

Exchange symmetry, spin pairs and Pauli exclusion

GRE undergraduate preparation · local supported objectives

Choose the physical question

Reasoning

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

Reasoning

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

Reasoning

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

Reasoning

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

Reasoning

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 reasoning 1

Reasoning

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

Worked relation 2

Reasoning

Apply this relation only under the conditions just stated.

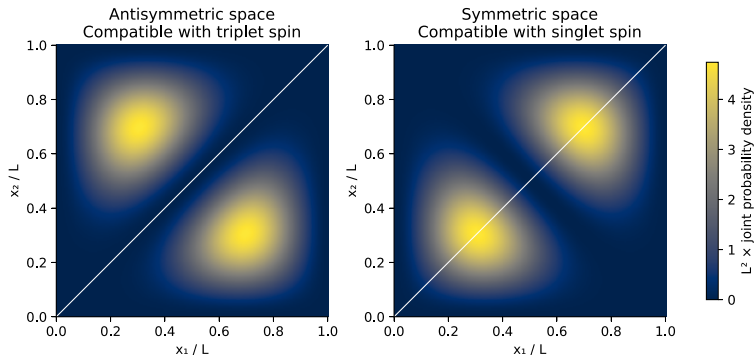
$$\psi_{\pm} = [a(1)b(2) \pm b(1)a(2)]/\sqrt{2}.$$

Worked reasoning 3

Reasoning

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 $a = b$.

Read the original diagram



- Original GRE teaching diagram: Exchange symmetry, spin pairs and Pauli exclusion
- Identify the axes, units, directions and the stated model.

Independent transfer · attempt

Reasoning

Two electrons access three orthonormal spatial orbitals, with no energy restriction. Count singlet states and triplet states, including spin projections. Reconcile the sum with choosing two complete states from six. **[5]**

Independent transfer · reasoning

Reasoning

Symmetric spatial states: three double occupations plus three different-orbital symmetric pairs, giving six singlets. Antisymmetric space has three orbital pairs; each permits three triplet spin projections, giving nine triplet states. Total is 15, equal to $\binom{6}{2}$. Award double occupations, singlet total, antisymmetric pairs, triplet total and reconciliation. Counting only the three triplet multiplets would omit their spin projections.

Check assumptions and limits

Reasoning

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.

Keep the technical distinctions

Reasoning

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.

Check yourself

- Define spin singlet and give its condition of use.
- Define Slater determinant and give its condition of use.
- Redo the original transfer with a changed parameter; check a limiting case.