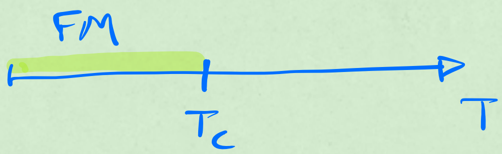
Lecture 5.12.2022

Q1



$-J\,\hat{S}_i\cdot\hat{S}_j \sim$ MAF

Classical spins

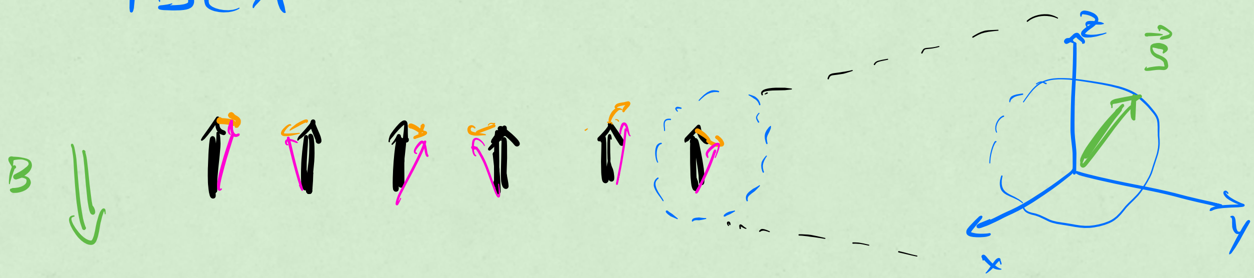
$|\vec{S}| = 1$

Ising, xy, Heisenberg

Q2

$$\langle \vec{S}(\underline{r})\cdot\vec{S}(0)\rangle \sim ?$$

IDEA



$$\mathcal{H} = -J\sum_{\langle \underline{n}\,\underline{n}'\rangle} \vec{S}(\underline{n})\cdot\vec{S}(\underline{n}') + g\mu_B B\sum_{\underline{n}} S^z(\underline{n})$$

$$\simeq E_{g.s.} + \mathcal{H}_{h.o.}$$ step 1

Lecture: 5.12.2022

7.2 The Classical Heisenberg model

In this section we discuss the classical version of the Heisenberg spin Hamiltonian, without uniaxial anisotropy ($D = 0$). The substitution of the quantum-spin operators by classical spins is somewhat justified when the relative spacing between levels inside each multiplet $S(\underline{n})$ becomes smaller and smaller. Moreover, when correlations among spins develop, cooperative effects create a sort of *collective* large spin which behaves classically. In formulas, the replacement of quantum-spin operators by classical vectors reads

$$\hat{\mathbf{S}}(\underline{n}) \to \vec{S}(\underline{n}) \equiv (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)\ . \tag{7.8}$$

Since the classical spin on the r.h.s. has unitary modulus, the factor $S\,(S+1)$ needs to be re-absorbed into the definition of g to recover the Curie law at $T \gg J$ (the exchange interaction constant can be rescaled similarly). The spin Hamiltonian then reads

$$\mathcal{H} = -\frac{1}{2} J \sum_{|\underline{n}-\underline{n}'|=1} \underline{\vec{S}(\underline{n}) \cdot \vec{S}(\underline{n}')} + g\mu_{\mathrm{B}} B \sum_{\underline{n}} S^z(\underline{n})\,, \tag{7.9}$$

and the partition function

$$\mathcal{Z} = \int d\Omega_1 \int d\Omega_2 \cdots \int d\Omega_N e^{-\beta\mathcal{H}\left(\{\vec{S}(\underline{n})\}\right)}\,, \tag{7.10}$$

with $d\Omega_{\underline{n}} = \sin\theta_{\underline{n}} d\theta_{\underline{n}} d\varphi_{\underline{n}}$ being the solid-angle element of the spin located at the site $\underline{n}$.

Stability against linear excitations

With the classical spin Hamiltonian (7.9), the minimal energy is obtained by aligning all the magnetic moments along the direction of the applied field (spins along negative z direction). We consider how the energy increases due to *small* deviations from this configuration. Our goal is to simplify the original problem by means of an *effective* Hamiltonian that is formally equivalent to the one describing a system of coupled harmonic oscillators. To this end, we may write

$$S^z(\underline{n}) = -\sqrt{1 - \sum_{\alpha=x,y} \left(S^\alpha(\underline{n})\right)^2} \simeq -1 + \frac{1}{2}\sum_{\alpha=x,y} \left(S^\alpha(\underline{n})\right)^2 \tag{7.11}$$

$$\text{with the hypothesis} \qquad \underline{\left(S^\alpha(\underline{n})\right)^2 \ll \left(S^z(\underline{n})\right)^2}\ ,$$

$(S^x)^2 + (S^y)^2 + (S^z)^2 = 1$

small

with α labeling, in this case, the *transverse* spin components. The approximation in Eq. (7.11) affects the Hamiltonian as follows:

$$
\begin{aligned}
\mathcal{H} \simeq & -\frac{1}{2} J \sum_{|\underline{n}-\underline{n}'|=1} \overbrace{\left[1-\frac{1}{2}\sum_{\alpha}(S^{\alpha}(\underline{n}))^2\right]}^{\sim S^z(\underline{n})} \times \overbrace{\left[1-\frac{1}{2}\sum_{\alpha'}(S^{\alpha'}(\underline{n}'))^2\right]}^{\sim S^z(\underline{n}')} \\
& -\frac{1}{2} J \sum_{|\underline{n}-\underline{n}'|=1} \overbrace{\sum_{\alpha} S^{\alpha}(\underline{n}) S^{\alpha}(\underline{n}')}^{S^x(\underline{n})S^x(\underline{n}')+(y)} - g\mu_{\mathrm{B}} B \sum_{\underline{n}} \overbrace{\left[1-\frac{1}{2}\sum_{\alpha}(S^{\alpha}(\underline{n}))^2\right]}^{\sim S^z(\underline{n})} \\
= & -\frac{1}{2} z_n N J - g\mu_{\mathrm{B}} B N + \frac{1}{2} z_n J \frac{1}{2}\left[\sum_{\underline{n}}\sum_{\alpha}(S^{\alpha}(\underline{n}))^2 + \sum_{\underline{n}'}\sum_{\alpha'}(S^{\alpha'}(\underline{n}'))^2\right] \\
& -\frac{1}{2} J \sum_{|\underline{n}-\underline{n}'|=1} \sum_{\alpha} S^{\alpha}(\underline{n}) S^{\alpha}(\underline{n}') + \frac{1}{2} g\mu_{\mathrm{B}} B \sum_{\underline{n}}\sum_{\alpha}(S^{\alpha}(\underline{n}))^2 + \mathcal{O}\left((S^{\alpha})^4\right) \\
\simeq & E_{g.s.} + \mathcal{H}_{h.o.}
\end{aligned}
\tag{7.12}
$$

where, by nothing that the double summations $\sum_{\underline{n}}\sum_{\alpha}$ and $\sum_{\underline{n}'}\sum_{\alpha'}$ are actually the same, we have defined

$$
\begin{aligned}
\mathcal{H}_{h.o.} = & \frac{1}{2} z_n J \sum_{\underline{n}}\sum_{\alpha}(S^{\alpha}(\underline{n}))^2 - \frac{1}{2} J \sum_{|\underline{n}-\underline{n}'|=1} \sum_{\alpha} S^{\alpha}(\underline{n}) S^{\alpha}(\underline{n}') \\
& + \frac{1}{2} g\mu_{\mathrm{B}} B \sum_{\underline{n}}\sum_{\alpha}(S^{\alpha}(\underline{n}))^2
\end{aligned}
\tag{7.13}
$$

Not well behaving

well behaving

and the constant ground-state energy

$$
E_{g.s.} = -\frac{1}{2} z_n N J - g\mu_{\mathrm{B}} B N \,. \tag{7.14}
$$

The Hamiltonian $\mathcal{H}_{h.o.}$, written in Eq. (7.13), is equivalent to the Hamiltonian of N coupled harmonic oscillators which can be decoupled by the usual Fourier transform in the discrete space:

$$
\left\{
\begin{array}{l}
S^{\alpha}(\underline{n}) = \frac{1}{\sqrt{N}} \sum_{\underline{q}} \tilde{S}^{\alpha}(\underline{q})\, e^{-i\underline{q}\cdot\underline{n}} \\
\tilde{S}^{\alpha}(\underline{q}) = \frac{1}{\sqrt{N}} \sum_{\underline{n}} S^{\alpha}(\underline{n})\, e^{i\underline{q}\cdot\underline{n}}
\end{array}
\right.
\tag{7.15}
$$

with the orthogonality relation

$$
\sum_{\underline{n}} e^{i(\underline{q}-\underline{q}')\cdot\underline{n}} = N\delta_{\underline{q},\underline{q}'} \,. \tag{7.16}
$$

$$\int |f(x)|^2 dx = \frac{1}{2\pi}\int |\tilde{f}(q)|^2 dq$$

For simplicity we assume unitary lattice constant. It is convenient to evaluate the two relevant summations appearing in the Hamiltonian of Eq. (7.13) separately. The first summation reads

$$\sum_{\underline{n}}(S^\alpha(\underline{n}))^2 = \frac{1}{N}\sum_{\underline{n}}\sum_{\underline{q},\underline{q}'}\tilde{S}^\alpha(\underline{q})\tilde{S}^\alpha(\underline{q}')\, e^{-i(\underline{q}+\underline{q}')\cdot\underline{n}} = \sum_{\underline{q}}|\tilde{S}^\alpha(\underline{q})|^2\,. \tag{7.17}$$

This is nothing but the Parseval's formula for the discrete-lattice Fourier transform. For what concerns the second summation on the right-hand side of Eq. (7.13), we first rewrite it as

$$\sum_{|\underline{n}-\underline{n}'|=1} S^\alpha(\underline{n})S^\alpha(\underline{n}') = \sum_{\underline{n}}\sum_{\underline{\delta}} S^\alpha(\underline{n})S^\alpha(\underline{n}+\underline{\delta}) \tag{7.18}$$

where $\underline{\delta}$ is a vector connecting the site $\underline{n}$ with its nearest neighbors. For simplicity, we will consider just a linear ($z_n = 2$), square ($z_n = 4$) and simple-cubic ($z_n = 6$) lattice for D=1, 2 and 3, respectively. Passing to the Fourier space one finds

$$\begin{aligned}\sum_{\underline{n}}\sum_{\underline{\delta}}S^\alpha(\underline{n})S^\alpha(\underline{n}+\underline{\delta}) &= \sum_{\underline{n}}\sum_{\underline{\delta}}\frac{1}{N}\sum_{\underline{q},\underline{q}'}\tilde{S}^\alpha(\underline{q})\tilde{S}^\alpha(\underline{q}')\, e^{-i(\underline{q}+\underline{q}')\cdot\underline{n}}\, e^{-i\underline{q}'\cdot\underline{\delta}} \\ &= \sum_{\underline{\delta}}\sum_{\underline{q}}|\tilde{S}^\alpha(\underline{q})|^2\, e^{-i\underline{q}\cdot\underline{\delta}} = \sum_{\underline{q}}|\tilde{S}^\alpha(\underline{q})|^2 \sum_{\{\underline{\delta}>0\}} 2\cos(\underline{q}\cdot\underline{\delta})\,;\end{aligned} \tag{7.19}$$

the notation $\{\underline{\delta} > 0\}$ means that the summation extends over half of the nearest neighbors of the spin located at site $\underline{n}$: it consists of $z_n/2$ terms. Eqs. (7.17) and (7.19) enable us to decouple the *elastic* Hamiltonian given in Eq. (7.13), which then reads

$$\begin{aligned}\mathcal{H}_{h.o.} =& \frac{1}{2}J\sum_{\underline{q}}\sum_{\alpha}\left(z_n - \sum_{\{\underline{\delta}>0\}}2\cos(\underline{q}\cdot\underline{\delta})\right)|\tilde{S}^\alpha(\underline{q})|^2 \\ &+ \frac{1}{2}g\mu_{\mathrm{B}}B\sum_{\underline{q}}\sum_{\alpha}|\tilde{S}^\alpha(\underline{q})|^2 \\ =& \frac{1}{2}\sum_{\alpha}\sum_{\underline{q}}\Gamma(\underline{q})|\tilde{S}^\alpha(\underline{q})|^2\,,\end{aligned} \tag{7.20}$$

with

$$\Gamma(\underline{q}) = J[z_n - \sum_{\{\underline{\delta}>0\}} 2\cos(\underline{q}\cdot\underline{\delta})] + g\mu_{\mathrm{B}}B\,. \tag{7.21}$$

$\Gamma(q) = \hbar\omega(q)$

1D case $\quad 2J(1-\cos q)$

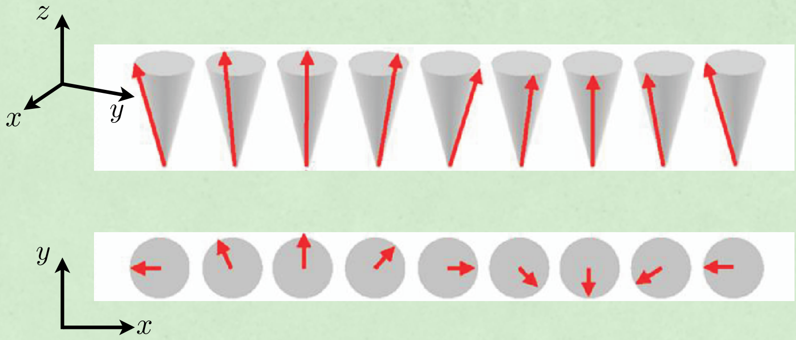


Figure 7.3: Sketch of a spin-wave excitation for the 1D Heisenberg model, with period equal to eight lattice units.

Indeed, for the Heisenberg model, the linear excitations associated with the quadratic Hamiltonian in Eq. (7.13) are spin waves with dispersion relation $\hbar\omega(\underline{q}) = \Gamma(\underline{q})$. Spin waves are collective excitations analogous to phonons. Similarly to phonons, spin waves are also quantized and the specific dependence of $\Gamma(\underline{q})$ on the wave vector (especially for $q \simeq 0$) determines the behavior of the magnetization at low temperature (in the absence of anisotropy). The dispersion curve $\Gamma(\underline{q})$ can be measured, e.g., by inelastic neutron scattering.

Coming back to our goal, we proceed by evaluating the average of fluctuations, namely those terms in Eq. (7.11) that we have assumed to be *small* for linearizing the Hamiltonian (7.9). The approximated Hamiltonian, Eq. (7.20), consists of N independent quadratic degrees of freedom so that the equipartition theorem can be applied:

$$\frac{1}{2}\Gamma(\underline{q})\,\langle|\tilde{S}^\alpha(\underline{q})|^2\rangle_{th} = \frac{1}{2}k_{\rm B}T \qquad \Rightarrow \qquad \boxed{\langle|\tilde{S}^\alpha(\underline{q})|^2\rangle_{th} = \frac{k_{\rm B}T}{\Gamma(\underline{q})}\,;} \tag{7.22}$$

$\langle\ldots\rangle_{th}$ denotes thermal average performed using the Hamiltonian $\mathcal{H}_{h.o.}$ in Eq. (7.20). Thermal averages of the squared transverse components in real space read

back to real space

$$\langle(S^\alpha(\underline{n}))^2\rangle_{th} = \frac{1}{N}\sum_{\underline{q},\underline{q}'}\langle\tilde{S}^\alpha(\underline{q})\tilde{S}^\alpha(\underline{q}')\rangle_{th}\, e^{-i(\underline{q}+\underline{q}')\cdot\underline{n}} = \frac{1}{N}\sum_{\underline{q}}\langle|\tilde{S}^\alpha(\underline{q})|^2\rangle_{th}\,, \tag{7.23}$$

where we have used the fact that transverse components fluctuate randomly so that $\langle\tilde{S}^\alpha(\underline{q})\tilde{S}^\alpha(\underline{q}')\rangle_{th} = \delta_{\underline{q},\underline{q}'}\langle|\tilde{S}^\alpha(\underline{q})|^2\rangle_{th}$. Note that the right-hand side of Eq. (7.23) is independent of the lattice site, thus the label $\underline{n}$ will be dropped henceforth from $\langle (S^\alpha(\underline{n}))^2\rangle_{th}$. In order to evaluate whether the considered linear excitations are able or not to destroy ferromagnetism, we shall let the field $B \to 0^+$. First, we approximate the summation on the right-hand side of Eq. (7.23) with an integral

$$\langle (S^\alpha)^2\rangle \simeq \frac{k_\mathrm{B}T}{(2\pi)^\mathrm{D}} \int \frac{d^\mathrm{D}q}{\Gamma(\underline{q})}\,. \tag{7.24}$$

Since what matters is the behavior for small values of q (i.e., the effect of fluctuations at large spatial scales), the denominator of the integral can be linearized as

Q1 small q

$$\Gamma(\underline{q}) \simeq Jz_n - 2J\sum_\mu (1-\frac{1}{2}q_\mu^2) + g\mu_\mathrm{B}B = Jz_n - 2J(\frac{z_n}{2} - \frac{1}{2}q^2) + g\mu_\mathrm{B}B = Jq^2 + g\mu_\mathrm{B}B \tag{7.25}$$

with μ=1...D and $q^2 = \sum_\mu q_\mu^2$, which yields

Q2 $B \to 0^+$

$$\langle (S^\alpha)^2\rangle \simeq \frac{k_\mathrm{B}T}{(2\pi)^\mathrm{D}} \int \frac{d^\mathrm{D}q}{Jq^2 + \cancel{g\mu_\mathrm{B}B}} \tag{7.26}$$

Spontaneous Mag

When taking the limit $B \to 0^+$, the integral in Eq. (7.26) has an infrared divergence[2] for D$\leq$2. The consequences of such a divergence can be appreciated more effectively by setting a lower bond to the integral: $q_{min} = \pi/N_\alpha$, with N_α being of the order of the linear size of the system in lattice units. Depending on the dimensionality of the lattice we have

$$\langle (S^\alpha)^2\rangle \sim \frac{k_\mathrm{B}T}{J}\int_{q_{min}} \frac{q^{\mathrm{D}-1}\,dq}{q^2} \Rightarrow \begin{cases} \mathrm{D}=1 & \langle (S^\alpha)^2\rangle \sim \frac{k_\mathrm{B}T}{J} N_\alpha \\ \mathrm{D}=2 & \langle (S^\alpha)^2\rangle \sim \frac{k_\mathrm{B}T}{J}\ln(N_\alpha) \\ \mathrm{D}=3 & \langle (S^\alpha)^2\rangle < \infty \end{cases} \tag{7.27}$$

In order to understand what a divergence with increasing N_α means, it is convenient to enumerate the mathematical steps that we followed according to their physical sense:

- We assumed the system to be in a ferromagnetic state at $T = 0$, namely, with all the spins aligned along the same direction.
- We let each spin deviate by a small amount from its direction of alignment, z.

[2] A possible ultraviolet divergence does not matter *i*) because the lattice unit sets a physical upper limit to large values of q *ii*) because we are interested in fluctuations acting on large spatial scales corresponding to $q \sim 0$.

$$\langle (S^{\perp})^2 \rangle_{th} \sim \frac{k_B T}{J} \frac{1}{(2\pi)^D} \int \frac{d^D q}{q^2}$$

$\underline{D=1}$ $\quad d^D q \sim dq \qquad q_{min} = \frac{\pi}{N_\alpha} \qquad q_{max} = \pi$

$$\langle (S^{\perp})^2 \rangle_{th} \sim \frac{k_B T}{J} \int_{q_{min}}^{q_{max}} \frac{dq}{q^2} \sim \frac{k_B T}{J} \frac{1}{q_{min}} \sim \boxed{\frac{k_B T}{J} N_\alpha}$$

$$\langle (S^{\perp})^2 \rangle \xrightarrow[N_\alpha \to \infty]{} \infty \qquad \text{whatever } T \text{ is !!!}$$

$\underline{D=2}$ $\quad d^2 q = 2\pi q \, dq$

$$\langle (S^{\perp})^2 \rangle \sim \frac{k_B T}{J} \int_{q_{min}}^{q_{max}} \frac{\cancel{q} \, dq}{q^{\cancel{2}}} = \frac{k T}{J} \ln(N_\alpha) \xrightarrow[N_\alpha \to \infty]{} \infty$$

No FM at any finite T

$\underline{D=3}$ $\quad d^3 q = 4\pi q^2 dq$

$$\langle (S^{\perp})^2 \rangle \sim \frac{k T}{J} \int_{q_{min}}^{q_{max}} \frac{\cancel{q^2} \, dq}{\cancel{q^2}} < \infty \quad N_\alpha \to \infty$$

FM is possible $T < T_c$

1D Heisenberg | (analogy 1D Ising model Landau)

$\langle (S^{\perp})^2 \rangle < \epsilon$

$N \frac{KT}{J} < \epsilon \Rightarrow N < \epsilon \frac{J}{KT}$ $\bar{N}(T)$

by analogy with 1D Ising

linear exc. destroy FM $\xi(T) \sim \bar{N}(T) \sim \frac{J}{K_B T}$ 1D Heisenberg

DWs destroy FM $\xi(T) \sim e^{2J/K_B T}$ 1D Ising

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question MFA

MFA Ising $m = th\left(\frac{zJm}{KT}\right)$

$\alpha = x, y, z$ Heisenberg $m^\alpha = \mathcal{L}\left(\frac{zJ\, m^\alpha}{KT}\right)$

$\alpha = x, y$ XY $m^a = F\left(\frac{zJ\, m^a}{KT}\right)$

MF CRITICAL EXP are exact for $D \geq 4$

SOLUTION QUIZ

dimension	**Ising**	**XY**	**Heisenberg**
1D	SRO	SRO	SRO
2D	LRO	q-LRO	SRO/q-LRO
3D	LRO	LRO	LRO

Para = paramagnetism, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle = 0$

SRO = short-range order, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle \sim \mathrm{e}^{-r/\xi}$

q-LRO = quasi-long-range order, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle \sim r^{-\eta}$

LRO = long-range order, $\langle \vec{S}(\underline{r}) \cdot \vec{S}(0) \rangle =$ constant.