

Singlet and Triplet States

Podcast Learn & Fun *

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In quantum mechanics, *spin* is a fundamental property of particles such as electrons, protons, and neutrons. Spin represents intrinsic angular momentum and can take on discrete values. For example, electrons possess a spin quantum number $s = \frac{1}{2}$, meaning they can have one of two possible spin orientations: spin-up ($m_s = +\frac{1}{2}$) or spin-down ($m_s = -\frac{1}{2}$). When multiple particles are involved, such as two electrons, their spins can combine in various ways to form different quantum states. Among these combinations, the *singlet* and *triplet* states are particularly important and arise in systems with two interacting particles.

Singlet State

The singlet state occurs when two particles (such as electrons) pair their spins in such a way that their total spin cancels out. This results in a total spin quantum number $S_{\text{total}} = 0$, which signifies a state where the spins of the two particles are oppositely aligned. Mathematically, the singlet state is represented by a quantum superposition of the two possible spin states of the particles. The wavefunction for the singlet state is given by:

$$|\psi_{\text{singlet}}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ represent the spin-up and spin-down states of an electron, respectively. The minus sign between the two terms indicates that the singlet state is *antisymmetric* with respect to the exchange of the two particles, meaning if the two particles are swapped, the wavefunction changes its sign:

$$|\psi_{\text{singlet}}(1, 2)\rangle = -|\psi_{\text{singlet}}(2, 1)\rangle$$

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In other words, the two electrons are in a state where one is always spin-up and the other is always spin-down. This anti-alignment is a key feature of the singlet state. Because the total spin is zero, the singlet state is often considered the lowest energy configuration for two interacting particles, as it minimizes the system's energy due to the favorable pairing of spins.

Triplet State

The triplet state, on the other hand, occurs when two particles have spins that are more aligned with each other, resulting in a total spin of $S_{\text{total}} = 1$. This means that the two particles are not oppositely aligned, as in the singlet state, but instead their spins are either parallel or partially parallel, leading to three possible orientations of the total spin. These orientations correspond to three possible values of the magnetic quantum number $m_{\text{total}} = 1, 0, -1$, which describe the projection of the total spin along a chosen axis.

The triplet states for two electrons can be written as:

$$|\psi_{\text{triplet}}(m_{\text{total}})\rangle = \begin{cases} |\uparrow\uparrow\rangle & \text{for } m_{\text{total}} = 1, \\ \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & \text{for } m_{\text{total}} = 0, \\ |\downarrow\downarrow\rangle & \text{for } m_{\text{total}} = -1. \end{cases}$$

These three states correspond to the three different possible values of m_{total} and represent the cases where the spins of the two electrons are both aligned (either both spin-up or both spin-down) or in a mixed alignment. Unlike the singlet state, the triplet state is *symmetric* with respect to the exchange of the two particles. Therefore, swapping the two electrons does not change the sign of the wavefunction:

$$|\psi_{\text{triplet}}(1, 2)\rangle = |\psi_{\text{triplet}}(2, 1)\rangle$$

The triplet state involves more correlated spins, with parallel or partially parallel configurations. This type of alignment leads to higher energy compared to the singlet state due to the Pauli exclusion principle and electrostatic repulsion between the particles.

Differences Between Singlet and Triplet States

The singlet and triplet states have several key differences, both in their quantum numbers and physical implications. The singlet state has a total spin

of $S_{\text{total}} = 0$ and a single possible value for the magnetic quantum number ($m_{\text{total}} = 0$), whereas the triplet state has a total spin of $S_{\text{total}} = 1$ and three possible values for m_{total} ($m_{\text{total}} = 1, 0, -1$). This results in the singlet state having only one substate, while the triplet state has three substates.

Moreover, the wavefunction for the singlet state is antisymmetric, meaning that swapping the two particles changes the sign of the wavefunction. In contrast, the wavefunction for the triplet state is symmetric with respect to particle exchange. The singlet state is typically lower in energy due to the opposite spin alignment, which reduces repulsive interactions between the particles. The triplet state, with parallel or mixed spin alignments, generally results in higher energy due to increased repulsion between the particles.

These differences also lead to distinct physical phenomena. For instance, the singlet and triplet states play an important role in spectroscopy, particularly in fluorescence and phosphorescence. A singlet-triplet transition, which involves a change in the spin state, is typically *spin-forbidden*, making such transitions less probable and leading to slower emission rates in phosphorescence. Additionally, the spin arrangements in these states impact magnetic properties, such as *magnetic susceptibility* and other related behaviors.

Applications and Implications

The singlet and triplet states have broad applications in various fields of physics and chemistry. In quantum mechanics, these states are vital for understanding *quantum entanglement*, where the quantum state of one particle is intrinsically linked to the state of the other. This entanglement is often utilized in *quantum information processing* and *quantum computing*, where the ability to manipulate entangled states forms the foundation of many proposed quantum algorithms.

Moreover, the singlet and triplet states influence the behavior of systems in *magnetism* and *molecular physics*. The different spin configurations lead to distinct energy levels and magnetic properties, which are crucial for understanding the behavior of materials at the quantum level. For example, materials with unpaired electrons often exhibit paramagnetism, and the interaction between spins in different states can influence the material's macroscopic properties.

Conclusion

In summary, the singlet and triplet states represent different configurations of spin for a two-particle system, with the singlet state corresponding to an anti-aligned pair of spins and the triplet state corresponding to parallel or partially parallel spins. The singlet state has lower energy due to spin-pairing, while the triplet state has higher energy due to spin alignment. These states play a crucial role in various physical processes, including quantum entanglement, spectroscopy, and magnetism. Understanding the properties and differences between these states is essential in fields such as atomic physics, quantum chemistry, and material science.