Ferromagnetic and antiferromagnetic orders; similarities and differences, low-energy excitations

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Compared to electrons, spins are weakly fluctuating objects which form "classical" states – ordered magnets. That this is the case we know from neutron scattering and magnetic force microscopy. The ordered magnets consist of individual spins pointing in a particular direction of space. How do we arrive at such a conclusion theoretically, starting from the (quantum) Heisenberg Hamiltonian?

The Hamiltonian reads $H_{spin} = J \sum_{i,\delta} \vec{S}_i \cdot \vec{S}_{i+\delta}$, that is,

$$H_{spin} = J \sum_{i,\delta} \left[S_i^z S_{i+\delta}^z + \frac{1}{2}\left(S_i^+ S_{i+\delta}^- + S_i^- S_{i+\delta}^+ \right) \right].$$

Note that the spin operators satisfy the su(2) algebra, defined through the commutation relations

$$[S_i^+, S_j^-] = 2 S_i^z \delta_{ij}; \quad [S_i^z, S_j^\pm] = \pm S_i^\pm \delta_{ij} .$$

Let us define the spin coherent states, which will here play the role of a complete set of classical spin states. They can be defined in general for spin S:

$$|\hat{\Omega}\rangle = e^{-i\phi S_z} e^{i\theta S_y} |S, S\rangle$$

$\longrightarrow M_s = S$

here $\hat{\Omega} \equiv (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ is a unit vector (defined by spherical polar angles θ and φ)

Note that $|\hat{\Omega}\rangle$ is a <u>coherent superposition</u> of quantum-mechanical spin states. Let us make this more concrete in the special case $S=\frac{1}{2}$.

To find $|\hat{\Omega}\rangle$ we need to know how S_y (or an operator function of S_y, i.e., $e^{i\theta S_y}$) acts on the eigenstate $|S=\frac{1}{2}, M_S=\frac{1}{2}\rangle$ of S_z. To this end, we first express the eigenstates of S_z in the eigenbasis of S_y:

$$|\tfrac{1}{2},\tfrac{1}{2}\rangle_y = \frac{1}{\sqrt{2}}\left\{|\tfrac{1}{2},\tfrac{1}{2}\rangle - i|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right\},$$
$$|\tfrac{1}{2},-\tfrac{1}{2}\rangle_y = \frac{1}{\sqrt{2}}\left\{|\tfrac{1}{2},\tfrac{1}{2}\rangle + i|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right\},$$

where $S_y|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle_y = \pm\frac{1}{2}|\tfrac{1}{2},\pm\tfrac{1}{2}\rangle_y$

$$\Rightarrow |\hat{\Omega}\rangle = e^{-i\phi S_z} e^{i\theta S_y}\frac{1}{\sqrt{2}}\left(|\tfrac{1}{2},\tfrac{1}{2}\rangle_y + |\tfrac{1}{2},-\tfrac{1}{2}\rangle_y\right)$$
$$= e^{-i\phi S_z}\frac{1}{\sqrt{2}}\left(e^{i\frac{\theta}{2}}|\tfrac{1}{2},\tfrac{1}{2}\rangle_y + e^{-i\frac{\theta}{2}}|\tfrac{1}{2},-\tfrac{1}{2}\rangle_y\right) =$$
$$= \frac{e^{-i\phi S_z}}{2}\left\{e^{i\frac{\theta}{2}}\left(|\tfrac{1}{2},\tfrac{1}{2}\rangle - i|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right) + e^{-i\frac{\theta}{2}}\left(|\tfrac{1}{2},\tfrac{1}{2}\rangle + i|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right)\right\} =$$
$$= e^{-i\phi S_z}\left\{\cos(\tfrac{\theta}{2})|\tfrac{1}{2},\tfrac{1}{2}\rangle + \sin(\tfrac{\theta}{2})|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right\} =$$

$$\Leftrightarrow \boxed{|\hat{\Omega}\rangle = e^{-i\frac{\phi}{2}}\cos\left(\frac{\theta}{2}\right)|\tfrac{1}{2},\tfrac{1}{2}\rangle + e^{i\frac{\phi}{2}}\sin\left(\frac{\theta}{2}\right)|\tfrac{1}{2},-\tfrac{1}{2}\rangle}$$

The meaning of these spin coherent states becomes clearer if we determine the expectation value of the spin operator $\langle\hat{\Omega}|\vec{S}|\hat{\Omega}\rangle$. Let us do this componentwise.

$$\langle\hat{\Omega}|\hat{S}_x|\hat{\Omega}\rangle = \frac{1}{2}\left\{\langle\hat{\Omega}|S_+|\hat{\Omega}\rangle + \langle\Omega|S_-|\Omega\rangle\right\}$$

$$= \frac{1}{2}\left\{\langle\hat{\Omega}|e^{i\frac{\phi}{2}}\sin\left(\frac{\theta}{2}\right)|\tfrac{1}{2},\tfrac{1}{2}\rangle\right.$$

$$\left. + \langle\hat{\Omega}|e^{-i\frac{\phi}{2}}\cos\left(\frac{\theta}{2}\right)|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right\} =$$

$$= \frac{1}{2}\left\{e^{i\frac{\phi}{2}}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)\underbrace{\langle\tfrac{1}{2},\tfrac{1}{2}|\tfrac{1}{2},\tfrac{1}{2}\rangle}_{1}\right.$$

$$\left. + e^{-i\frac{\phi}{2}}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)\langle\tfrac{1}{2},-\tfrac{1}{2}|\tfrac{1}{2},-\tfrac{1}{2}\rangle\right\} =$$

$$= \frac{1}{2}\cos(\phi)\, 2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) = \boxed{\frac{1}{2}\cos\phi\sin\theta}.$$

In a similar manner we obtain

$$\langle\hat{\Omega}|\hat{S}_y|\hat{\Omega}\rangle = \frac{1}{2}\sin\phi\sin\theta, \quad \langle\hat{\Omega}|\hat{S}_z|\hat{\Omega}\rangle = \frac{\cos\theta}{2}.$$

Thus overall we have

$$\boxed{\langle\hat{\Omega}|\hat{\vec{S}}|\hat{\Omega}\rangle = \frac{1}{2}(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \equiv \frac{1}{2}\hat{\Omega}}!$$

Thus the spin coherent states translate the su(2) algebra of spins into classical vectors ("arrows in space")!

$\Rightarrow$ The <u>classical energy</u> of the Heisenberg Hamiltonian is then

$$\langle \Psi_{cl} | H_{spin} | \Psi_{cl} \rangle \, , \quad \text{where } |\Psi_{cl}\rangle = \prod_i |\hat{\Omega}_i\rangle$$

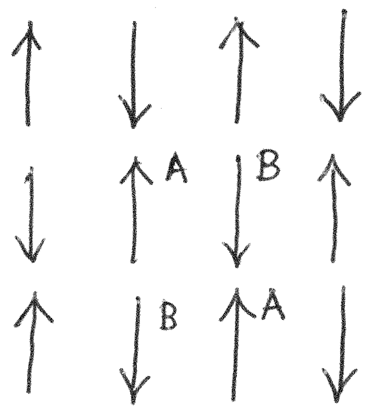
$$\Rightarrow \langle \Psi_{cl} | H_{spin} | \Psi_{cl} \rangle = J S^2 \sum_{i,\delta} \hat{\Omega}_i \cdot \hat{\Omega}_{i+\delta}$$

$$= J S^2 \sum_{i,\delta} \Big\{ \sin(\theta_i) \sin(\theta_{i+\delta}) \cos(\phi_{i+\delta} - \phi_i) + \cos(\theta_i) \cos(\theta_{i+\delta}) \Big\}$$

$\Rightarrow$ the classical ground state now depends on the lattice geometry, details of the couplings, etc. On <u>cubic lattices</u> and with nearest-neighbour couplings we have:

1) $J > 0$: the energy is minimized if the nearest neighbours point in opposite (antiparallel) directions!

For this to be possible the lattice must be <u>bipartite</u>! Such a state is called an <u>antiferromagnetic</u> or <u>Néel state</u>.



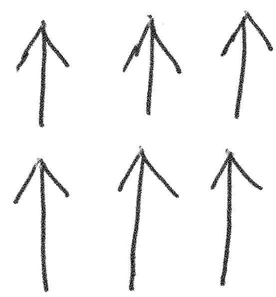
The Néel (or <u>staggered</u>) <u>order parameter</u> is

$$\boxed{O_{AFM} = \frac{1}{N} \left\langle \Psi_{cl}^{0} \left| \sum_{i \in A} S_i^z - \sum_{i \in B} S_i^z \right| \Psi_{cl}^{0} \right\rangle}$$

(if the z-axis is chosen as the preferred one)

2) $J < 0$: the energy is minimized if all θ_i and ϕ_i are the same, i.e., if all "spins" point in the same direction!

This is <u>ferromagnetic state</u>.



Choosing again the z axis as the preferred one, the ferromagnetic order parameter is given by

$$\boxed{O_{FM} = \frac{1}{N} \left\langle \Psi_{cl}^{0} \left| \sum_{i} S_i^z \right| \Psi_{cl}^{0} \right\rangle}$$

The first and obvious difference between ferromagnets and antiferromagnets is that ferromagnets are obtained for $J<0$ on an arbitrary lattice, while antiferromagnets exist for $J>0$ <u>only on bipartite lattices</u>!

What ferromagnets and antiferromagnets have in common is that they spontaneously break the spin-rotational symmetry (remember, we were talking about this symmetry in the context of the Hubbard model!). This means that individual spins cannot rotate freely anymore, although the absolute orientation of the order parameter is undetermined.

What is very different in the two cases is that a ferromagnet is an exact eigenstate of the Heisenberg Hamiltonian, while an antiferromagnet is not!

Ferromagnets have collective excitations but they are of a different kind than those that we have found in crystals, charge-neutral Fermi liquids, etc. (modes with linear dispersion at small q)!

Let us demonstrate this: the lowest-lying excitations in the system are of the type

spin flip on site l

$$|l\rangle \equiv S_l^- |0\rangle$$

where $|0\rangle$ is the ferromagnetic ground state (all "spins" pointing, say, in the z direction)

Thus these states are characterized by $S_{TOT} = N \cdot \frac{1}{2}$ and $M_{tot} = N \cdot \frac{1}{2} - 1$.

How H_{spin} acts on such a state:

$$H_{spin}|l\rangle = J\sum_{i,\delta}\left(S_i^z S_{i+\delta}^z + \frac{1}{2}S_i^+ S_{i+\delta}^- + \frac{1}{2}S_i^- S_{i+\delta}^+\right) \times |l\rangle$$

$$= J\sum_{i,\delta}\Big\{\left(\frac{1}{2}-\delta_{il}\right)\left(\frac{1}{2}-\delta_{i+\delta,l}\right)|\vec{l}\rangle + \frac{1}{2}\delta_{il}|i+\delta\rangle + \frac{1}{2}\delta_{i+\delta,l}|i\rangle\Big\}$$

$$= \Big(NE_0 - \frac{1}{2}J\sum_{i,\delta}\left(\delta_{il}+\delta_{i+\delta,l}\right)\Big)|l\rangle + \frac{J}{2}\sum_{\delta}\left(|l+\delta\rangle + |l-\delta\rangle\right)$$

$$= NE_0 + z|J| - \frac{1}{2}|J|\sum_{\delta}\left(|l+\delta\rangle + |l-\delta\rangle\right)$$

$\Rightarrow$ By carrying out the Fourier transformation

$$|q\rangle = \frac{1}{\sqrt{N}}\sum_{l} e^{iql}|l\rangle$$

we get

$$H_{spin}|q\rangle = (NE_0 + z|J|)|q\rangle - |J|\sum_{\delta}\left(e^{i\vec{q}\cdot\vec{\delta}} + e^{-i\vec{q}\cdot\vec{\delta}}\right)|q\rangle$$

$\Leftrightarrow$

$$H_{spin} |\vec{q}\rangle = \left\{ NE_0 + |J| \sum_{\delta=1}^{d} \left(1 - \frac{e^{i\vec{q}\cdot\vec{\delta}} + e^{-i\vec{q}\cdot\vec{\delta}}}{2}\right)\right\} |\vec{q}\rangle$$

$$\Longleftrightarrow \quad H_{spin} |\vec{q}\rangle = \left(NE_0 + 2|J| \sum_{\delta=1}^{d} \sin^2\left(\frac{\vec{q}\cdot\vec{\delta}}{2}\right)\right) |\vec{q}\rangle$$

$$\Longleftrightarrow \quad \boxed{H_{spin} |\vec{q}\rangle = \left(NE_0 + \hbar \omega_q \right) |\vec{q}\rangle}$$

where $\boxed{\hbar \omega_q \equiv 2|J| \sum_{\alpha=1}^{d} \sin^2\left(\frac{q_\alpha}{2}\right)}$

for small q, $\boxed{\omega_q \propto q^2} \longrightarrow$ particle-like dispersion!

Since antiferromagnets belong to the same general class of systems as crystalline solids, we can anticipate the existence of the same type of low-energy modes. Unlike in crystals where they originate from broken translational symmetry, in antiferromagnets they are a consequence of the breaking of spin-rotational symmetry. Physically, they represent precessional motion of the spins around the Néel ordered state.

Let us start from the quantum equations of motion; more precisely, let us look at the equation of motion of the <u>spin-flip operators</u>

$$\dot{S}_i^+ = \frac{1}{i}\left[S_i^+, H_{spin}\right] \iff$$

$$(\#) \quad \dot{S}_i^+ = \frac{2J}{i}\left\{ - S_{i+\delta}^z S_i^+ + S_{i+\delta}^+ S_i^z \right\}$$

We assume the Néel order parameter to be oriented along the z axis, an in the <u>classical limit</u>, all spins are pointing upwards on the A sublattice and downwards on the B sublattice.

In this limit we can therefore take $S_i^z \to +S$ on the A sublattice and $S_i^z \to -S$ on the B sublattice. By substituting this into Eq. (#) we obtain

$$\dot{S}_{i\in A}^+ = \frac{JS}{i}\left[z\, S_{i\in A}^+ + \sum_\delta S_{i+\delta\in B}^+\right],$$

$$\dot{S}_{i\in B}^+ = -\frac{JS}{i}\left[z\, S_{i\in B}^+ + \sum_\delta S_{i+\delta\in B}^+\right].$$

We can solve these equations using the Ansatz

$$S_{i\in A,B}^+ = u_{A,B}\, e^{i(\vec{q}\vec{r}_{i\in A,B} - \omega_q t)}$$

$\Longrightarrow$ we find that the problem reduces to

$$\begin{pmatrix} zJS - \omega_{\vec{q}} & zJS\gamma_{\vec{q}} \\ -zJS\gamma_{\vec{q}} & -zJS - \omega_{\vec{q}} \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = 0$$

with $\boxed{\gamma_{\vec{q}} = \frac{1}{z} \sum_{\vec{\delta}} e^{i\vec{q}\cdot\vec{\delta}}}$.

Solution of the above system yields the dispersion relation

$$\boxed{\omega_q = zJS\sqrt{1-\gamma_q^2}}$$

it is not difficult to show that $\sqrt{1-\gamma_q^2} = q + \mathcal{O}(q^2)$ at small q!

These are the spin-waves (anti-ferromagnons). Their general behavior is very familiar: in the limit $q \to 0$ they correspond with the Goldstone-mode with $\omega = cq$ and spin-wave velocity $\boxed{c = zJS}$.