

# Exchange

- How do spins interact?
- Magnetostatic dipole-dipole coupling

$$H_{d-d} = -\frac{\mu_0}{4\pi r^3} [3(\mathbf{m} \cdot \mathbf{r})(\mathbf{m}' \cdot \mathbf{r}) - \mathbf{m} \cdot \mathbf{m}']$$

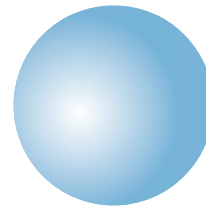
- This is rather weak,  $\approx$  1K for even large spins
- Electrostatic interaction usually dominates, just as it does inside atoms
- Indirectly leads to spin coupling through Pauli principle

# Exchange

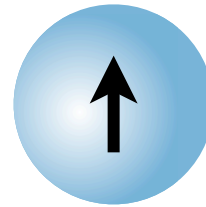
- Generally think of exchange interactions between spins as due to hopping of electrons from one orbital to another
- Many types of exchange, complicated by varieties of orbitals involved, including those on non-magnetic atoms
- We will just discuss the simplest case

# Direct exchange

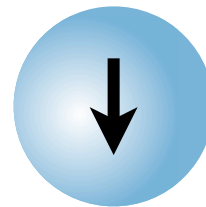
Assume individual  
 $S=1/2$  ions



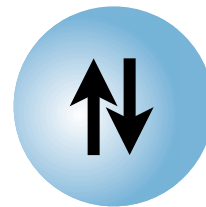
$$E=0$$



$$E=\varepsilon$$



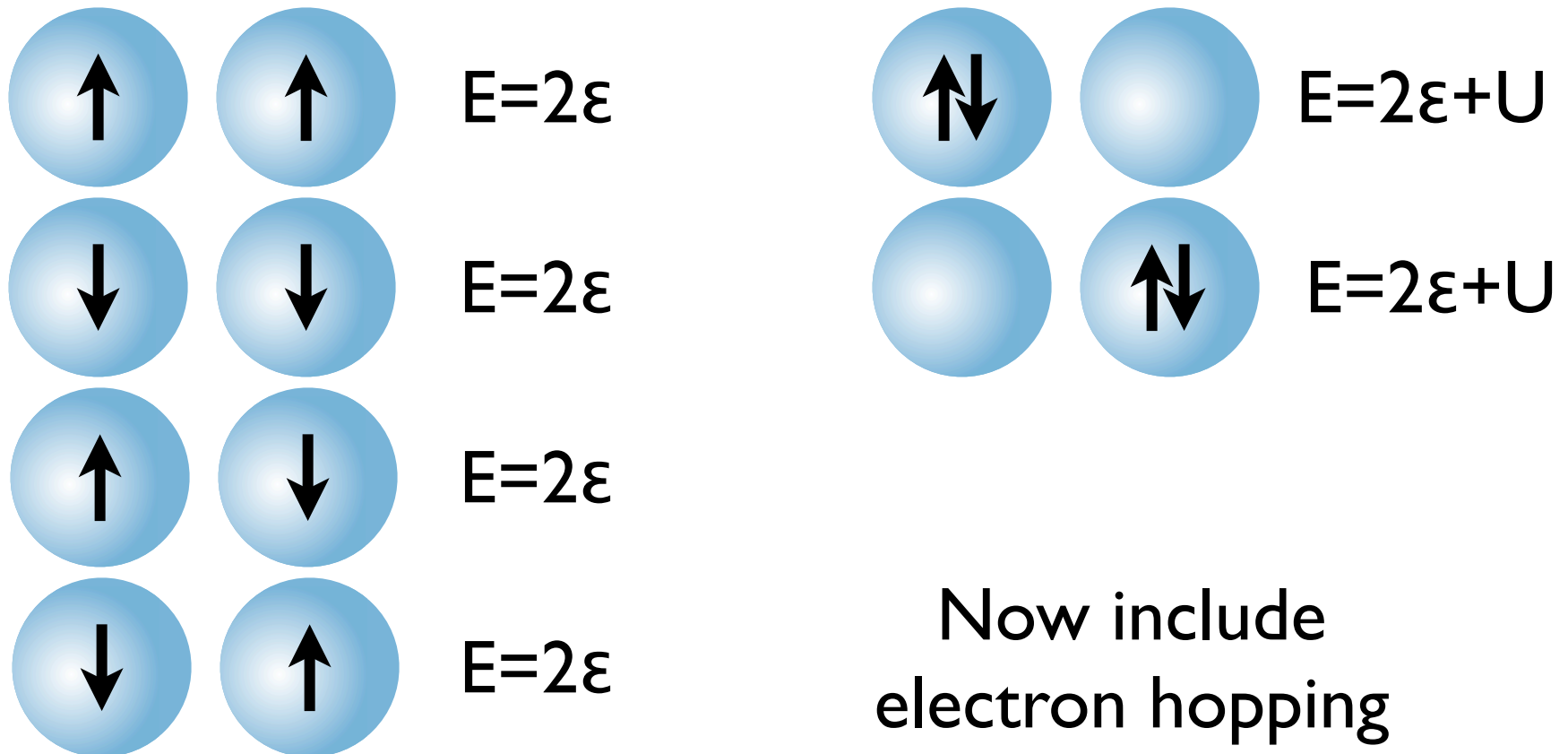
$$E=\varepsilon$$



$$E=2\varepsilon+U$$

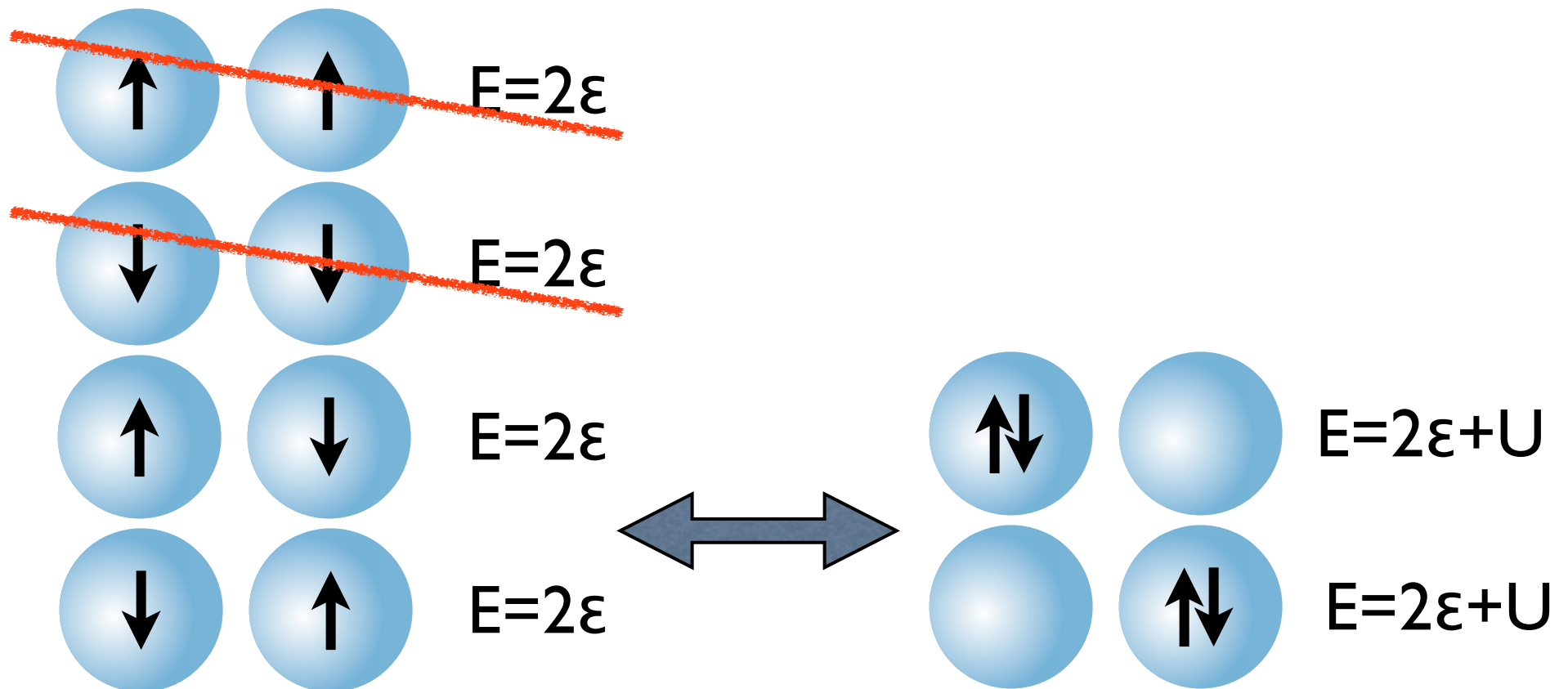
# Direct exchange

- Two ions, 2 electrons. With no contact:



# Direct exchange

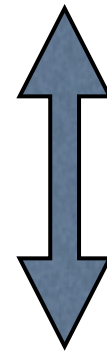
- Hopping? Prohibited by Pauli for parallel spins ( $S=1$ )



# Direct exchange

- Since spin is conserved, only  $S=0$  state can hop

$$\frac{1}{\sqrt{2}} \left( \begin{array}{cc} \uparrow & \downarrow \\ \downarrow & \uparrow \end{array} - \begin{array}{cc} \downarrow & \uparrow \\ \uparrow & \downarrow \end{array} \right) \quad \text{parity } P=-1$$

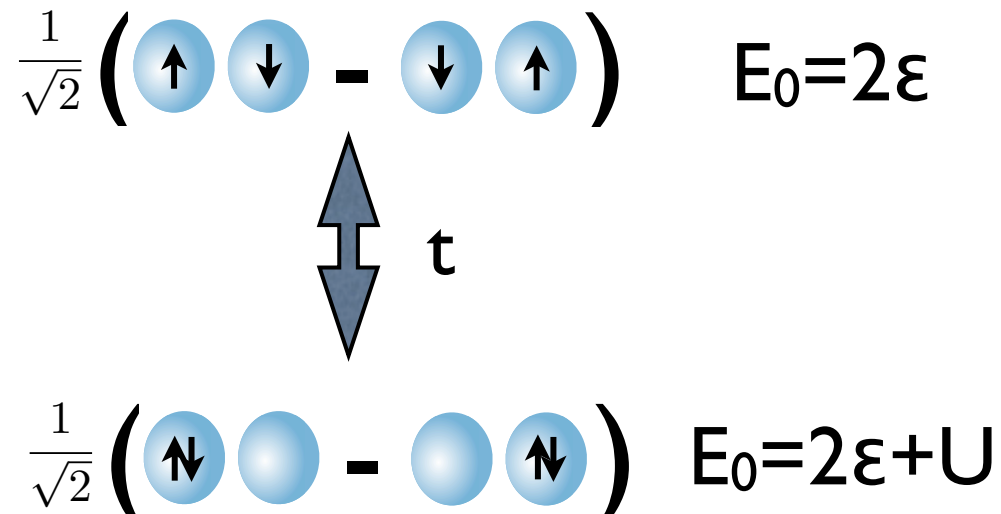


amplitude =  $t$

$$\frac{1}{\sqrt{2}} \left( \begin{array}{cc} \uparrow\downarrow & \bullet \\ \bullet & \uparrow\downarrow \end{array} - \begin{array}{cc} \bullet & \uparrow\downarrow \\ \uparrow\downarrow & \bullet \end{array} \right) \quad \text{parity } P=-1$$

# Direct exchange

- Since spin is conserved, only  $S=0$  state can hop



$$H = \begin{pmatrix} 2\varepsilon & t \\ t & 2\varepsilon + U \end{pmatrix}$$

$$E_- \approx 2\varepsilon - \frac{t^2}{U}$$

singlet energy  
lowered by  $O(t^2/U)$

# Direct exchange

- Write as an “effective Hamiltonian”:

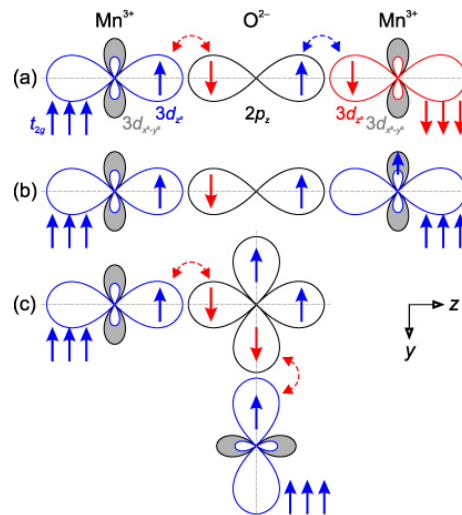
$$\begin{aligned} H_{\text{eff}} &= -\frac{t^2}{U} \hat{P}_{S=0} \\ &= -\frac{t^2}{U} \left[ 1 - \frac{1}{2} (\mathbf{S}_i + \mathbf{S}_j)^2 \right] \\ &= \text{const.} + J \mathbf{S}_i \cdot \mathbf{S}_j \end{aligned}$$

- With  $J \sim t^2/U$ . Note this is typically *antiferromagnetic* interaction: favors singlet/anti-parallel spins

$J$  can be as large as 1000K, or as small as a few K

# Other exchanges

- Super-exchange: exchange due to electrons hopping through an intermediate orbital



usually antiferromagnetic

this can be ferromagnetic

# Other exchanges

- RKKY exchange:
  - interaction of spins mediated by delocalized metallic electrons
  - only in a metal, obviously
- Double exchange
  - more exotic exchange in some metals with some localized electrons

# Magnetic order

- In a crystal with a periodic lattice of spins, exchange interactions typically induce an *ordered* state at low temperature
- For example, the ferromagnetic Heisenberg model:

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad J > 0$$

- Wants every spin parallel to its neighbor, so they choose a global axis

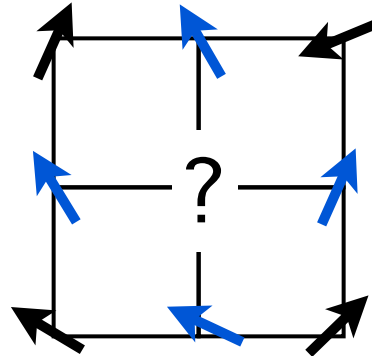
$$\langle \mathbf{S}_i \rangle = \mathbf{m}$$

# Mean field theory

- When  $kT \gtrsim J$ , spins will fluctuate thermally, and  $\mathbf{m}$  will be reduced.
- We can study this with *mean field theory*

$$\begin{aligned} H &= -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\ &\rightarrow -J \sum_{\langle ij \rangle} [\langle \mathbf{S}_i \rangle \cdot \mathbf{S}_j + \mathbf{S}_i \cdot \langle \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle] \\ &= -zJ \sum_i \mathbf{m} \cdot \mathbf{S}_i + \text{const.} \end{aligned}$$

# Mean field theory



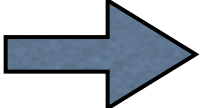
$$g\mu_B \mathbf{H}_{\text{eff}} = J \langle \uparrow + \uparrow + \leftarrow + \uparrow \rangle$$

- This reduces the problem to independent spins in an *effective* “exchange field”
- Note: this exchange field can be a thousand times larger than physical laboratory fields!

# Mean field theory

- Define  $h = z J m$  ( $= g \mu_B H_{\text{eff}}$ )
- Then we know for a single spin

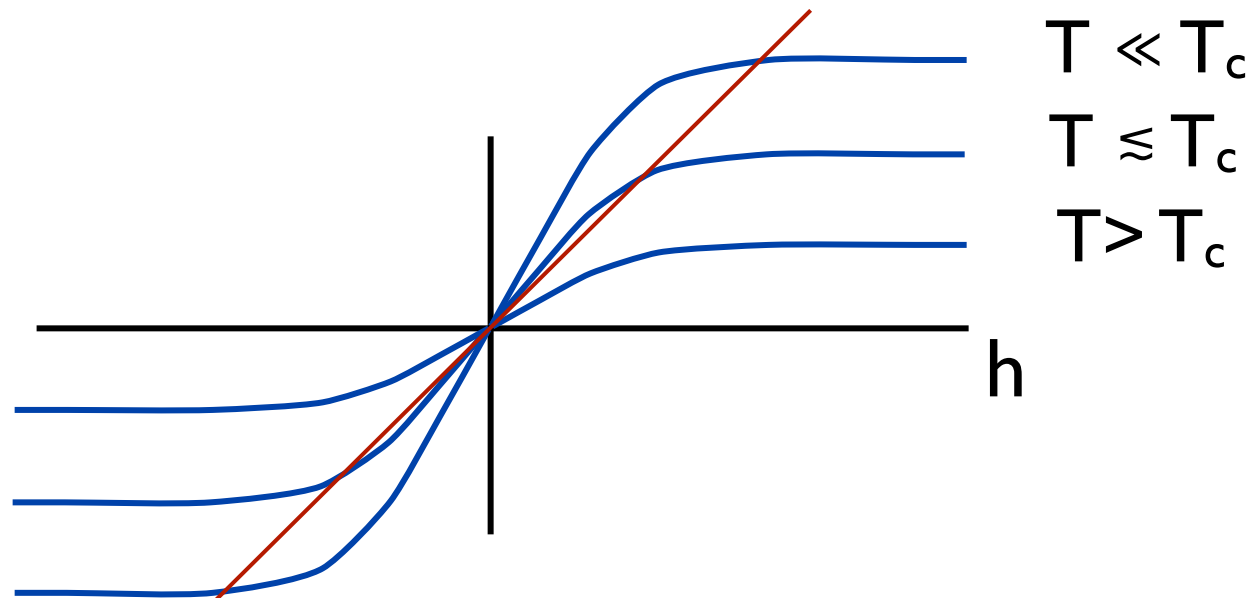
$$|\langle \mathbf{S}_i \rangle| = m = S B_S(\beta h S)$$


$$m = S B_S(\beta z J S m)$$

- For example for  $S=1/2$

$$m = \frac{1}{2} \tanh \left[ \frac{z J m}{2kT} \right]$$

# Mean field theory



- Non-zero solution for  $m_e$  appears only for  $T < T_c$
- equality of slopes implies  $kT_c = zJ/4$  ( $= \frac{zJS(S+1)}{3}$ )