



Figure 6.2: Schematic picture of the origin of the superexchange interaction. The figure shows the charge density for the wavefunctions in a singlet state (solid line) and a triplet state (dotted line)

where the two magnetic atoms are separated by a nonmagnetic ion with a closed shell, commonly in an insulating magnetic oxide where the oxygen ion is O^{2-} . This is called *superexchange*. The second case is in a magnetic d- or f-band metal, where there are itinerant s- or p-like electronic states. A magnetic interaction mediated by conduction electrons is called *itinerant exchange*.

Superexchange can be visualised in Fig. 6.2. We have in mind here a Mott insulating state, so that the direct overlap between the d-electrons on the nearest magnetic ions is too small to overcome the local Coulomb repulsion. Furthermore, because the mediating O ion is almost completely full, there is only a little overlap between the d-wavefunction and the oxygen neighbour. This small overlap is, however, just enough to generate an exchange interaction.

As usual, if we consider the spatial wavefunctions for the singlet and triplet states, they will be of the form

$$\psi = \frac{1}{\sqrt{2}}[\psi_A(1)\psi_B(2) \pm \psi_A(2)\psi_B(1)] \quad (6.9)$$

where the $+$ sign goes with the spin singlet, and the $-$ sign with the triplet. Because the triplet state has a node, it has less possibility for both electrons to spill over onto the O ion than does the singlet. Consequently the singlet state has a somewhat lowered kinetic energy (the electrons a little less localised) and this is enough to lower its energy below the triplet state. So for superexchange J is *negative* favouring antiparallel, or *antiferromagnetic* alignment of spins. Values of J for transition metal oxides range from a few