Notes on magnetism and the spin wave theory

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Contents

(Classical) Ground states 3

Spin-wave theory 5

Ferromagnetism 5

Anti-ferromagnet 7

Goldstone mode 8

XY model 10

Operator method based on Cauchy-Schwarz inequality 11

Low-temperature expansion 13

Average magnetization 14

Experimental techniques 15

Neutron scattering 15

Nuclear magnetic resonance 16

Homework 18

In the previous chapter, we have introduced the Hubbard model and related t-J model for strongly-correlated systems such as cuprates. What we focus there is the electronic properties, such as metal-to-insulator transition and potential superconductivity. In this chapter, we will consider magnetism, which is another important property of physical systems. The main focus will be the Heisenberg model,

$$\hat{H} = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{1}$$

where J_{ij} are the Heisenberg interactions between the nearest neighbor spins. This model is the basis to study the magnetism. One can just take this model comes from the t-J model, by setting electronic kinetic term vanishing. Nevertheless, the Heisenberg model can be derived independent of the Hubbard or t-J model. The value of J in the Heisenberg model can be estimated from the second perturbation theory. That is, $J \sim \frac{t^2}{U}$, where U is the energy cost of the intermediate state.

$\boldsymbol{S}$ is the local spin operator, for example, for the spin-1/2,

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

$\boldsymbol{S}$ is not necessarily 1/2, but can be larger — physically this corresponds to multiple electrons per atom; or, in rare-earth materials, to effects of spin-orbit coupling replacing spin by total angular momentum. In this case,

$$\boldsymbol{S}^2 = S(S+1), \tag{3}$$

$$S^z|S, m >= m|S, m > \tag{4}$$

$$S^{\pm}|S, m >= \sqrt{(S \mp m)(S \pm m + 1)}|S, m \pm 1 > \tag{5}$$

`How to write down the spin-1 operator?`

Here, I would like to say, the origin of magnetism is a long-standing problem. In history, people thought (classical) magnetism is associated with circulating currents. In this lecture note, I would like to take spin as an intrinsic degree of freedom, and the magnetism comes from the interactions among spins. Another thing is, magnetism occurs both in metals such as iron as well as in certain types of insulators. Some of magnetic effects in metals can be understood within the Landau Fermi-liquid theory. Here we will also study novel many-body effects in insulating magnets.

(CLASSICAL) GROUND STATES

We start by discuss the ground states of the Heisenberg model. In the fully quantum systems, the ground state is not easy to get. In many cases we have to deal with them case by case. We will show several examples in one-dimension later. Here, we first discuss the classical limit. That is, we can first take the large-S limit, and treat the spin classically as unit vector,

$$\boldsymbol{S} = (\sin\theta\sin\phi, \sin\theta\cos\phi, \cos\theta) \tag{6}$$

where θ, ϕ is polar angle to label the direction of the spin in the phase space. When we just minimize the spin configuration to get the lowest energy, which relates to the ground state.

$$E = J\sum_{ij} \sin\theta_{ij}\sin\phi_{ij} + \sin\theta_{ij}\cos\phi_{ij} + \cos\theta_{ij} \tag{7}$$

We start with the simplest case, the nearest spin is co-parallel (the phase difference is only limited to 0 or π). One see that, if $J < 0$, the minimal energy is achieved by $\theta_{ij} = 0$,

$$E_0 = JN < 0, \tag{8}$$

This is the ferromagnetic state. If $J > 0$, the minimal energy is achieved by $\theta_{ij} = \pi$,

$$E_0 = -JN < 0, \tag{9}$$

This is the anti-ferromagnetic state.

The similar analysis can be generalized to two-dimension. For example, the anti-ferromagnetic square lattice, the ground state is (π, π) antiferromagnetic order (zero temperature).

Next we can consider a less non-trival case. The spin is co-plane, the spins lay down in the same plane, but not in the parallel way. The famous example is the antiferromagnetic 120-degree order on the triangular lattice. Similarly, there is non-coplane magnetic order. I will give some example below.

Let us consider $J_1 - J_2 - J_\chi$ model on the square lattice:

$$H = J_1 \sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j + J_2 \sum_{\langle\langle ij\rangle\rangle} \mathbf{S}_i\cdot\mathbf{S}_j + J_\chi \sum_{ijk\in\triangle} \mathbf{S}_i\cdot(\mathbf{S}_j\times\mathbf{S}_k) \tag{10}$$

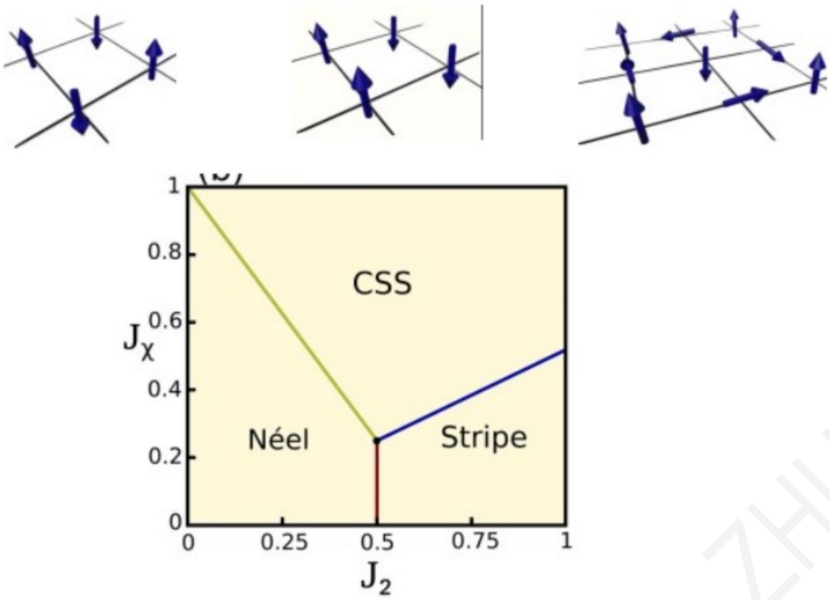

FIG. 1: The phase diagram for the heisenberg model on the square lattice.

where $\langle\rangle$ refers to the nearest-neighbor sites, and $i, j, k \in \triangle$ referes to the three neighboring sites of the smalles triangle taken clockwise. $J_1 = 1$ as the energy limit.

For the neel (π, π) phase, the energy is

$$E_{neel} = -2N \times J_1 + 2N \times J_2 \tag{11}$$

For the stripe phase,

$$E_{stripe} = -2N \times J_2 \tag{12}$$

For the non-coplane chiral spin state phase

$$E_{css} = -4N/4 \times J_2 - 8N/4 \times J_\chi \tag{13}$$

By comparing the energy, we map out a classical phase diagram as shown here.

In summary, there are three types of magnetic order: co-linear, co-plane and non-coplane. They can be realized in different lattice through interactions.

SPIN-WAVE THEORY

In cases where the Neel state is a reasonable starting point, we may try to improve upon it by considering spin wave corrections, i.e. allowing "quantum fluctuations". To discuss this idea, we take the case of large S (for which the fractional difference between Neel and singlet bonds is even smaller, 1/S).

Ferromagnetism

We can introduce the Holstein-Primakoff transformation

$$S^+ = \sqrt{2S - a^+ a}\; a \tag{14}$$

$$S^- = a^+\; \sqrt{2S - a^+ a} \tag{15}$$

$$S^z = (S - a^+ a) \tag{16}$$

where a, a^+ is bosonic operator

$$[a, a^+] = 1, [a, a] = [a^+, a^+] = 0 \tag{17}$$

We can prove this transformation keep the original commutation relation

$$\begin{aligned}[S^+, S^-] &= \sqrt{2S - a^+ a} a a^+ \sqrt{2S - a^+ a} - a^+(2S - a^+ a) a \\ &= (a^+ a + 1)(2S - a^+ a) - a^+ a(2S - a^+ a) - a^+ a = 2(S - a^+ a) = 2S^z\end{aligned} \tag{18}$$

By inserting the HP transformation into the hamiiltonian,

$$\begin{aligned}H &= -J \sum_{i,j} (S - a_i^+ a_i)(S - a_j^+ a_j) + \frac{1}{2} \sqrt{2S - a_i^+ a_i} a_i a_j^+ \sqrt{2S - a_j^+ a_j} \\ &+ \frac{1}{2} a_j^+ \sqrt{2S - a_j^+ a_j} \sqrt{2S - a_i^+ a_i} a_i \\ &\approx -NJzS^2 + 2ZJS \sum_i a_i^+ a_i - JS \sum_{i,j} (a_i^+ a_j + a_j^+ a_i)\end{aligned} \tag{19}$$

The first is the ground state energy, while the second term is the spin excitation energy. Let us make the Fourier transformation

$$a_k = \frac{1}{\sqrt{N}} \sum_i e^{-ikr_i} a_i \tag{20}$$

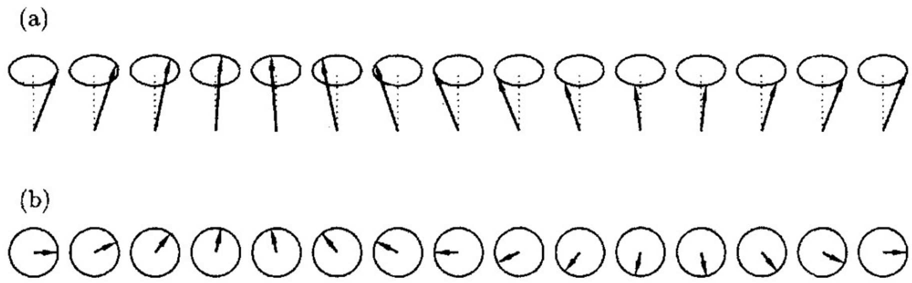

FIG. 2: The spin wave configuration: (Top panel) the side view and (Bottom panel) the top view.

The hamiltonian becomes

$$H = E_0 + \sum_k \omega_k a_k^+ a_k \tag{21}$$

where $\omega_k = 2ZJS(1 - \sum_\delta e^{ik\delta})$ is the magnon energy.

For the sc lattice,

$$\omega_k = 2ZJS(1 - \cos(k\delta)) \approx JSk^2\delta^2 \tag{22}$$

There is a simple idea to understand the spin wave. We consider the ground state of the system, $|0>$, which consists of all the spins lying along the +z direction. Now to create an excitation, flip a spin at site j. This excitation therefore has integer spin and is a boson. If we apply the Hamiltonian to this new state, we get

$$H|j>= 2[(-NS^2J + 2SJ)|j> -SJ|j+1> -SJ|j-1>] \tag{23}$$

which is not a constant multiplied by $|j>$, so this state is not an eigenstate of the Hamiltonian. Nevertheless, we can diagonalize the Hamiltonian by looking for plane wave solutions of the form

$$|k>= \frac{1}{\sqrt{N}} \sum_j e^{ikR_j} |j> \tag{24}$$

The state $|k>$ is essentially a flipped spin delocalized (smeared out) across all the sites. And the eigenenergy is

$$E(k) = 4JS(1 - \cos(ka)) \tag{25}$$

If we work at very low temperatures we may be able to estimate the magnetization using the free boson approximation, if the density of these (thermally excited) bosons is low so that their interactions have negligible effects. Calling the magnetization $M = S = N/2$ for the ground state, we have

$$M = N/2 - \sum_k a_k^+ a_k \approx N/2 - \frac{V}{(2\pi)^d} \int d^d k \frac{1}{e^{\beta A k^2} - 1} \tag{26}$$

For $d \leq 2$ there is an infrared divergence in the integral signaling the fact that the magnetization is destroyed at any non-zero temperature, and the rotation symmetry is restored. Thus $d = 2$ is the so-called "lower critical dimension" for the Heisenberg ferromagnet. In statistical mechanics, this is called Hohenberg-Mermin-Wagner theorem. We will discuss it in detail later.

In $d = 3$,

$$M = \frac{N}{2}(1 - (T/T_0)^{3/2}) \tag{27}$$

where $T_0 \sim J/k_B$. This result tells us that thermal fluctuations do not immediately destroy the magnetization in $d = 3$, but rather do so gradually with a characteristic 3/2 power law as the temperature is raised.

Anti-ferromagnet

We also assume the lattice is bipartite, so that we can divide sites into class A and B such that the nearest neighbour of an A site is always of type B. We will then use a Holstein-Primakoff representation of spins to allow us to parameterise small fluctuations about the N´eel state, i.e.

$$\begin{aligned} i \in A, S_i^z = S - a_i^+ a_i, S_i^+ = \sqrt{2S - a_i^+ a_i} a_i \\ i \in B, S_i^z = b_i^+ b_i - S, S_i^+ = b_i^+ \sqrt{2S - b_i^+ b_i} \end{aligned} \tag{28}$$

It can be shown that these definitions satisfy the spin commutation relations, and the Neel state corresponds to the vacuum state, i.e. no population of the modes a^+, b^+. Quantum fluctuations describe the occupations of these modes in the ground state; thermal fluctuations to the additional occupation at finite temperature. If we assume the occupation of fluctuations is small, $a^+ a, b^+ b \ll S$, then we may neglect the terms in the square root, and neglect any products of operators higher than second order, and thus write:

$$H = J \sum_{ij} [-S + S(a_i^+ a_i + b_j^+ b_j + S(a_i^+ b_j^+ + a_i b_j))] \tag{29}$$

At quadratic level, it is straightforward to transform this expression into a ground state energy plus a cost of occupying excitations by making a Bogoliubov transform. We will outline this, and show how this procedure shows that the lowest energy state does not correspond to no bosons, but to a finite occupation, and thus the ground state energy is less than the N´eel estimate. To perform this transformation there are two steps: Fourier transformation to see that the Hamiltonian is diagonal in momentum space (whereas it is off-diagonal in site index), and Bogoliubov transformation to find superpositions of particle and hole operators.

$$H = 2ZJS\sum_k a_k^+ a_k + b_k^+ b_k + 2ZJS\sum_k \gamma_k (a_k^+ b_k^+ + a_k b_k) \tag{30}$$

$$= JS\sum_k \begin{pmatrix} a_k^+ & b_{-k} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ b_{-k}^+ \end{pmatrix} \tag{31}$$

$$= JS\sum_k \begin{pmatrix} \alpha_k^+ & \beta_{-k} \end{pmatrix} \begin{pmatrix} \sqrt{1-\gamma_k^2} & 0 \\ 0 & \sqrt{1-\gamma_k^2} \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_{-k}^+ \end{pmatrix} \tag{32}$$

$$= JS\sum_k \sqrt{1-\gamma_k^2}(\alpha_k^+ \alpha_k + \beta_k^+ \beta_k) + \sqrt{1-\gamma_k^2} \tag{33}$$

For the long-wave limit ($ka \ll 1$), the dispersion of sc lattice gives

$$E_k \approx JS|k| \tag{34}$$

So the spin wave is linear in k for anti-ferromagnet.

GOLDSTONE MODE

Spin wave is important collective excitations, which can be viewed as Goldstone bosons associated with the broken symmetry. Here we shall prove the lattice version of Goldstone's theorem for the Heisenberg model.

The essence of Goldstone's theorem is that for a Hamiltonian with short-ranged interactions, spontaneously broken continuous symmetry implies the existence of low-energy excitations called Goldstone modes. If the ground state has momentum $\boldsymbol{q}_0$, the energy of the Goldstone mode vanishes as $\boldsymbol{q} \to \boldsymbol{q}_0$. (e.g. On the square lattice, for FM $\boldsymbol{q}_0 = (0, 0)$;

for AFM $\boldsymbol{q}_0 = (\pi, \pi)$.) In the condensed matter physics, Goldstone modes appear in many systems: spin waves in $O(N)$ Heisenberg models, sound mode in the superfluid.

We consider the short-range Heisenberg model

$$H = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{35}$$

Its spin (static) structure factor is

$$S(\mathbf{q}) = \frac{1}{N} \sum_{i,j} \langle \mathbf{S}(\mathbf{r}_i) \cdot \mathbf{S}(\mathbf{r}_j) \rangle e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \tag{36}$$

For magnetic order, structure factor diverges at typical momentum $\mathbf{q}_0$.

Goldstone's theorem If the spin correlation diverges at some wave vector $\boldsymbol{q}_0$: $\lim_{\mathbf{q}\to\mathbf{q}_0} S(\mathbf{q}) \to \infty$, then there exists a Goldstone mode labelled by the momentum $\mathbf{q}$, whole energy $E(\boldsymbol{q})$ vanishes at $\boldsymbol{q}_0$:

$$\lim_{\boldsymbol{q}\to\boldsymbol{q}_0} E(\boldsymbol{q}) = 0 \tag{37}$$

Proof. Let us recall the single-mode approximation as studied in the superfluidity, the energy gap of low-energy excitation is

$$\Delta_k = E_k - E_0 = \frac{\langle \Psi_k | H - E_0 | \Psi_k \rangle}{\langle \Psi_k | \Psi_k \rangle} \equiv \frac{f(k)}{S(k)} \tag{38}$$

where $S(k)$ is the structure factor. Here $f(\boldsymbol{k})$ is a double commutator function

$$f(\mathbf{k}) \equiv N^{-1} \langle [S^x_{-\boldsymbol{k}}, [H, S^x_{\boldsymbol{k}}]] \rangle \tag{39}$$

which has explicit upper bound since

$$\begin{aligned} f(\mathbf{k}) &= iN^{-1} \sum_{ijl} e^{i\mathbf{k}\cdot(\mathbf{x}_l - \boldsymbol{x}_i)} J_{jl} \langle [S^x_i, (S^z_j S^y_l - S^y_j S^z_l)] \rangle \\ &= N^{-1} \sum_{jl} J_{jl} [\cos(\mathbf{k} \cdot (\mathbf{x}_j - \boldsymbol{x}_l)) - 1] \langle S^y_j S^y_l + S^z_j S^z_l \rangle \\ &\leq \frac{k^2}{2N} \sum_{jl} |J_{jl}| |\mathbf{x}_j - \boldsymbol{x}_l|^2 |\langle S^y_j S^y_l + S^z_j S^z_l \rangle| \\ &\leq \overline{J} k^2 S(S+1) \end{aligned} \tag{40}$$

where we define $\overline{J} = \frac{1}{2N} \sum_{jl} |J_{jl}| |\mathbf{x}_j - \boldsymbol{x}_l|^2 < \infty$ which should satisfy the locality condition and $|\langle S^y_j S^y_l + S^z_j S^z_l \rangle| \leq |\langle \boldsymbol{S} \cdot \boldsymbol{S}_l \rangle| \leq S(S+1)$.

Thus, we get

$$\Delta_k = \frac{f(k)}{S(k)} \leq \frac{\overline{J}k^2 S(S+1)}{S(k)} \to 0, (\boldsymbol{k} \to \boldsymbol{k}_0) \tag{41}$$

If the ground state has broken continuous symmetry, there exist Goldstone modes. This follows directly from $S(\mathbf{k}_0) \to \infty$. However, please note that the inverse statement is not true, i.e. existence of gapless excitations doesnot imply true long-range order or symmetry broken. Notable counterexamples are $S = 1/2$ Heisenberg antiferromagnet in one-dimension which is a quantum spin liquid.

In symmetry-breaking phases, the low-energy degrees of freedom are often those giving rise to the order parameter. This is particularly true when a continuous symmetry is broken spontaneously, as guaranteed by the Goldstone theorem, which states that there is a gapless collective mode (known as a “Goldstone mode”) associated with each spontaneously broken continuous symmetry. The gapless mode is nothing but the long-wavelength fluctuation of the order parameter.

XY MODEL

Let us consider the XY (or rotator) model with periodic boundary conditions. (Actually, this is a preparation for future study. We will come back to this model again in future.) We include an external field in the x direction:

$$H = -\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j - \sum_j \vec{h} \cdot \vec{S}_j = -\sum_{\langle i,j\rangle} \cos(\theta_i - \theta_j) - h \sum_j \cos\theta_j \tag{42}$$

where $\vec{S}_i = (\cos\theta_i, \sin\theta_i)$ lays down in the xy plane. Let N denote the number of sites in the rectangle and define

$$m = \frac{1}{N} \sum_j \langle \cos\theta_j \rangle \tag{43}$$

There are two ways to calculate it. One is to prove it using a phenomenogical method, and the other one is a direct calculation. We will derive the Mermin-Wegner theorem :

$$\lim_{h \to 0} m = 0 \tag{44}$$

which states that long-ranged magnetic order only survives at the finite temperature in $d > 2$ but is unstable in $d \leq 2$.

Operator method based on Cauchy-Schwarz inequality

In the first method, we define two quantity:

$$A = \sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j} \sin\theta_j \tag{45}$$

$$B = -\sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j} \frac{\partial H}{\partial \theta_j} \tag{46}$$

Here $\mathbf{k}$ is summed of the appropriate set of momenta. For simplicity, we take a square lattice, $\mathbf{k} = (k_1, k_2)$ with $k_i = 2\pi l_i / L$ where $l_i = 0, 1, 2, ..., L-1$.

The proof will rely on the Cauchy Schwarz inequality

$$\langle \overline{A} B\rangle^2 \leq \langle \overline{A} A\rangle \langle \overline{B} B\rangle \tag{47}$$

$$0 \leq (|v|u - |u|v)\cdot(|v|u - |u|v) = |u|^2 v\cdot v + |v|^2 u\cdot u - 2|u||v|u\cdot v \tag{48}$$

$$\Rightarrow 2|u||v|u\cdot v \leq 2|u|^2|v|^2$$

$$\Rightarrow u\cdot v \leq |u||v| \tag{49}$$

Next we calculate the different terms one by one. We need one trick as

$$e^{-\beta H}\frac{\partial H}{\partial \theta_l} = -\frac{1}{\beta}\frac{\partial}{\partial \theta_l} e^{-\beta H} \tag{50}$$

$$\begin{aligned}
\langle \overline{A} B\rangle &= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_l)} \langle \sin\theta_j \frac{\partial H}{\partial \theta_l}\rangle \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_l)} \frac{1}{Z}\int d\theta e^{-\beta H}\sin\theta_j \frac{\partial H}{\partial \theta_l} \\
&= \sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_l)} \frac{1}{Z\beta}\int d\theta \sin\theta_j \frac{\partial e^{-\beta H}}{\partial \theta_l} \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_l)} \frac{1}{Z\beta}\int d\theta e^{-\beta H} \frac{\partial}{\partial \theta_l}\sin\theta_j \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_l)} \frac{1}{\beta}\delta_{j,l}\langle\cos\theta_j\rangle = -\frac{Nm}{\beta}
\end{aligned} \tag{51}$$

For another term,

$$
\begin{aligned}
\langle \overline{B}B\rangle &= \sum_{j,l} e^{\mathbf{ik}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\langle\frac{\partial H}{\partial\theta_j}\frac{\partial H}{\partial\theta_l}\rangle \\
&= \sum_{j,l} e^{\mathbf{ik}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta e^{-\beta H}\frac{\partial H}{\partial\theta_j}\frac{\partial H}{\partial\theta_l} \\
&= -\sum_{j,l} e^{\mathbf{ik}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta\frac{\partial H}{\partial\theta_j}\frac{\partial e^{-\beta H}}{\partial\theta_l} \\
&= \sum_{j,l} e^{\mathbf{ik}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta\frac{\partial}{\partial\theta_j}\frac{\partial}{\partial\theta_l}e^{-\beta H}
\end{aligned}
\tag{52}
$$

Since

$$
\frac{\partial H}{\partial\theta_j} = \sum_{|m-j|=1}\sin(\theta_j-\theta_m)+h\sin\theta_l \tag{53}
$$

$$
\frac{\partial^2 H}{\partial\theta_j\partial\theta_l} = \delta_{j,l}\sum_{|m-l|=1}\cos(\theta_l-\theta_m)-\delta_{|j-l|=1}\cos(\theta_l-\theta_j)+\delta_{j,l}h\cos\theta_l \tag{54}
$$

we have

$$
\begin{aligned}
\langle \overline{B}B\rangle &= \frac{1}{\beta}[\sum_l\sum_{|m-l|=1}\langle\cos(\theta_l-\theta_m)\rangle-\sum_{j,l,|j-l|=1}e^{ik(j-l)}\langle\cos(\theta_j-\theta_l)\rangle+h\sum_l\langle\cos\theta_l\rangle] \\
&= \frac{1}{\beta}\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)})\langle\cos(\theta_j-\theta_l)\rangle+hNm/\beta
\end{aligned}
\tag{55}
$$

The last one

$$
\begin{aligned}
\langle \overline{A}A\rangle &= \sum_{j,l}e^{ik(j-l)}\langle\sin\theta_j\sin\theta_l\rangle \\
&\Rightarrow \sum_k\langle\overline{A}A\rangle = N\sum_l\langle\sin^2\theta_j\rangle \le N^2
\end{aligned}
\tag{56}
$$

Then we can write the Cauthy inequality as

$$
\begin{aligned}
&\langle\overline{A}A\rangle \ge \frac{\langle\overline{A}B\rangle^2}{\langle\overline{B}B\rangle} \\
&N^2 \ge \sum_k\frac{\langle\overline{A}B\rangle^2}{\langle\overline{B}B\rangle} \\
&= \frac{1}{\beta}\sum_k\frac{N^2m^2}{\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)})\langle\cos(\theta_j-\theta_l)\rangle+hNm} \\
&(\langle\cos(\theta_j-\theta_l)\rangle\le 1)\Rightarrow 1\ge\frac{1}{\beta}\sum_k\frac{m^2}{\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)})+hNm}
\end{aligned}
\tag{57}
$$

Then we use the condition $1-\cos x \leq x^2/2$, we have

$$\begin{aligned} \sum_{j,l,|j-l|=1} (1-e^{ik(j-l)}) &\leq Nk^2 \\ \Rightarrow 1 &\geq \frac{1}{\beta}\int d^2k \frac{m^2}{ck^2+hm} \end{aligned} \tag{58}$$

At last we take the zero field limit,

$$1 \geq \frac{1}{\beta}\int d^2k \frac{m^2}{ck^2} \tag{59}$$

Since $\int d^2k\frac{1}{k^2} = \infty$, this implies that

- $T=0, m\neq 0$: The magnetic order is possible only at zero temperature;
- $T\neq 0, m=0$: At finite temperature, the magnetic order should be zero.

Another point is interesting, the integral $\int d^dk\frac{1}{k^2}$ is divergent when $d\leq 2$, but it is regular $d>2$. So, in three dimension, the order at finite temperature is possible.

Low-temperature expansion

The second method to calculate the magnetization is shown below.

In a low-temperature expansion, the angle difference between two spins will be small: $|\theta_i-\theta_j| \ll 2\pi$. In this small fluctuation regime, we can approximate the cosine term in the hamiltonian to extract the long-range behavior.

$$\begin{aligned} H &= -J\sum_{<i,j>}\cos(\theta_i-\theta_j) \\ &= -JN + \frac{J}{2}\sum_{<i,j>}(\theta_i-\theta_j)^2 \\ &= E_0 + \frac{J}{4}\sum_{\mathbf{r},\mathbf{a}}(\theta(\mathbf{r}+\mathbf{a})-\theta(\mathbf{r}))^2 \\ &\simeq E_0 + \frac{J}{2}\int d^2r(\nabla\theta(\mathbf{r}))^2 \ . \end{aligned} \tag{60}$$

In the last line, we have taken the continuum limit, and replaced the field θ_i by a continuous one, $\theta(\mathbf{r})$, as slowly varying function of $\mathbf{r}$. From this, we can extract a lot of information about the magnetization and correlation functions.

Average magnetization

We calculate the average magnetization in the x direction for the 2D XY model (y is identical). We have:

$$\langle S_x \rangle =< \cos\theta(\mathbf{r}) >=< \cos\theta(0) > \tag{61}$$
$$= \frac{Tr_{\{\theta_i\}} \cos\theta(0) e^{-\beta H}}{Tr_{\{\theta_i\}} e^{-\beta H}} \tag{62}$$
$$= Re\left(\frac{1}{\mathcal{Z}} \int \mathcal{D}[\theta_i] e^{-\beta H + i\theta(0)}\right) \tag{63}$$

where $\mathcal{Z}$ is the partition function $Tr_{\{\theta_i\}} e^{-\beta H}$, and in the first line, we took advantage of translation invariance to set the spin at site $\mathbf{r} = 0$. In order to calculate that expression, we Fourier transform the θ variable, with periodic boundary conditions. We then have

$$\theta(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \theta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{64}$$
$$\theta(\mathbf{r} = 0) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \theta_{\mathbf{k}} \tag{65}$$

This leads to, after Gaussian integral:

$$< S_x >= \exp\left(-\frac{T}{2J} I_d(L)\right), \tag{66}$$

with $I_d(L)$ a geometric factor written as (by setting a momentum UV cut-off $\Lambda \sim \pi/a$)

$$I_d(L) = S_d \int_{\pi/L}^{\pi/a} dk k^{d-3} = \begin{cases} L^{2-d}, d < 2 \\ \ln\left(\frac{L}{a}\right), d = 2 \\ \frac{1}{d-2}\left(\frac{\pi}{a}\right)^{d-2}, d > 2 \end{cases} \tag{67}$$

Therefore,

$$\lim_{L\to\infty} \langle S_x \rangle = \begin{cases} 0, d \leq 2 \\ \exp(-\frac{S_d}{2Ja^{2-d}} AT), d > 2 \end{cases} \tag{68}$$

Then, for any $T \neq 0$ and $d = 2$, the logarithmic divergence of this geometric factor will force $< S_x >= 0$. This is directly the statement of the Mermin-Wagner theorem. Hence there can be no ordered low-temperature phase (in the conventional long-range order) in the 2D XY model.

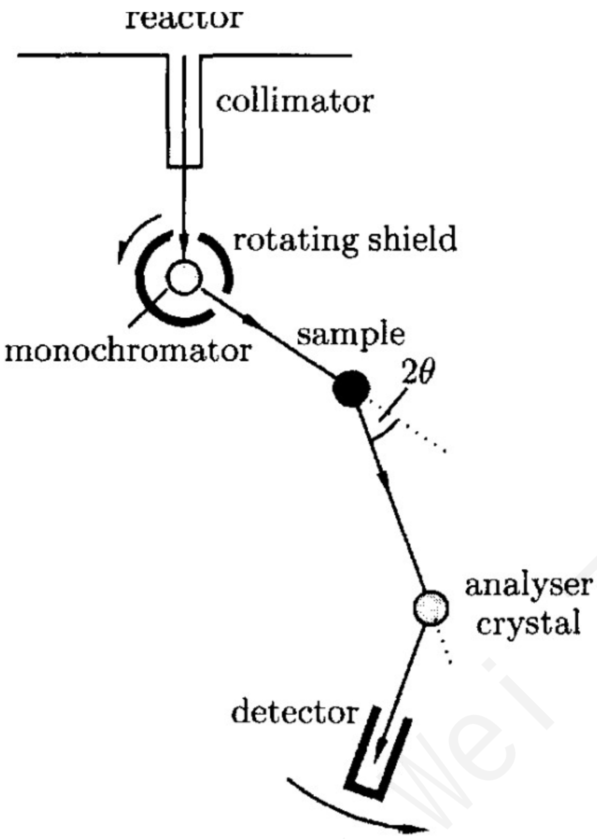

FIG. 3: The spin wave configuration.

EXPERIMENTAL TECHNIQUES

Neutron scattering

Spin wave dispersions can be measured using a technique known as inelastic neutron scattering, because neutron is charge neutral but spin is one. The magnitude of the incident neutron wave vector k is now no longer equal to the magnitude of the scattered neutron wave vector k'. The energy of the neutron also changes from E to E'.

This is because the neutron has produced in the sample an excitation of energy $\hbar\omega$ and wave vector q. Conservation of energy and momentum implies that

$$E = E' + \omega, k = k' + q + G \tag{69}$$

so that a measurement of k, k', E and E' allows a determination of ω and q. Neutrons have energies similar to the energies of atomic and electronic processes, i.e. in the meV to eV range. magnon energies are typically in the range $10^{-3} - 10^{-2}$ eV and therefore can be effectively measured using inelastic neutron scattering.

Nuclear magnetic resonance

The local environment of a magnetic moment can be studied by using a variety of experimental techniques which involve magnetic resonance.

The most commonly used form of magnetic resonance is nuclear magnetic resonance (NMR). This technique is greatly employed in medical imaging, where it goes by the name of magnetic resonance imaging (MRI) to avoid the use of the dreaded word "nuclear". Some people may be devastated to discover that the average human body contains over 10^{27} nuclei; by mass we are 99.98% nuclear! MRI measures NMR in the protons in a patient's body and provides a safe, non-invasive technique of yielding detailed cross-sectional images.

To perform any NMR experiment, one needs a nucleus with a non-zero spin. Nuclei which are commonly studied include 1H (proton), 2H (deuteron) and 13C. In a simple NMR experiment, a sample is placed inside a coil which is mounted between the pole pieces of a magnet. The magnet produces a magnetic field B along a particular direction, say the z-direction. We have already seen that the quantity m_z, the z component of the angular momentum of the nucleus, can only take integral values between $-I$ and I.

The energy E of the nucleus is the energy of a magnetic moment in the magnetic field B_z,

$$E = -g_N \mu_N m_I B_z \tag{70}$$

Exciting transitions between adjacent pairs of levels with a radiofrequency (RF) field is the basis of nuclear magnetic resonance. The RF field B_x is applied in the x-direction, and leads to a perturbation of the system which is proportional to B_x. The matrix element of the perturbation is proportional to $\langle m_j' | B_x I_x | m_j \rangle$ and is zero unless $m_j' = m_j \pm 1$. The allowed transitions are therefore described by the selection rule $\Delta m_j = \pm 1$.

There are two ways to perform the experiment: you could keep the frequency of the RF field constant and vary the magnetic field or you could keep the magnetic field constant and vary the frequency of the RF field. It is usually the former which is performed. A crucial factor is to have a highly homogeneous magnet to produce the constant field B0. If this is not the case, different parts of the sample will sit in slightly different magnetic fields and will come into resonance at slightly different points of the magnetic field sweep, causing the measured resonance to be extremely broad, maybe so much that it is washed out altogether.

In order to understand the transitions which we are inducing in a little more detail, let us consider how a two-level spin system (I =1/2)will absorb energy from the RF coil. We will label the lower level $-$ and the upper level $+$. Hence the probability per unit time of these so-called stimulated transitions between levels + and —is independent of the direction of the transition and occurs at a rate W which is proportional to the size of the RF power used to excite transitions. At time t, if there are $N_-(t)$ spins in the lower level. $WN_-(t)$ will be excited per unit time into the upper level. If there are $N_+(t)$ spins in the upper level, $WN_+(t)$ will be excited per unit time into the lower level. Thus

$$\begin{aligned} \frac{dN_+(t)}{dt} &= WN_-(t) - WN_+(t) \\ \frac{dN_-(t)}{dt} &= WN_+(t) - WN_-(t) \end{aligned} \tag{71}$$

which gives

$$\begin{aligned} \frac{dN_+(t) - N_-(t)}{dt} &= -2W(N_+(t) - N_-(t)) \\ N_+(t) - N_-(t) &= (N_+(0) - N_-(0))e^{-2Wt} \end{aligned} \tag{72}$$

An initial difference in population tends exponentially to zero when driven by a stimulated electromagnetic transition.

HOMEWORK

1. Please repeat the classical phase diagram in Fig. 1a of the following paper: Quantum Phase Diagram of the Triangular-Lattice XXZ Model in a Magnetic Field, Daisuke Yamamoto, Giacomo Marmorini, and Ippei Danshita, Phys. Rev. Lett. 112, 127203 (2014). 10.1103/PhysRevLett.112.127203