

Exchange symmetry, spin pairs and Pauli exclusion

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Two electrons can share one spatial orbital if their complete spatial-plus-spin state has the required antisymmetry.

Prerequisites: 5, 36.

- Construct normalised symmetric and antisymmetric two-orbital spatial states
- Combine spatial and spin symmetry to produce allowed two-electron states
- Count complete-state occupations and interpret exchange-induced correlations

Exchange complete particle labels

For identical particles, exchanging every coordinate and spin label changes a fermionic total wavefunction by a minus sign and leaves a bosonic one unchanged. Mathematical slots 1 and 2 label arguments, not permanently distinguishable particles. For two distinct orthonormal orbitals a and b, spatial combinations are $\Psi_{\pm} = [a(1)b(2) \pm b(1)a(2)]/\sqrt{2}$. Orthogonality makes these combinations normalised and gives exchange eigenvalues ± 1 . If the two orbitals are identical, the antisymmetric combination is identically zero and the displayed symmetric formula is not correctly normalised; the double-occupation spatial state is simply $a(1)a(2)$. Recheck normalization whenever orbitals or their overlaps change.

Pair spatial and spin symmetry

Two spin-1/2 particles have one spin singlet $(\uparrow\downarrow - \downarrow\uparrow)/\sqrt{2}$ with total spin $S=0$; it is antisymmetric under exchange. The three triplets $\uparrow\uparrow$, $(\uparrow\downarrow + \downarrow\uparrow)/\sqrt{2}$ and $\downarrow\downarrow$ have $S=1$ and are symmetric. Electrons require an antisymmetric total state, so a symmetric spatial state pairs with the singlet, while an antisymmetric spatial state pairs with a triplet. Two electrons in the same spatial orbital can form the singlet, but cannot form a triplet there in this simple two-electron state. Pauli exclusion prevents occupation of the same complete single-particle state, including spin. Opposite-spin electrons in one orbital are two different complete states; describing exclusion as one electron per orbital discards this distinction.

Count complete states

For two spatial orbitals a,b and two spin states each, there are four complete single-particle states. Two identical electrons have $\text{choose}(4,2)=6$ occupation patterns: two double-occupation singlets, one different-orbital singlet, and three different-orbital triplets. For three spatial orbitals, there are six complete states and $\text{choose}(6,2)=15$ patterns. Counting ordered assignments overcounts identical particles. Spinless bosons

in two orbitals instead have three occupations: both in a, one in each, both in b. These counts assume no additional energy restriction and the stated accessible single-particle states; restricting total energy or spin projection changes the allowed subset.

Interpret the joint density

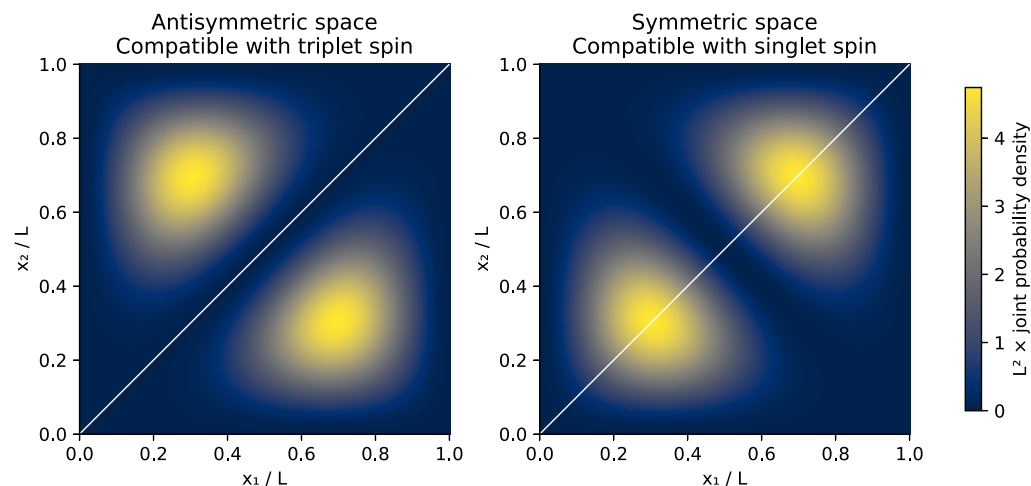
An antisymmetric spatial state satisfies $\Psi_{-}(x,x)=0$, so its joint position density vanishes on the coincidence line. A symmetric spatial state need not vanish there. The difference arises from interference between exchanged amplitudes, even for noninteracting particles; it is not a separately imposed classical repulsive force. For a well of length L, choose $a(x)=\sqrt{(2/L)}\sin(\pi x/L)$, $b(x)=\sqrt{(2/L)}\sin(2\pi x/L)$. At $x_1=L/4$ and $x_2=3L/4$, the antisymmetric spatial amplitude is $-2/L$ and its density is $4/L^2$; the symmetric amplitude is zero. These are joint probability densities per two lengths, not dimensionless probabilities at exact points. Physical spin compatibility still decides which total electronic state uses each spatial combination.

Worked method

For orthonormal different orbitals a and b, symmetric and antisymmetric spatial states are

$$\Psi_{\pm} = [a(1)b(2) \pm b(1)a(2)]/\sqrt{2}.$$

A two-electron total state must be antisymmetric under simultaneous exchange of position and spin. Thus symmetric space pairs with the spin singlet; antisymmetric space pairs with triplet spin. If both electrons occupy a, the spatial product is symmetric and only singlet spin is allowed. The different-orbital normalisation formula cannot simply be reused for $a = b$.



Exchange symmetry, spin pairs and Pauli exclusion: original GRE teaching diagram.

Check conditions and vocabulary

Exchange all spatial and spin arguments. Do not confuse antisymmetric space with antisymmetric total state, or use the distinct-orbital $\sqrt{2}$ factor for two identical orbitals.

spin singlet: Antisymmetric two-spin-1/2 state with total spin $S=0$.

Slater determinant : Antisymmetric fermionic construction from complete single-particle states; duplicate states make it vanish.