

38.1 Exchange symmetry, spin pairs and Pauli exclusion

Name: _____ Class: _____ Date: _____

Total: 11 marks

KEY WORDS spin singlet • Slater determinant

Objective

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. Original public practice; not an ETS paper.

1 Key knowledge and worked examples

For orthonormal distinct orbitals, $\Psi_{\pm} = [a(1)b(2) \pm b(1)a(2)]/\sqrt{2}$. Fermionic total states are antisymmetric under simultaneous exchange of spatial and spin labels. Identical-orbital normalisation needs a separate treatment.

The spin singlet is antisymmetric and pairs with symmetric electron space. Triplet spin is symmetric and pairs with antisymmetric space. Same-orbital double occupation permits the singlet, not a triplet.

Two orbitals $\times$ two spin states give four complete states and $\text{choose}(4,2)=6$ two-electron occupations. Three orbitals give $\text{choose}(6,2)=15$. Exclusion is per complete state, not per spatial orbital.

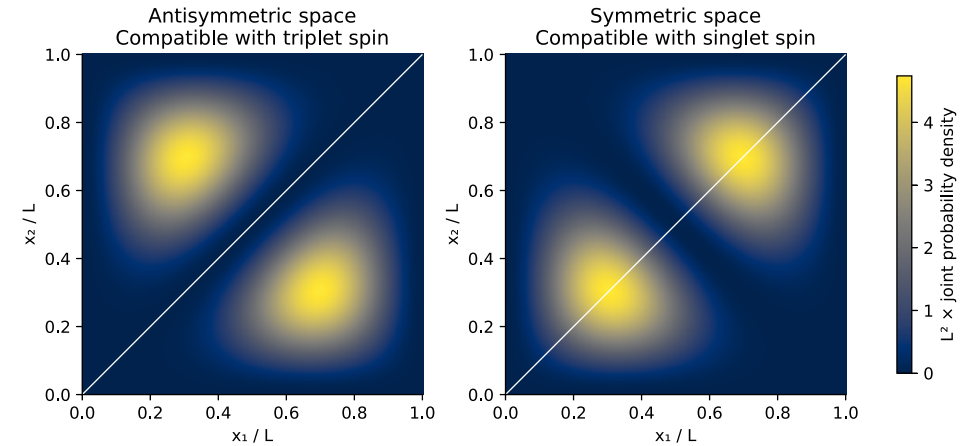
Antisymmetric spatial density vanishes at $x_1=x_2$. Exchange interference changes correlations without introducing a classical force. Joint position density has units inverse length squared and must be integrated for an interval probability.

■ 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 $a = b$.



2 Practice

2.1 Choose one answer. Two electrons share the same spatial orbital. Which spin state is allowed for their antisymmetric total state? [1]

- A $\uparrow\uparrow$
- B $\downarrow\downarrow$
- C Symmetric $\uparrow\downarrow + \downarrow\uparrow$ triplet
- D Antisymmetric $\uparrow\downarrow - \downarrow\uparrow$ singlet
- E Any spin state

2.2 Choose one answer. Two spinless identical bosons can use two spatial orbitals without an energy restriction. Occupation patterns number: [1]

- A 1
- B 2
- C 3
- D 4
- E 6

2.3 Two electrons access three spatial orbitals, each with two spin states. Complete-state occupation patterns number _____. Show your relation and units. [2]

[2]

[5]

Solutions

2.1 D The same-orbital spatial product is symmetric; the spin factor must be antisymmetric.

Compare the rejected options: $\uparrow\uparrow$; $\downarrow\downarrow$; Symmetric $\uparrow\downarrow+\downarrow\uparrow$ triplet; Any spin state. Use the stated model and conditions.

2.2 C Allowed patterns are (2,0), (1,1) and (0,2); particle labels do not create separate versions of (1,1).

Compare the rejected options: 1; 2; 4; 6. Use the stated model and conditions.

2.3 15. Six complete states give $\text{choose}(6,2)=15$.

2.4 True. At $x_1=x_2$ the two products are equal and their difference vanishes.

3.1 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.