Lecture XIV. Jorge Quintanilla, Magnetism and Superconductivity (PH752)

In this lecture we continue to develop the mean field theory of antiferromagnetism. In the previous lecture we computed the magnetic susceptiblity of an antiferromagnet in the disordered (i.e. paramagnetic) state. We saw that unlike a ferromagnet, where the susceptiblity is enhanced by interactions between magnetic moments, compared to the non-interacting case, in an antiferromagnet the zero-field susceptibility is suppressed compared to the non-interacting case. Now we will work out the mean field theory of the antiferromagnetic instability that leads, in this case, to an ordered state below a critical temperature called the Neel temperature, T_N (after Louis Neel).

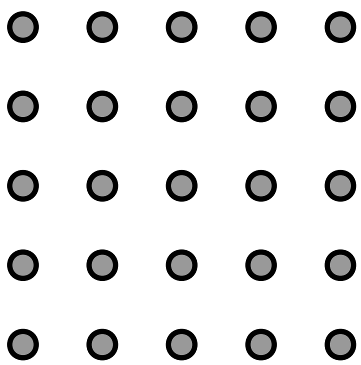
1 Mean field theory of the antiferromagnetic state

Unlike the ferromagnetic state, which always takes the same form (all magnetic moments aligned in the same way), ferromagnetism can take many forms depending on the exact type of anti-ferromagnetic interactions in the system. We will assume here the simplest possible type of interaction, where each magnetic moment interacts antiferromagnetically with its immediate neighbours, and that's it:

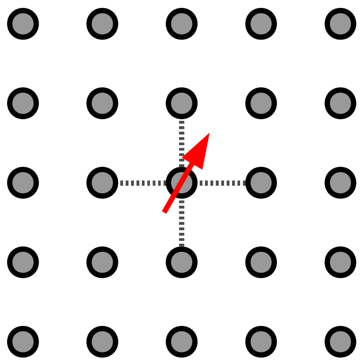
$$J_{i,j} = \begin{cases} -J < 0 & \text{if } i \text{ and } j \text{ are nearest neighbours,} \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

We will also assume, unlike the case of ferromagnetism, that there is no externally-applied field (this introduces considerable complications in the case of the anti-ferromagnetic state - see Blundell).

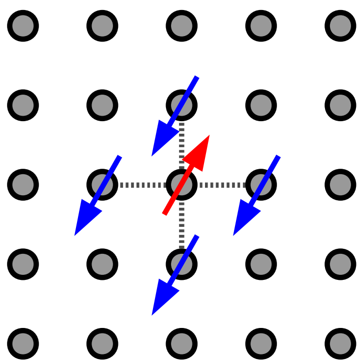
Let us now think of what kind of magnetic order we should find at low temperatures in this case. To illustrate it, consider the simple case of a square lattice:



We are saying that the magnetic moment on a certain site j interacts only with its z nearest neihgbours (in this square lattice example, $z = 4$):

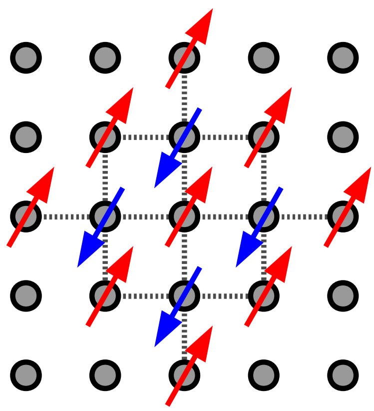


Since the exchange constant $-J$ is always negative, it will tend to align the four neighbouring magnetic moments in the opposite direction to that adopted by the $j^{\underline{\text{th}}}$ one:

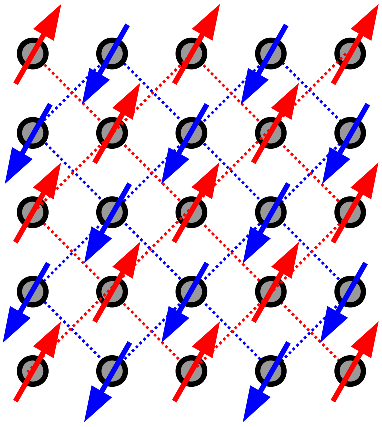


This is the reason why the susceptibility is suppressed (see the last lecture): since each magnetic moment wants to point against the direction chosen by the surrounding ones, there is a penalty, coming from interactions, for aligning all the magnetic moments in the same direction.

What kind of magnetic order can such interaction lead to? It is easy to guess if we forget now about the magnetic moment that we coloured in red and think of the four moments coloured in blue. Each of them has four neighbours (including the red magnetic moment) and each of those neighbours will tend to be anti-aligned to the corresponding blue spin - i.e. they will tend to adopt the same orientation as the original red spin:



Clearly as this propagates through the lattice we end up with two square sublattices, one made up of "red" magnetic moments and another one composed of "blue" ones:



We will call the two sublattices the "A" sublattice and the "B" sublattice. This suggests that we look for solutions of the form

$$\langle \mu_{z,j} \rangle = \begin{cases} \mu_A & \text{if } j \text{ is in the "A" sublattice;} \\ \mu_B = -\mu_A & \text{if } j \text{ is in the "B" sublattice;} \end{cases} \tag{2}$$

to the mean-field self-consistency equations

$$\mathbf{B}_{eff,j} \approx \sum_{i \neq j} \frac{J_{i,j}}{g_J^2 \mu_B^2} \langle \boldsymbol{\mu}_i \rangle + \mathbf{B}$$

(Lect. XI, Eq. 9)

$$\langle \mu_{j,z} \rangle = \mu_z^{\text{sat}} \mathcal{B}_{j_{\text{tot}}} \left(\frac{\mu_z^{\text{sat}} B_{\text{eff},j}}{k_B T} \right)$$

(Lect. XI, Eq. 12)

Substituting the above type of solution, with the interaction given by Eq. (1), above, and applied magnetic induction $\mathbf{B} = 0$, the first of the above self-consistency equations reduces to[12]

$$\left. \begin{matrix} B_{eff,A} \\ B_{eff,B} \end{matrix} \right\} = \sum_{\langle i,j \rangle} \frac{-J}{g_J^2 \mu_B^2} \times \left\{ \begin{matrix} \mu_B \\ \mu_A \end{matrix} \right\} = \pm \sum_{\langle i,j \rangle} \frac{J}{g_J^2 \mu_B^2} \times \left\{ \begin{matrix} \mu_A \\ \mu_A \end{matrix} \right\} \tag{3}$$

$$\Rightarrow B_{eff,B} = -B_{eff,A} \text{ and } B_{eff,A} = \lambda \mu_A \,, \tag{4}$$

where

$$\lambda \equiv \sum_{\langle i,j \rangle} \frac{J}{g_J^2 \mu_B^2}. \tag{5}$$

The second self-consistency equation in turn becomes

$$\left. \begin{matrix} \mu_A \\ \mu_B \end{matrix} \right\} = \left\{ \begin{matrix} \mu_A \\ -\mu_A \end{matrix} \right\} = \mu_z^{\text{sat}} \mathcal{B}_{j_{\text{tot}}} \left(\frac{\mu_z^{\text{sat}}}{k_B T} \times \left\{ \begin{matrix} B_{eff,A} \\ -B_{eff,B} \end{matrix} \right\} \right) \tag{6}$$

$$= \mu_z^{\text{sat}} \mathcal{B}_{j_{\text{tot}}} \left(\pm \frac{\mu_z^{\text{sat}}}{k_B T} \times B_{eff} \right) \tag{7}$$

$$= \pm \mu_z^{\text{sat}} \mathcal{B}_{j_{\text{tot}}} \left(\frac{\mu_z^{\text{sat}}}{k_B T} \times B_{eff} \right) \tag{8}$$

[12] We introduce the notation $\sum_{\langle i,j \rangle} \ldots$ meaning sum over all values of i and j subject to the constraint that the $i^{\underline{\text{th}}}$ and $j^{\underline{\text{th}}}$ ions are nearest neighbours.

i.e.

$$\frac{\mu_A}{\mu_z^{\text{sat}}} = \mathcal{B}_{j_{\text{tot}}}\left(\frac{\mu_z^{\text{sat}}}{k_B T}B_{eff}\right) . \tag{9}$$

Defining, as before,

$$y \equiv \frac{\mu_z^{\text{sat}} B_{eff}}{k_B T} \tag{10}$$

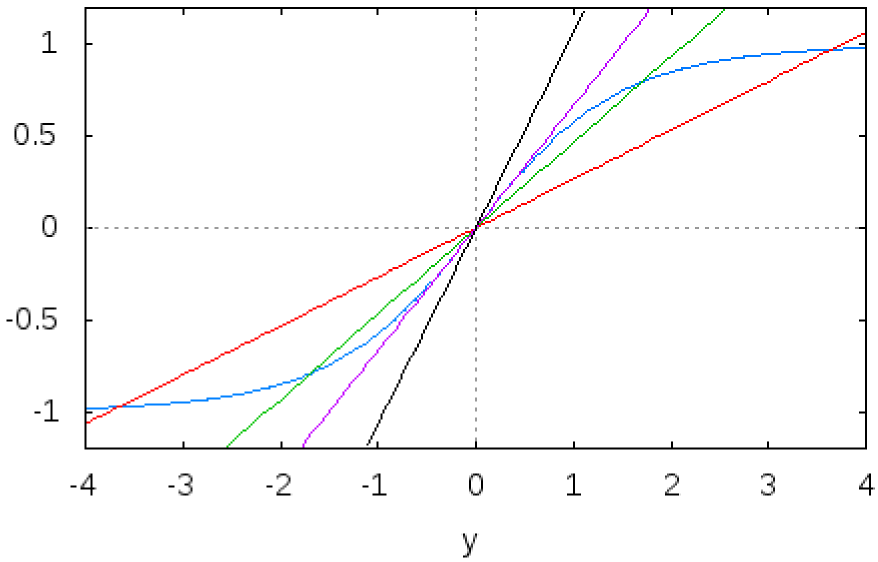
Lect. XII, Eq. 11)

we have

$$\boxed{\frac{\mu_A}{\mu_z^{\text{sat}}} = \tilde{T} y \text{ with } \tilde{T} = \frac{k_B}{\lambda \left(\mu_z^{\text{sat}}\right)^2}} \tag{11}$$

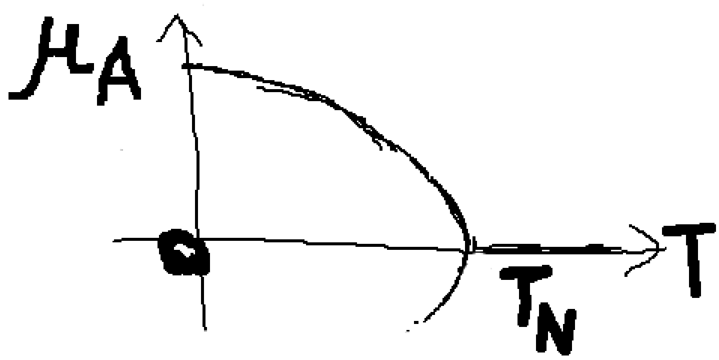
$$\text{and } \boxed{\frac{\mu_A}{\mu_z^{\text{sat}}} = \mathcal{B}_{j_{\text{tot}}}(y)} . \tag{12}$$

These self-consistency equations are entirely analogous to the ones we obtained for the ferromagnetic state in Lecture XII, with the magnetic moment in the A sublattice playing the role of the uniform magnetic moment. We solve the equation graphically in the same



way as before

and find the same temperature-dependence of the magnetic moment *in the A sublattice* that we found back then for the *uniform* magnetic moment:



The critical temperature at which the magnetic moment becomes finite, T_N, is obtained in the same way as the Curie temperature [this is left as an exercise] and is given by

$$\boxed{k_B T_N = \frac{1}{3}\lambda \mu^2 = -\frac{2}{3} J z j_{\text{tot}} \left(j_{\text{tot}} + 1\right)} , \tag{13}$$

where as usual $\mu = \sqrt{\langle \hat{\boldsymbol{\mu}}^2 \rangle} = g_J \, |\mu_B| \, \sqrt{j_{\mathrm{tot}} \, (j_{\mathrm{tot}} + 1)}$ is the r.m.s. expectation value of the magnetic moment strength and z is the number of nearest nieghbours ($z = 4$ is the square lattice example).

Note, however, that unlike ferromagnetism the magnetization in the antiferromagnetic state is

$$M = \rho \frac{\mu_A + \mu_B}{2} = 0 \tag{14}$$

in the anti-ferromagnetic state. The staggered magnetization,

$$M_{\mathrm{staggered}} \equiv \rho \frac{\mu_A - \mu_B}{2}, \tag{15}$$

on the other hand does become finite as we go through T_N and can be taken as the order parameter of the antiferromagnetic instability. It is the susceptibility to develop such staggered magnetization that diverges as the system undergoes the antiferromagnetic instability at T_N (rather than the magnetic susceptibility which, as we saw in the preivous lecture, never diverges for an antiferromagnet).

2 Broken symmetry

The different nature of ferromagnetism and antiferromagnetism can be better appreciated in terms of the concept of **broken symmetry**.[13]

Let us go back to the general Heisenberg Hamiltonian,

$$\mathcal{H} = -\sum_j \sum_{i \neq j} \frac{J_{i,j}}{g_J^2 \mu_B^2} \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j - \sum_j \boldsymbol{\mu}_j \cdot \mathbf{B}.$$

(Lect. XI, Eq. 5)

In the absence of an externally-applied magnetic induction ($\mathbf{B}$=0) the above Hamiltonian becomes

$$\mathcal{H} = -\sum_j \sum_{i \neq j} \frac{J_{i,j}}{g_J^2 \mu_B^2} \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j, \tag{16}$$

which is symmetric under the reversal of all the magnetic moments in the system. That is to say that under the operation

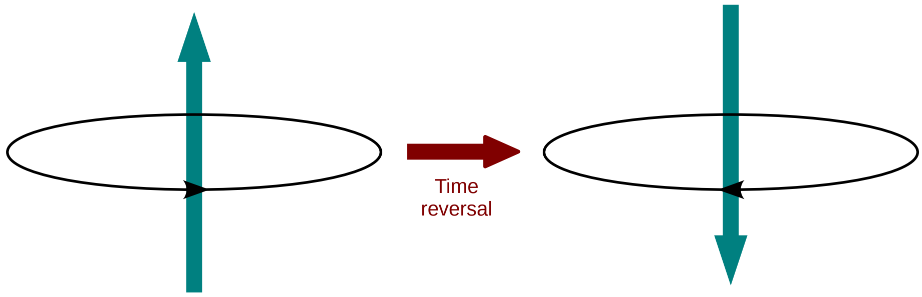
$$\boldsymbol{\mu}_j \to -\boldsymbol{\mu}_j \text{ for all } j \tag{17}$$

the Hamiltonian stays exactly the same. This is because the dot product

$$\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j \tag{18}$$

does not change when I reverse both $\boldsymbol{\mu}_i$ and $\boldsymbol{\mu}_j$.

Such symmetry under the inversion of all the magnetic moments can also de regarded as a symmetry under time reversal, since in order to flip a magnetic moment all we need to do is reverse the currents giving rise to it, which could be achieved by turning time backwards so as to reverse the trajectories of all the charges:[14]



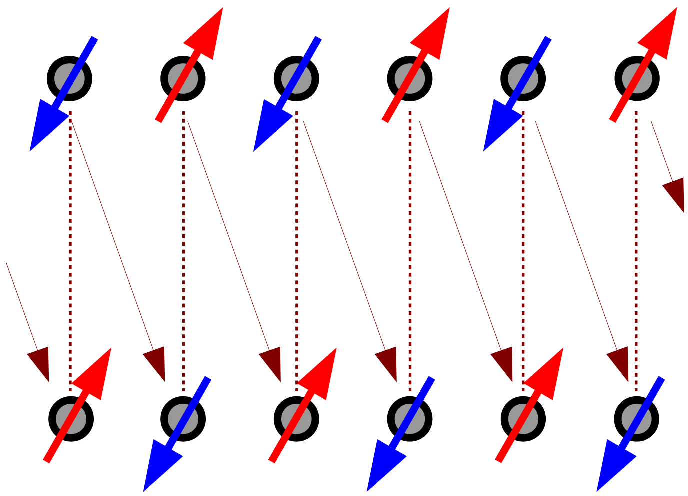
[13] The wonder and deep implications of broken symmetry are beautifully brought forth in Nobel laureate Phil W. Anderson's classic essay "More is different", *Science* **177**, 393-396 (1972).

[14] Of course, spin does not emerge from circulating currents in any trivial way, but nevertheless it behaves in the same way as orbital angular momentum under time reversal.

In the paramagnetic state, the time-reversal operation (inverting all the magnetic moments) would leave all observables unchanged. In particular the magnetization, which is zero in the paramagnetic state (remember that there is no applied field in this discussion), would remain zero after time-reversal. In contrast, in the ferromagnetic state, where the magnetic moments have spontaneously chosen to point in one particular direction, time reversal would have the effect of inverting the magnetization, so it would have a macroscopically-observable effect. We thus say that **ferromagnetism breaks time-reversal symmetry**.

Time-reversal symmetry breaking is a notable phenomenon: how does the system decide which value of the magnetisation to adopt, given that the Hamiltonian (which describes fully the dynamics of the system) cannot distinguish between values related by time-reversal symmetry? The key to this conundrum is the divergence of the susceptibility to magnetise as the Curie temperature is approached from above. Because of this, any small perturbation, e.g. a tiny applied magnetic field (e.g. the Earth's magnetic field), will make a macroscopic region of the magnet point in one direction rather than another.

In antiferromagnets, time-reversal symmetry is also broken, since flipping all the magnetic moments in the sample would have the effect of swapping the A and B sublattices, changing the sign of the staggered magnetization. However, in addition, another symmetry is broken, namely the symmetry under lattice translations. This says that if all the sites on the lattice are displaced by exactly one lattice constant in the same direction, so that each occupies the site of one of its nearest neighbours, the Hamiltonian, again, stays the same (this is obviously only valid for inifinite systems with no boundaries - but for all practical purposes within this discussion any macroscopic chunk of matterial can be ocnsidered infinite). This symmetry holds true in the paramagnetic state, and also for a ferromagnet (since all sites develop the same magnetization and therefore are still equivalent). However, when we carry out the operation in the antiferromagnetic state we find that it has the effect of interchanging the A and B sublattices, which is the same as flipping all the magnetic moments, again changing the sign of the order parameter (that is, the staggered magnetization):



Thus the antiferromagnetic state breaks time-reversal symmetry and, in addition, also the symmetry under lattice translations.