

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.

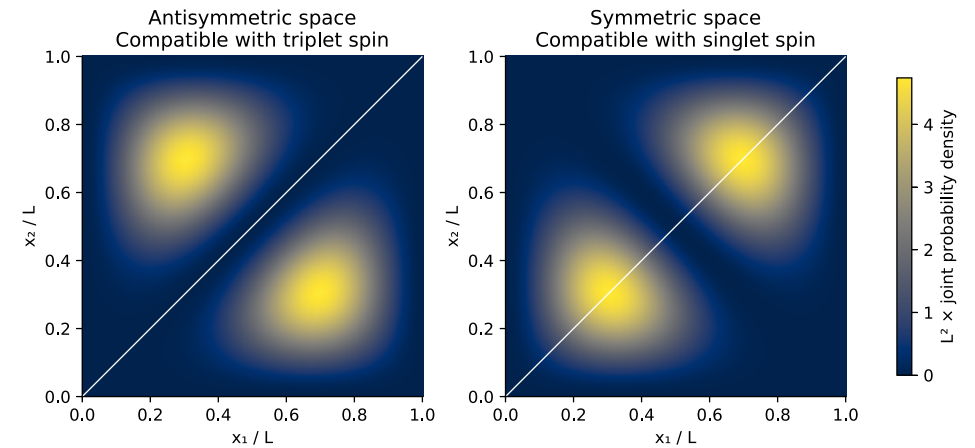
Antisymmetric spatial density vanishes at $x_1=x_2$. Exchange interference changes correlations without introducing a classical force. Joint position density has units inverse length squared and must be integrated for an interval probability.

■ 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]

2.4 Decide whether this claim is true. Justify it: An antisymmetric two-orbital spatial state must have zero amplitude when the two spatial arguments coincide. [2]

3 Exam-style questions

3.1 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]