Spin waves

Part I

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Why spin waves ?

Time-dependent phenomenon \longrightarrow precession of the spin



Theory developed to describe the excited states of the Heisenberg Hamiltonian

$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$

And determine exchange interaction (and anisotropies) via experiments

Why spin waves ?

Bulk systems

 ω ~A few THz, meV, cm⁻¹ in bulk system k ~ 0.1 A-1

Observed by neutron scattering in (k, ω) space, but also NMR, optical techniques (Raman, $\omega = 0$)

Part I

General considerations Ferromagnet Antiferromagnet Failure of the theory

Part II

Neutron scattering Examples





$$\mathcal{H} = \sum_{m,n} J_{m,n} \ \vec{S}_m.\vec{S}_n$$



A spin experiences a molecular field due to interaction with its neighbours

Long range ordering

Depending on interactions, this molecular field can induce a new periodicity



Example : AF ordering



New periodicity, « magnetic unit cell »



$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$

m labels the unit cell

i labels the ion within the unit cell

New periodicity, « magnetic unit cell »



$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$

m labels the unit cell

i labels the ion within the unit cell

Define Interactions



$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$



 $J_{m,1,n,1}$

 $J_{m,1,m,2}$

 $J_{m,1,n,2}$

Define Interactions

$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$

 $J_{m,1,m,1}$





 $J_{m,1,m,2}$

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 $J_{m,1,n,2}$



Define Interactions

$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$

 $J_{m,1,m,1}$

 $J_{m,1,n,1}$

 $J_{m,1,m,2}$









Mermin and Wagner theorem : no spontaneous broken symmetry at finite temperature in 1 and 2 dimension





A spin experiences a molecular field due to the interaction with its neighbors



 $J_{m,n}$



Classical mechanics

$$\mathcal{H} = -\vec{S}.\vec{h}$$

 $\frac{d}{dt} \vec{S} = \vec{S} \times \vec{h} \qquad \text{Equation of motion}$

$$\frac{d}{dt} \begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix} = \begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ h \end{pmatrix} = h \begin{pmatrix} S^y \\ -S^x \\ 0 \end{pmatrix}$$

$$S^{+} = S^{x} + i S^{y} \qquad S^{x} = \frac{S^{+} + S^{-}}{2}$$
$$S^{-} = S^{x} - i S^{y} \qquad S^{y} = \frac{S^{+} - S^{-}}{2i}$$

Classical mechanics

$$\frac{d}{dt} \begin{pmatrix} S^+\\ S^-\\ S^z \end{pmatrix} = \begin{pmatrix} -ih & & \\ & ih & \\ & & 0 \end{pmatrix} \begin{pmatrix} S^+\\ S^-\\ S^z \end{pmatrix}$$
$$\omega = h$$

$$S^{+}(t) = S^{+}(t=0) e^{-i\omega t}$$

$$S^{-}(t) = S^{-}(t=0) e^{+i\omega t}$$

$$S^{z}(t) = S^{z}(t=0)$$

The spin precesses around S^z with a frequency ω proportional to h

1 degree of freedom

$$(S^{x})^{2} + (S^{y})^{2} = \frac{S^{+}S^{-} + S^{-}S^{+}}{2} = \frac{S^{+}(t=0)S^{-}(t=0) + S^{-}(t=0)S^{+}(t=0)}{2}$$

Quantum mechanics

Spin operators in the local basis

$$\begin{split} \vec{S} &= \left(S^{1}, S^{2}, S^{3}\right) \\ S^{3} |\ell\rangle &= \ell \ |\ell\rangle \qquad \ell = -S, ..., S \\ S^{+} |\ell\rangle &= \sqrt{S(S+1) - \ell(\ell+1)} \ |\ell+1\rangle \\ S^{-} |\ell\rangle &= \sqrt{S(S+1) - \ell(\ell-1)} \ |\ell-1\rangle \\ \left[S^{+}, S^{-}\right] &= 2 \ S^{3} \end{split}$$

Eigenvalues

$$\begin{aligned} \mathcal{H} &= -\vec{S}.\vec{h} = -h \ S^3 \\ E_\ell &= h \ \ell \qquad \ell = -S, ..., S \end{aligned}$$



Quantum mechanics



Coupled spins

Back to the problem of coupled spins ...



Transformation to local basis





Classical mechanics

$$\mathcal{H} = \sum_{m,n,i,j} J_{m,i,n,j} \ \vec{S}_{m,i}.\vec{S}_{n,j}$$

Equation of motion :

N coupled ...

... non linear equations



 $\frac{d}{dt} \vec{S}_{m,i} = \vec{S}_{m,i} \times \left(-\sum_{n,j} J_{m,i,n,j} \vec{S}_{n,j} \right)$

Classical mechanics

1. Molecular field : small deviations around the direction of the ordered moment

$$\vec{S} = \langle \vec{S} \rangle + \delta \vec{S} \longrightarrow \vec{S}_{m,i} = \langle \vec{S}_{m,i} \rangle + \delta \vec{S}_{m,i}$$

2. Take advantage of the new periodicity (Fourier transform) : reduce the number of coupled equations



3. Exchange
$$J_{m,i,n,j} = J_{m,i,m+\Delta,j} = \sum_{q} e^{iq\Delta} J_{q,i,j}$$

Classical mechanics

1. Fourier transform



$$\frac{d}{dt} \vec{S}_{m,i} = \vec{S}_{m,i} \times \left(-\sum_{n,j} J_{m,i,n,j} \vec{S}_{n,j} \right)$$
$$\frac{d}{dt} \vec{S}_{k,i} = -\sum_{k'} \vec{S}_{k-k',i} \times \sum_{j} J_{k',i,j} \vec{S}_{k',j}$$

2. Ordered moment + small deviations : linearization $\vec{S}_{k,i} = \langle \vec{S}_i \rangle \, \delta_{k=0} + \delta \vec{S}_{k,i}$

$$\frac{d}{dt} \,\delta\vec{S}_{k,i} \approx -\left(\sum_{k'} \,\delta\vec{S}_{k-k',i} \times \sum_{j} J_{k',i,j} \langle\vec{S}_{j}\rangle \,\delta_{k'=0} + \sum_{k'} \,\langle\vec{S}_{i}\rangle \,\delta_{k-k'=0} \times \sum_{j} J_{k',i,j} \,\delta\vec{S}_{k',j}\right) \\ \approx \sum_{j} \left(\delta_{i,j} \sum_{\ell} J_{0,i,\ell} \,\langle\vec{S}_{\ell}\rangle \times - \langle\vec{S}_{i}\rangle \times J_{k,i,j}\right) \,\delta\vec{S}_{k,j}$$

$$\vec{h}_{k,i,j} \quad \text{effective magnetic field acting on } \delta\vec{S}_{k,j}$$

Classical mechanics

Effective magnetic field acting on $\delta \vec{S}_{k,j}$

$$\frac{d}{dt} \begin{pmatrix} \delta S_{k,i}^x \\ \delta S_{k,i}^y \\ \delta S_{k,i}^z \end{pmatrix} = \sum_j \vec{h}_{k,i,j} \times \begin{pmatrix} \delta S_{k,j}^x \\ \delta S_{k,j}^y \\ \delta S_{k,j}^z \end{pmatrix}$$

Local coordinates (use local transformation)

$$\frac{d}{dt} \begin{pmatrix} \delta \sigma_{k,i}^+ \\ \delta \sigma_{k,i}^- \\ \delta \sigma_{k,i}^3 \end{pmatrix} = \sum_j \left(R_i^T \vec{h}_{k,i,j} \times R_j \right) \begin{pmatrix} \delta \sigma_{k,j}^+ \\ \delta \sigma_{k,j}^- \\ \delta \sigma_{k,j}^3 \end{pmatrix}$$

L magnetic ions per magnetic unit cell : L coupled linear equations

Approximations :

- 1. Ordered phase
- 2. Small deviations around the ordered moment : « linear spin wave theory » (large S, low T)

From the general equations of motion

$$\frac{d}{dt} \ \delta \vec{S}_{k,i} \approx \sum_{j} \left(\delta_{i,j} \sum_{\ell} J_{0,i,\ell} \ \langle \vec{S}_{\ell} \rangle \times \ - \ \langle \vec{S}_{i} \rangle \times J_{k,i,j} \right) \ \delta \vec{S}_{k,j}$$

back to the simple ferromagnetic case :

$$\frac{d}{dt} \delta \vec{S}_k \approx (J_0 - J_k) \langle \vec{S} \rangle \times \delta \vec{S}_k$$

$$\frac{d}{dt} \begin{pmatrix} \delta S_k^x \\ \delta S_k^y \\ \delta S_k^z \end{pmatrix} \approx (J_0 - J_k) \begin{pmatrix} 0 \\ 0 \\ \langle S \rangle \end{pmatrix} \times \begin{pmatrix} \delta S_k^x \\ \delta S_k^y \\ \delta S_k^z \end{pmatrix} = (J_0 - J_k) \langle S \rangle \begin{pmatrix} -\delta S_k^y \\ \delta S_k^x \\ 0 \end{pmatrix}$$

$$\frac{d}{dt} \begin{pmatrix} \delta S_k^+ \\ \delta S_k^- \\ \delta S_k^z \end{pmatrix} = \begin{pmatrix} -i\omega_k \\ i\omega_k \\ 0 \end{pmatrix} \begin{pmatrix} \delta S_k^+ \\ \delta S_k^- \\ \delta S_k^z \end{pmatrix}$$

$$\delta S_k^+(t) = \delta S_k^+(t=0) e^{-i\omega_k t}$$

$$\delta S_k^-(t) = \delta S_k^-(t=0) e^{+i\omega_k t}$$

$$\delta S_k^z(t) = \delta S_k^z(t=0)$$

Coupled precessions of the spins around the ordered moment; propagate through the lattice



The dispersion relation connects the wavevector and the frequency ω (energy)

$$\omega_k = -\left(J_0 - J_k\right) \langle S \rangle$$



Back to quantum mechanics : spin waves are (quasi) independent Bose modes

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$$\mathcal{H} = \sum_{k} \omega_k \ b_k^+ b_k \qquad \langle E \rangle = \sum_{k} \omega_k \ n_B(\omega_k) \qquad n_B(E) = \frac{1}{e^{E/k_B T} - 1}$$

Check the approximations (correction to the magnetization)

$$\langle S \rangle \approx S - \sum_{k} n_{B}(\omega_{k})$$
$$\sum_{k} \longrightarrow \int dk^{d} = \int dk \; \frac{k^{d-1}}{(2\pi)^{d}}$$
$$n_{B}(E) \longrightarrow \frac{k_{B}T}{E}$$
$$\omega_{k} \sim 2 \; |J| \; \langle S \rangle \; \frac{k^{2}a^{2}}{2}$$

$$\sum_{k} n_B(\omega_k) \longrightarrow \int dk \; \frac{k^{d-1}}{(2\pi)^d} \; \frac{T}{k^2}$$

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The thermal fluctuations prevents long range ordering for

$$d \leq 2$$

Breakdown of the spin wave theory is consistent with Mermin and Wagner theorem



$$J_{k,1,2} = J_k = J(1 + e^{-ika})$$
$$J_{k,2,1} = J_k^* = J(1 + e^{ika})$$
$$J_{k,1,1} = J_{k,2,2} = 0$$
$$\langle \vec{S}_1 \rangle = -\langle \vec{S}_2 \rangle = \langle \vec{S} \rangle$$

From the general equations of motion

$$\frac{d}{dt} \,\delta \vec{S}_{k,i} \approx \sum_{j} \left(\delta_{i,j} \sum_{\ell} J_{0,i,\ell} \,\langle \vec{S}_{\ell} \rangle \times \, - \,\langle \vec{S}_{i} \rangle \times J_{k,i,j} \right) \,\delta \vec{S}_{k,j}$$

$$\frac{d}{dt} \,\delta \vec{S}_{k,1} = J_0 \,\langle \vec{S}_2 \rangle \times \,\delta \vec{S}_{k,1} - J_k \,\langle \vec{S}_1 \rangle \times \delta \vec{S}_{k,2}$$

$$\frac{d}{dt} \,\delta \vec{S}_{k,2} = J_0 \,\langle \vec{S}_1 \rangle \times \,\delta \vec{S}_{k,2} - J_k \,\langle \vec{S}_2 \rangle \times \delta \vec{S}_{k,1}$$

Local coordinates (use local transformation)

4 : There are 2 degrees of freedom

$$\frac{d}{dt} \begin{pmatrix} \delta \sigma_{k,1}^{+} \\ \delta \sigma_{k,2}^{-} \end{pmatrix} = -i \langle S \rangle \begin{pmatrix} J_{0} & -J_{k} \\ J_{k} & -J_{0} \end{pmatrix} \begin{pmatrix} \delta \sigma_{k,1}^{+} \\ \delta \sigma_{k,2}^{-} \end{pmatrix}$$

$$\frac{d}{dt} \begin{pmatrix} \delta \sigma_{k,2}^{+} \\ \delta \sigma_{k,1}^{-} \end{pmatrix} = -i \langle S \rangle \begin{pmatrix} J_{0} & -J_{k} \\ J_{k} & -J_{0} \end{pmatrix} \begin{pmatrix} \delta \sigma_{k,2}^{+} \\ \delta \sigma_{k,1}^{-} \end{pmatrix}$$

$$\frac{d}{dt} \delta \sigma_{k,1}^{3} = \frac{d}{dt} \delta \sigma_{k,2}^{3} = 0$$
3 : Exchange the role of sublattices 1 and 2 (degenerate modes)

2 : Projection on e3 is constant

Additional transformation to decouple sublattice 1 and 2

$$\delta \sigma_{k,1}^+ = u_k \,\delta A_k + v_k \,\delta B_k$$

$$\delta \sigma_{k,2}^- = v_k \,\delta A_k + u_k \,\delta B_k$$

$$\left(\begin{array}{cc}J_0 & -J_k\\J_k & -J_0\end{array}\right)$$

Spin wave energies

$$\omega_k = \pm \langle S \rangle \sqrt{J_0 - J_k^2}$$

$$\delta \sigma_{k,2}^{+} = u_k \, \delta A_k + v_k \, \delta B_k$$

$$\delta \sigma_{k,1}^{-} = v_k \, \delta A_k + u_k \, \delta B_k$$

Details of the transformation :

$$u_k^2 - v_k^2 = 1$$

$$u_k^2 = \frac{1}{2} \left(+1 + \frac{J_0 \langle S \rangle}{\omega_k} \right)$$
$$v_k^2 = \frac{1}{2} \left(-1 + \frac{J_0 \langle S \rangle}{\omega_k} \right)$$
$$u_k v_k = \frac{J_k \langle S \rangle}{2 \omega_k}$$













Check the approximations (correction to the magnetization)

$$\langle S \rangle \approx S - \sum_{k} v_{k}^{2} + (u_{k}^{2} + v_{k}^{2}) n_{B}(\omega_{k})$$

$$\langle S \rangle \approx S + \frac{1}{2} - \sum_{k} \frac{J_{0} \langle S \rangle}{\omega_{k}} \left(n_{B}(\omega_{k}) + \frac{1}{2} \right)$$



$$\sum_{k} \frac{J_0 \langle S \rangle}{\omega_k} \left(n_B(\omega_k) + \frac{1}{2} \right) \longrightarrow \int dk \; \frac{k^{d-1}}{(2\pi)^d} \frac{1}{k} \left(\frac{T}{k} + \frac{1}{2} \right)$$

Breakdown of the spin wave theory is consistent with Mermin and Wagner theorem

Summary

Spin waves : excited states of the Heisenberg Hamiltonian

L ions per magnetic unit cell : L branches

Approximations

1) Ordered phase

2) Small deviations around the ordered moment : large S, low T

Quasi independent modes (bosons) and important role of quantum fluctuations (low dimension)



Spin $\frac{1}{2}$: no long range order, no spin waves A spin 1 excitation = 2 spinons : continuum and no dispersion relation

Kagome Lattice Degenerate ground state : no long range order The system keeps fluctuating : liquid and co-planar regimes (order by disorder)





 Beyond spin wave theory : calculate the equation of motion for each spin (~ molecular dynamics) in classical mechanics (no approximation):

Propagative modes as well as soft modes



Robert et al, PRL 101, 117207 (2008)





 $\sqrt{3} \times \sqrt{3}$ Configuration





Thanks for your attention

Questions

Practical

To be continued ... Part II : how to observe spin waves ?



References

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Quantum mechanics

Holstein-Primakov representation of the spin « seen from the classical picture » :

$$S^{1} = S \cos \theta \sin \phi \qquad S^{+} = S \sin \phi \ e^{+i\theta}$$

$$S^{2} = S \sin \theta \sin \phi \qquad S^{-} = S \sin \phi \ e^{-i\theta}$$

$$S^{3} = S \cos \phi$$

New variable : deviation D

$$S^{3} = S - D \qquad \cos \phi = 1 - \frac{D}{S}$$
$$S^{+} = \sqrt{2S} \sqrt{1 - \frac{D}{2S}} \sqrt{D} e^{+i\theta}$$
$$S^{-} = \sqrt{2S} \sqrt{1 - \frac{D}{2S}} \sqrt{D} e^{-i\theta}$$
$$S^{3} = S - D$$



Quantum mechanics

Deviation D n_b Boson field : $n_b = b^+ b = 0, 1, 2, ..., \infty$ $[b, b^+] = 1$ $S^+ = \sqrt{2S} \sqrt{1 - \frac{n_b}{2S}} b$ $S^+ \approx \sqrt{2S} b$ $S^- = \sqrt{2S} b^+ \sqrt{1 - \frac{n_b}{2S}}$ $S^- \approx \sqrt{2S} b^+$ $S^3 = S - n_b$