers of two identical particles results in multiplying the state by ± 1.

Outline

A convenient notation

If λ_i is a complete set of eigenvalues for single particles and $|\lambda_i\rangle$ are the corresponding eigenvectors, then any multi-particle state of N non-interacting particles is fully specified in the explicit notation

$$|\lambda_1; \lambda_2; \cdots \lambda_N\rangle = |\lambda_1\rangle \otimes |\lambda_2\rangle \otimes \cdots \otimes |\lambda_N\rangle,$$

i.e., by giving the quantum numbers of each particle. However, one could also try to specify the same state in a new notation

$$|n_1, n_2, \cdots\rangle, \qquad (\sum_i n_i = N),$$

i.e., by specifying n_i, the number of particles in each state i. However, this notation loses the ordering of tensor products, which, as we saw, is an important part of the specification of quantum states.
To do this, we first extend our considerations to **Fock space**, which is the direct sum of Hilbert spaces for different particle numbers—

$$\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_N \oplus \cdots$$

Boson creation and annihilation operators

Introduce operators which change the number of particles, *i.e.*, connect the Hilbert spaces of operators with two different numbers of particles. Let a_i be the operator which decreases the number of particles in state $|i\rangle$ by 1, *i.e.*,

$$a_i|n_1, n_2, \cdots, n_i, \cdots\rangle = \sqrt{n_i}|n_1, n_2, \cdots, n_i - 1, \cdots\rangle.$$

This "particle annihilation operator" is clearly not Hermitean; label its adjoint by $a_i^\dagger$. Clearly,

$$a_i^\dagger|n_1, n_2, \cdots, n_i, \cdots\rangle = \sqrt{1 + n_i}|n_1, n_2, \cdots, n_i + 1, \cdots\rangle.$$

Now $a_i a_i^\dagger$ and $a_i^\dagger a_i$ are both Hermitean operators, which act on Hilbert spaces of fixed number of particles. From the definitions, clearly

$$[a_i, a_i^\dagger]|n_1, n_2, \cdots, n_i, \cdots\rangle = |n_1, n_2, \cdots, n_i - 1, \cdots\rangle.$$

Similar arguments when the indices are different lead to the basic commutation relations

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0.$$

Fermion creation and annihilation operators

Fermions are created and annihilated by operators which satisfy the relation

$$\{a_i, a_j^\dagger\} = a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}, \quad \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0.$$

The last two relations imply that $a_j^2 = (a_j^\dagger)^2 = 0$ when acting on any quantum state. As a result, the number of particles in any quantum state is either 0 or 1 ($n_i = 0$, 1 for all i).
A multi-particle state is obtained from the unique state $|0\rangle$ without any particles (vacuum state) by the action of multiple creation operators—

$$|n_1, n_2, n_3, \cdots\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}(a_3^\dagger)^{n_3}\cdots|0\rangle.$$

The permutation symmetry of particles is then subsumed into the operator commutation (or anti-commutation) rules. Hence this definition of multi-particle states is exactly the same as the ones given earlier by the explicit symmetrization and anti-symmetrization formulae.

Rewriting the operators

Note that particle creation and annihilation operators are not the same as ladder operators we have encountered earlier. Ladder operators work on the Hilbert space of states with fixed particle number, and change the states. Particle creation and annihilation operators connect Hilbert spaces with different numbers of particles. Bilinear operators such as $a_i a_j^\dagger$ or $a_j^\dagger a_i$ could be used as ladder operators in Hilbert spaces with fixed numbers of particles.
Rewriting the states allows us to rewrite the operators. Any single particle observable is

$$f = \sum_{ij} f_{ij} |\lambda_i\rangle\langle\lambda_j| = \sum_{ij} f_{ij} a_i^\dagger a_j,$$

Any two particle observable is

$$g = \sum_{ijkl} g_{ijkl} |\lambda_i; \lambda_j\rangle\langle\lambda_k; \lambda_l| = \sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_k a_l,$$

and so on. Thus, the boson and fermion creation and annihilation operators allow us to reformulate the quantum mechanics of many particle systems very efficiently. Further use of this formalism is made in quantum field theory and in a formulation of a truncated field theory called many-body theory.

Outline

Exchange effects in transitions

A two particle system is initially in the state $|a;b\rangle$ and makes a transition to the state where one of the particles is in state $|c\rangle$ whereas the other is in state $|d\rangle$. The transition probability is

$$\mathcal{P} = |\langle c;d|a;b\rangle|^2 + |\langle d;c|a;b\rangle|^2 = |\langle c|a\rangle|^2|\langle d|b\rangle|^2 + |\langle c|b\rangle|^2|\langle d|a\rangle|^2.$$

When the two particle states are symmetrized, *i.e.*, the initial state is $(1/\sqrt{2})(1 \pm P)|a;b\rangle$ and the final state is $(1/\sqrt{2})(1 \pm P)|c;d\rangle$, the transition probability is

$$\mathcal{P} = \left|\langle c;d|\frac{1}{2}(1 \pm P)(1 \pm P)|a;b\rangle\right|^2 = |\langle c|a\rangle\,\langle d|b\rangle \pm \langle d|a\rangle\,\langle c|b\rangle|^2\,.$$

In the second case there is interference between the two possibilities, and this interference is missing in the first case.

Ground state of He

The neglect of electron spins in atoms is approximately correct since the Coulomb force does not depend on spins. However, for two-electron atoms such as He, the ground state is actually

$$|100;100\rangle \otimes \left|\frac{1}{2}, m; \frac{1}{2}, m'\right\rangle,$$

where the two-particle spatial part of the state, $|100;100\rangle$, is symmetric by construction. However, the complete state must be antisymmetric under exchange of **all** quantum numbers of the system.
As a result, the outer product of two spin 1/2 states, must be completely antisymmetric. However, we have seen that the completely antisymmetric state belongs to total spin 0,

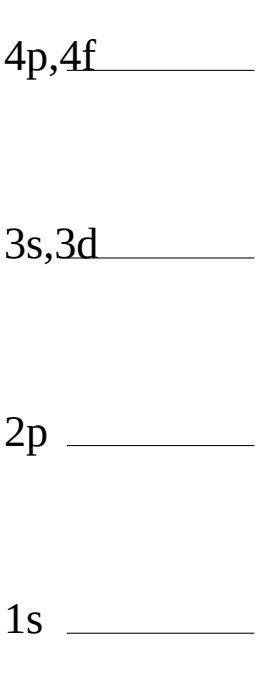
$$|0,0\rangle = \frac{1}{\sqrt{2}}\left\{\left|\frac{1}{2},\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle - \left|\frac{1}{2},-\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle\right\}.$$

The prediction that the ground state of He has spin 0 follows from purely quantum **exchange effects**.

Chemistry and nuclear physics

The fact that atoms have electrons distributed in many different orbitals, $|nlm\rangle$, is due to the fact that electrons are fermions, and hence, through the Pauli exclusion principle, must all occupy different states. Since each electron has spin $s = 1/2$, each orbital can be occupied by two electrons (with opposite s_z). This fact leads to the shell model of atoms as we know them, and to other consequences like finite valency in chemistry.

Since nuclei contain protons and neutrons, which are also fermions, a shell model also works for nuclei. This is somewhat more complicated by the fact that there are two different kinds of indistinguishable fermions.



The existence of colour

All baryons are made of three quarks. The u quark has charge $2e/3$ and spin $1/2$, and the d quark has charge $-e/3$ and spin $1/2$. The Δ^{++} is a baryon with spin $3/2$ and charge $2e$. Hence it must contain three u quarks. The quantum state of the Δ^{++} with maximum J_z must be

$$\left|\lambda_1, \frac{1}{2}, \frac{1}{2}, u; \lambda_2, \frac{1}{2}, \frac{1}{2}, u; \lambda_3, \frac{1}{2}, \frac{1}{2}, u\right\rangle,$$

since the total angular momentum must sum to $3/2$. There is evidence from various other properties that the spatial quantum numbers of the three quarks, λ_i, are equal. Hence the state must be symmetric. But this is impossible.

Various explanations were advanced in the 1960's, including exotic statistics under exchange of quarks. However, the simplest explanation, and the one that is now verified is that there is an extra quantum number in the problem, now called colour. Under the interchange of **all** quantum numbers, the state is antisymmetric.

Outline

References

1. Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz. The material in this lecture can be found in chapter 9. This chapter approximates the material in this lecture.
2. Quantum Mechanics (Vol 2), C. Cohen-Tannoudji, B. Diu and F. Laloë. Chapter 14 of this book discusses angular momentum. The presentation in this chapter includes some of the material from this lecture.
3. A Handbook of Mathematical Functions, by M. Abramowicz and I. A. Stegun. This is a handy place to look up useful things about various classes of functions.