Multiparticle systems: indistinguishability and consequences

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Outline

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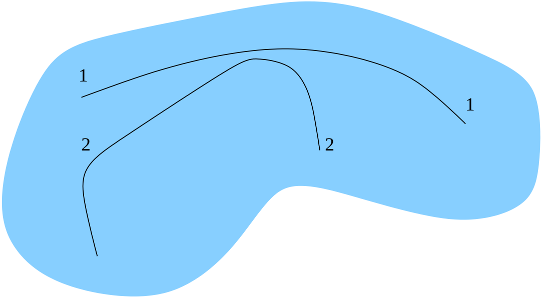
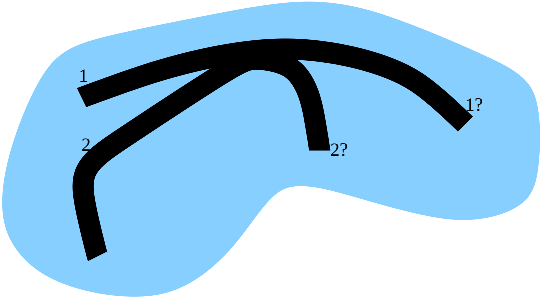
Classical identical particles



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 and identical particles

Single particle states are $|\lambda\rangle$, where λ stands for a complete set of eigenvalues. A 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 $|\lambda_2\rangle \otimes |\lambda_1\rangle$. If the two particles are identical, then the vector space with this basis is the same as the vector space with the previous basis. In that case P must be an unitary matrix. However, $P^2\,|\lambda_1;\lambda_2\rangle = |\lambda_1;\lambda_2\rangle$, *i.e.*, $P^2 = 1$, so its eigenvalues are ± 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 relativistic quantum mechanics one can prove a spin-statistics theorem: all bosons have integer spin and all fermions have half integer spin.

N-particle states: permutations

The states of N identical particles can be created by a simple extension of the previous argument. Any permutation of N objects can be built out of permutations of appropriately chosen pairs. Each pair-wise permutation multiplies the state by a fixed sign. So, successive permutations multiply the state by products of these signs.

Using the permutation operators P_α, one may write

$$|\lambda_1; \lambda_2; \cdots \lambda_N\rangle_{B,F} \propto \sum_\alpha (\pm 1)^\alpha P_\alpha \, |\lambda_1; \lambda_2; \cdots \lambda_N\rangle \, ,$$

where $(-1)^\alpha$ is -1 only if the permutation interchanges an odd number of pairs of fermions. The constant of proportionality must be chosen to normalize the state.

N-particle wavefunctions

The wavefunction of a non-interacting N-boson system is

$$\Psi_B^{\lambda_1,\lambda_2,\cdots\lambda_N}(r_1, r_2, \cdots, r_N) \propto \sum_P \prod_{i=1}^N \psi^{\lambda_i}(r_{P(i)}),$$

where the sum is over all $N!$ permutations of the labels. For the N-fermion wavefunction one gets the determinant

$$\Psi_F^{\lambda_1,\lambda_2,\cdots\lambda_N}(r_1, r_2, \cdots, r_N) \propto \begin{vmatrix} \psi^{\lambda_1}(r_1) & \psi^{\lambda_2}(r_2) & \cdots & \psi^{\lambda_N}(r_N) \\ \psi^{\lambda_1}(r_2) & \psi^{\lambda_2}(r_3) & \cdots & \psi^{\lambda_N}(r_1) \\ \vdots & \vdots & \cdots & \vdots \\ \psi^{\lambda_1}(r_N) & \psi^{\lambda_2}(r_1) & \cdots & \psi^{\lambda_N}(r_{N-1}) \end{vmatrix}.$$

This is called a Slater determinant.

Some consequences

- The 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 for interacting particles, when the multi-particle state cannot be written as tensor products of single particle states, the interchange of all quantum numbers of two identical particles results in multiplying the state by ± 1.

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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

Since the Coulomb force does not depend on spins, electron spins may be approximately neglected. But when there are 2 or more electrons, we must keep track of it. The ground state of He is

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

where the spatial part, $|100;100\rangle$, is obviously symmetric. But the complete state must be antisymmetric under exchange of all quantum numbers of the system. So, the spin part must be completely antisymmetric. So this must be a total spin 0 state

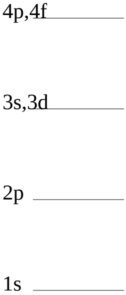
$$|0,0\rangle = \frac{1}{\sqrt{2}}\left\{\left|\frac{1}{2},\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle - \left|\frac{1}{2},-\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle\right\}.$$

The prediction that the ground state of He has spin 0 follows from purely quantum exchange effects. If the electrons is replaced by pions, which have $s=0$, the ground state would again have total spin zero. However, the excited states of He and $He(\pi)$ would be quite different. Exchange effects are removed if one of the electrons in He is replaced by a muon.

Shell model: 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 colour quantum number

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, 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: colour. Under the interchange of all quantum numbers, the state is antisymmetric.

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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.*,

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

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

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

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

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

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

Particle creation and annihilation operators are not ladder operators. Those work on states with fixed particle number. Particle creation and annihilation operators connect Hilbert spaces of different numbers of particles. Combinations like $a_j^\dagger a_i$ can 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

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

Any two particle observable is

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

and so on. So, creation and annihilation operators allow us to rewrite 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.

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Keywords and References

Keywords

Intrinsic properties, interchange operator, bosons, fermions, spin-statistics theorem, permutation, Slater determinant, Pauli's exchange principle, exchange effects, shell model, colour quantum number, Fock space, quantum field theory, many-body theory.

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