## Magnons of ferromgnetism Masatsugu Sei Suzuki Department of Physics, SUNY at Binghamton (Date: April 21, 2012)

A magnon is quantized spin wave. We find the magnon dispersion relation of  $\omega$  vs k.



#### 1. Magnon

The ground state of a simple ferromagnet has all spins parallel. Consider N spins each of magnitude S on a line or a ring, with nearest neighbor spins coupled by the Heisenberg interaction,

$$H = -2J\sum_{p=1}^{N} \mathbf{S}_{p} \cdot \mathbf{S}_{p+1}$$

where J is the exchange integral, and  $\hbar S_p$  is the angular momentum of the spin at the point p. If we treat  $S_p$  as a classical vector, then in the ground state,

$$\mathbf{S}_{p} \cdot \mathbf{S}_{p+1} = S^{2}$$

and the exchange energy of the system is

$$E_0 = -2NJS^2$$

What is the energy of the first excited state? We consider an excited state with one particular spin reversed.



$$E_1 = -2(N-2)JS^2 + 2 \cdot 2JS^2 = -2NJS^2 + 8JS^2$$

We can form an excitation of much lower energy if we let all the spins share the reversal. The elementary excitations of a spin system have a wave-like form, and called magnons.

### 2. Derivation of the magnon dispersion relation

The term in *H* which involve the *p*-th spin are

$$-2J\mathbf{S}_{p}\cdot(\mathbf{S}_{p-1}+\mathbf{S}_{p+1}),$$

The magnetic moment at the site p is

$$\boldsymbol{\mu}_p = -g\boldsymbol{\mu}_B \mathbf{S}_p \,.$$

Then we get

$$-2J\left(\frac{\boldsymbol{\mu}_p}{-g\,\boldsymbol{\mu}_B}\right)\cdot(\boldsymbol{S}_{p-1}+\boldsymbol{S}_{p+1})=-\boldsymbol{\mu}_p\cdot\boldsymbol{B}_p$$

where the effective magnetic field that acts on the *p*-th spin is

$$\boldsymbol{B}_{p} = -\frac{2J}{g\mu_{B}}(\boldsymbol{S}_{p-1} + \boldsymbol{S}_{p+1})$$

We know that

$$\frac{d(\hbar \boldsymbol{S}_p)}{dt} = \boldsymbol{\tau}_p = \boldsymbol{\mu}_p \times \boldsymbol{B}_p$$

$$\frac{d\boldsymbol{S}_{p}}{dt} = -\frac{g\mu_{B}}{\hbar}\boldsymbol{S}_{p} \times (-\frac{2J}{g\mu_{B}})(\boldsymbol{S}_{p-1} + \boldsymbol{S}_{p+1})$$
$$= \frac{2J}{\hbar}(\boldsymbol{S}_{p} \times \boldsymbol{S}_{p-1} + \boldsymbol{S}_{p} \times \boldsymbol{S}_{p+1})$$

In Cartesian components

$$\frac{dS_p^{x}}{dt} = \frac{2J}{\hbar} [S_p^{y} (S_{p-1}^{z} + S_{p+1}^{z}) - S_p^{z} (S_{p-1}^{y} + S_{p+1}^{y})]$$
$$\frac{dS_p^{y}}{dt} = \frac{2J}{\hbar} [S_p^{z} (S_{p-1}^{x} + S_{p+1}^{x}) - S_p^{x} (S_{p-1}^{z} + S_{p+1}^{z})]$$
$$\frac{dS_p^{z}}{dt} = \frac{2J}{\hbar} [S_p^{x} (S_{p-1}^{y} + S_{p+1}^{y}) - S_p^{y} (S_{p-1}^{x} + S_{p+1}^{x})]$$

If the amplitude of the excitation is small ( $|S_p^x| \ll S$ ,  $|S_p^y| \ll S$ ). We may obtain an approximate set of linear equations by taking all  $S_p^z = S$  and by neglecting terms in the product of  $S_x$  and  $S_y$  in  $\frac{d\mathbf{S}_p}{dt}$ ,

$$\frac{dS_{p}^{x}}{dt} = \frac{2JS}{\hbar} (2S_{p}^{y} - S_{p-1}^{y} - S_{p+1}^{y})$$
$$\frac{dS_{p}^{y}}{dt} = -\frac{2JS}{\hbar} (2S_{p}^{x} - S_{p-1}^{x} - S_{p+1}^{x})$$
$$\frac{dS_{p}^{z}}{dt} = 0$$

We look for travelling wave solutions of the above equations of the form.

$$S_p^x = \operatorname{Re}[u \exp[i(pka - \omega t)], \qquad S_p^y = \operatorname{Re}[v \exp[i(pka - \omega t)]]$$

or

where u and v are complex numbers, p is an integer, and a is the lattice constant. Then we get

$$-i\omega u = \frac{2JS}{\hbar}(2 - e^{-ika} - e^{-ika})v = \frac{4JS}{\hbar}[1 - \cos(ka)]v$$
$$-i\omega v = -\frac{2JS}{\hbar}(2 - e^{-ika} - e^{-ika})u = -\frac{4JS}{\hbar}[1 - \cos(ka)]u$$

These equations have a solution for u and v if the determinant of the coefficients is equal to zero.

$$\begin{vmatrix} i\omega & \frac{4JS}{\hbar} [1 - \cos(ka)] \\ -\frac{4JS}{\hbar} [1 - \cos(ka)] & i\omega \end{vmatrix} = 0$$

or

$$\hbar\omega = 4JS[(1 - \cos(ka))]$$

With this solution we find that

$$v = -iu$$

where u is assumed to be real. Then we have

$$S_p^{x} = \operatorname{Re}[u \exp[i(pka - \omega t)]]$$
  
=  $u \cos(pka - \omega t)$ ,  
$$S_p^{y} = \operatorname{Re}[ue^{-i\frac{\pi}{2}} \exp[i(pka - \omega t)]]$$
  
=  $u \sin(pka - \omega t)$ 

Circular precession:



## 3. Periodic boundary condition

The spin wave has the travelling wave form,

$$\psi = \exp[i(kx - \omega_k t)]$$

We assume the periodic boundary condition,

$$\psi(0) = \psi(L)$$

where L = Na and a is the lattice constant. Then we have

$$k = \frac{2\pi}{L}n$$

with  $n = 0, 1, 2, 3, \dots, N/2$  (the first Brillouin zone).

# 4. Magnon dispersion relation

$$\hbar\omega_k = 4JS[(1 - \cos(ka))]$$

For *ka*<<1,

$$\hbar\omega_k = 8JS\sin^2\frac{ka}{2} \approx 2JSa^2k^2.$$

The frequency is proportional to  $k^2$ .

((Note))

We note that the dispersion relation for a ferromagnetic cubic lattice with nearest-neighbor interactions,

$$\hbar\omega_{\mathbf{k}} = 2S[J(0) - J(\mathbf{k})]$$

with

$$J(\mathbf{k}) = \sum_{j} J_{ij} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}$$

where the summation is over the  $\delta$  vectors denoted by  $\delta$  which join the central atom to its nearest neighbors.

### 5. Quantization of spin waves

#### Holstein-Primakoff

The *z*-component of  $S_j$  at the *j*-th takes the values

$$S_j^z = S - n_j$$

where  $n_j = 0, 1, 2, ..., 2S$  (total number: 2*S*+1). Let  $|n_j\rangle$  be the eigen state of  $n_j$  with  $S_j^z = S - n_j$ . Note that  $n_j$  is the spin deviation operator. Here we introduce the operators  $a_j$  and  $a_j^*$ .

$$a_{j} | n_{j} \rangle = \sqrt{n_{j}} | n_{j} - 1 \rangle$$
$$a_{j}^{*} | n_{j} \rangle = \sqrt{n_{j} + 1} | n_{j} + 1 \rangle$$

 $a_j$  is the annihilation operator and  $a_j^*$  is the creation operator. The commutation relation is valid,

$$[a_{j}, a_{j}^{*}] = 1$$

and

$$a_j^*a_j|n_j\rangle = \sqrt{n_j}a_j^*|n_j-1\rangle = n_j|n_j\rangle.$$

Spin operators satisfy the following relations,

$$\left(S_{j}^{x}+iS_{j}^{y}\right)n_{j}\rangle = \sqrt{(S-M)(S+M+1)}\left|n_{j}-1\rangle$$
$$\left(S_{j}^{x}-iS_{j}^{y}\right)n_{j}\rangle = \sqrt{(S+M)(S-M+1)}\left|n_{j}+1\rangle$$

with

$$M = S - n_j.$$

Then we have the Holstein-Primakoff transformation,

$$S_{j}^{+} = S_{j}^{x} + iS_{j}^{y} = \sqrt{2S} \left(1 - \frac{a_{j}^{*}a_{j}}{2S}\right)^{1/2} a_{j}$$
$$S_{j}^{-} = S_{j}^{x} - iS_{j}^{y} = \sqrt{2S} a_{j}^{*} \left(1 - \frac{a_{j}^{*}a_{j}}{2S}\right)^{1/2}.$$

 $S_j^+$  and  $S_j^-$  can be approximated as follows ( $\frac{\langle a_j^* a_j \rangle}{S} \ll 1$ ).

$$S_{j}^{+} = \sqrt{2S} (1 - \frac{a_{j}^{*} a_{j}}{4S} + ...) a_{j}^{*}$$

$$S_{j}^{-} = \sqrt{2S}a_{j}^{*}(1 - \frac{a_{j}a_{j}}{4S} + ...)$$

The Hamiltonian H is described as

$$H = -2\sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = -2\sum_{\langle i,j \rangle} J_{ij} [S_i^{z} S_j^{z} + \frac{1}{2} (S_i^{-} S_j^{+} + S_i^{+} S_j^{-})],$$

Here we note

$$S_{j}^{z}S_{j}^{z} = (S - n_{i})(S - n_{j}) = S^{2} - (n_{i} + n_{j})S + n_{i}n_{j},$$

$$S_i^{-}S_j^{+} = 2S(a_i^{*} - \frac{a_i^{*}a_i^{*}a_i}{4S} + \dots)(a_j - \frac{a_j^{*}a_ja_j}{4S} + \dots)$$
$$= 2Sa_i^{*}a_j - \frac{1}{2}a_i^{*}a_j^{*}a_ja_j - \frac{1}{2}a_i^{*}a_i^{*}a_ia_j + \dots$$

$$S_{i}^{+}S_{j}^{-} = 2S(a_{i} - \frac{a_{i}^{*}a_{i}a_{i}}{4S} + \dots)(a_{j}^{*} - \frac{a_{j}^{*}a_{j}^{*}a_{j}}{4S} + \dots)$$
$$= 2Sa_{i}a_{j}^{*} - \frac{1}{2}a_{i}a_{j}^{*}a_{j}^{*}a_{j} - \frac{1}{2}a_{i}^{*}a_{i}a_{i}a_{j}^{*} + \dots$$

Then we get

$$H = -2\sum_{\langle i,j \rangle} J_{ij} [S^2 - (n_i + n_j)S + n_i n_j + S(a_i^* a_j + a_i a_j^*) - \frac{1}{4} (a_i^* a_j^* a_j a_j + a_i^* a_i^* a_i a_j + a_i a_j^* a_j^* a_j + a_i^* a_i a_i a_j^*) + \dots]$$

We neglect the fourth term and higher order terms such as  $a_i^* a_j^* a_j a_j$ .

$$H = -2\sum_{\langle i,j \rangle} J_{ij} [S^2 - (n_i + n_j)S + n_i n_j + S(a_i^* a_j + a_i a_j^*)]$$
  
=  $-2\sum_{\langle i,j \rangle} J_{ij} [S^2 - (n_i + n_j)S + n_i n_j + S(a_i^* a_j + a_j^* a_i)]$ 

because of  $[a_i, a_j^*] = 0$  for  $i \neq j$ . We introduce the Fourier transform  $a_q^+$  and  $a_q$ ,

$$a_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{j} a_{j} e^{i\mathbf{q}\cdot\mathbf{r}_{j}}$$
$$a_{\mathbf{q}}^{+} = \frac{1}{\sqrt{N}} \sum_{j} a_{j}^{*} e^{-i\mathbf{q}\cdot\mathbf{r}_{j}}$$

Commutation relation:

$$[a_{\mathbf{q}}, a_{\mathbf{q}}^{+}] = \frac{1}{N} \sum_{i,j} [a_{i}, a_{j}^{*}] e^{i\mathbf{q} \cdot (\mathbf{r}_{j} - \mathbf{r}_{j})} = \frac{1}{N} \sum_{i,j} \delta_{ij} e^{i\mathbf{q} \cdot (\mathbf{r}_{j} - \mathbf{r}_{j})} = 1$$

Similarly we get

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} a_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}_j}$$

We introduce

$$J(\mathbf{q}) = \sum_{j} J_{ij} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}.$$

Then the Hamiltonian can be expressed by

$$H = -2\sum_{\langle i,j \rangle} J_{ij} [S^{2} - (n_{i} + n_{j})S + n_{i}n_{j} + S(a_{i}^{*}a_{j} + a_{j}^{*}a_{i})]$$
  
=  $-2S^{2}\sum_{\langle i,j \rangle} J_{ij} + \sum_{q} 2S[J(0) - J(\mathbf{q})]a_{\mathbf{q}}^{*}a_{\mathbf{q}}$   
=  $E_{0} + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} a_{\mathbf{q}}^{*}a_{\mathbf{q}}$ 

where

$$\hbar\omega_{\mathbf{q}} = 2S[J(0) - J(\mathbf{q})]$$

is the magnon dispersion relation.

## ((Simple example))



 $J_{ij} = J$  only for the nearest- neighbor pairs.

$$J(\mathbf{q}) = \sum_{j} J_{ij} e^{i\mathbf{q}\cdot\mathbf{r}_{ij}} = J \sum_{j} e^{i\mathbf{q}\cdot\mathbf{r}_{j}} = J(e^{iqa} + e^{-iqa}) = 2J\cos(aq).$$

Then we have

$$\hbar\omega_{\mathbf{q}} = 2S[J(0) - J(\mathbf{q})] = 4JS(1 - \cos(qa)] = 2JS\sin^2(\frac{qa}{2})$$

which is the spin wave dispersion (magnon dispersion).



**Fig.** Dispersion curve of magnon.

# 6. Magnetization

The z-component of the magnetization is

$$M_{z} = g\mu_{B}\sum_{j} S_{j}^{z} = g\mu_{B}\sum_{j} (S - n_{j}) = g\mu_{B} (NS - \sum_{q} a_{q}^{*}a_{q})$$

The magnon is a boson.

$$M_{s}(0) - M_{s}(T) = \Delta M = g\mu_{B}\sum_{q} \left\langle a_{\mathbf{q}}^{*}a_{\mathbf{q}} \right\rangle = g\mu_{B}\sum_{q} \left\langle n_{\mathbf{q}} \right\rangle$$

The total number of magnons excited at a temperature T is

$$\sum_{q} \left\langle n_{\mathbf{q}} \right\rangle = \int d\omega D(\omega) < n(\omega) >$$

where  $D(\omega)$  is the number of magnon modes per unit frequency range.

$$D(\omega)d\omega = \frac{V}{(2\pi)^3} 4\pi q^2 dq = \frac{V}{(2\pi)^3} 4\pi q^2 \frac{dq}{d\omega} d\omega$$

We use the magnon dispersion relation,

$$\hbar\omega_q = \hbar\omega = 2JSa^2q^2$$
$$\frac{d\omega}{dq} = \frac{4JSa^2}{\hbar}q$$

Then the density of states is given by

$$D(\omega) = \frac{V}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \omega^{1/2}$$

The integral is taken over the allowed range of q, which is the first Brillouin zone. At T = 0 K, we may carry the integral between 0 and  $\infty$ , because  $\langle n(\omega) \rangle \rightarrow \infty$  exponentially as  $\omega \rightarrow \infty$ .

$$\Delta M = g\mu_B \frac{V}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \int_0^\infty \frac{\omega^{1/2} d\omega}{e^{\beta\hbar\omega} - 1}$$
$$= g\mu_B \frac{V}{4\pi^2} \left(\frac{k_B T}{2JSa^2}\right)^{3/2} \int_0^\infty \frac{x^{1/2} dx}{e^x - 1}$$

Since

$$\int_{0}^{\infty} \frac{x^{1/2} dx}{e^{x} - 1} = \frac{\sqrt{\pi}}{2} \zeta(\frac{3}{2}) = 0.0587(4\pi^{2})$$

we have

$$\frac{\Delta M}{M_s(0)} = \frac{V}{NSa^3} \left(\frac{k_B T}{2JS}\right)^{3/2} 0.0587 = \frac{1}{S} \left(\frac{k_B T}{2JS}\right)^{3/2} 0.0587$$

where  $M_s(0) = Ng\mu_B S$  and  $V = Na^3$ . This result is called the **Bloch**  $T^{3/2}$  law. The magnetization

$$M(T) = M_s(0) \left[1 - \frac{1}{S} \left(\frac{k_B T}{2JS}\right)^{3/2} 0.0587\right]$$

## 7. Heat capacity

The heat capacity is given by

$$C = \frac{dE}{dT} = \frac{\hbar^2}{k_B T^2} \int d\omega D(\omega) \frac{\omega^2}{(e^{\beta\hbar\omega} - 1)(1 - e^{-\beta\hbar\omega})}$$

where  $\beta = 1/(k_{\rm B}T)$ ,

$$E = \sum_{q} \hbar \omega_{q} \langle n_{q} \rangle = \int d\omega D(\omega) \hbar \omega \frac{1}{e^{\beta \hbar \omega} - 1}$$

$$\frac{d}{dT}\frac{1}{e^{\beta\hbar\omega}-1} = \frac{\hbar\omega}{k_B T^2}\frac{1}{(e^{\beta\hbar\omega}-1)(1-e^{-\beta\hbar\omega})}$$

Then we get

$$C = \frac{1}{k_B T^2} \frac{\hbar^2 V}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \int d\omega \frac{\omega^{5/2}}{(e^{\beta\hbar\omega} - 1)(1 - e^{-\beta\hbar\omega})}$$
$$= \frac{1}{k_B T^2} \frac{\hbar^2 V}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \left(\frac{k_B T}{\hbar}\right)^{7/2} \int_0^\infty \frac{x^{5/2} dx}{(e^x - 1)(1 - e^{-x})}$$
$$= k_B \frac{V}{4\pi^2 a^3} \left(\frac{k_B T}{2JS}\right)^{3/2} \int_0^\infty \frac{x^{5/2} dx}{(e^x - 1)(1 - e^{-x})}$$

Here we note that

$$\int_{0}^{\infty} \frac{x^{5/2} dx}{(e^x - 1)(1 - e^{-x})} = 4.45823$$

and  $V = Na^3$ . Then we have

$$C = k_B \frac{N}{4\pi^2} \left(\frac{k_B T}{2JS}\right)^{3/2} 4.45823$$

The heat capacity is proportional to  $T^{3/2}$ .

# 8. Spin wave theory (Feynman) S = 1/2.

We consider a spin wave theory which is described by Feynman. The Hamiltonian is

$$\hat{H} = -\frac{J}{2} \sum_{n} \hat{\boldsymbol{\sigma}}_{n} \cdot \hat{\boldsymbol{\sigma}}_{n+1}$$

where s is the Pauli operator. With this Hamiltonian we have a complete description of the ferromagnet.



 $\hat{\boldsymbol{\sigma}}_n \cdot \hat{\boldsymbol{\sigma}}_{n+1} = 2\hat{P}_{n,n+1} - 1$ 

where  $\hat{\boldsymbol{\sigma}}_n \cdot \hat{\boldsymbol{\sigma}}_{n+1}$  interchanges the spins of the *n*-th and (*n*+1)-th electrons.

For the ground state all spins are up  $(|+\rangle)$ , so if you exchange a particular pair of spins, one can get back the original state. The ground state is a stationary state: -J/2 for each pair of spins. That is, the energy of the system in the ground state is -J/2 per spin.

It is convenient to measure the energies with respect to the ground state. Our new Hamiltonian is



With this Hamiltonian, the energy of the ground state is zero. Here we define the state  $|x_{n}\rangle$  where all the spins except for the one on the spin at  $x_{n}$ .

$$\hat{H}|x_{5}\rangle = -J\sum_{n} (\hat{P}_{n,n+1} - 1)|x_{5}\rangle = -J(\hat{P}_{5,6} - 1)|x_{5}\rangle - J(\hat{P}_{4,5} - 1)|x_{5}\rangle$$
$$= -J(|x_{6}\rangle - 2|x_{5}\rangle + |x_{4}\rangle)$$

where

$$\hat{P}_{45}|x_5\rangle = |x_4\rangle, \ \hat{P}_{56}|x_5\rangle = |x_6\rangle, \ \hat{P}_{78}|x_5\rangle = |x_5\rangle, \text{ and } \ \hat{P}_{34}|x_5\rangle = |x_5\rangle.$$

Similarly,

$$\hat{H}|x_n\rangle = -J(|x_{n+1}\rangle - 2|x_n\rangle + |x_{n-1}\rangle$$
$$\hat{H}|x_{n+1}\rangle = -J(|x_{n+2}\rangle - 2|x_{n+1}\rangle + |x_n\rangle$$

Here we consider

$$|\psi\rangle = \sum_{n} C_{n} |x_{n}\rangle$$

Eigenvalue problem

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

or

$$\sum_{n} C_{n} \hat{H} \big| x_{n} \big\rangle = E \sum_{n} C_{n} \big| x_{n} \big\rangle$$

or

$$\sum_{n} C_{n} \hat{H} \big| x_{n} \big\rangle = E \sum_{n} C_{n} \big| x_{n} \big\rangle$$

or

$$\sum_{n} (-J)(C_{n} | x_{n+1} \rangle - 2C_{n} | x_{n} \rangle + C_{n} | x_{n-1} \rangle = E \sum_{n} C_{n} | x_{n} \rangle$$

or

$$\sum_{n} (-J)(C_{n-1} - 2C_n + C_{n+1}) |x_n\rangle = E \sum_{n} C_n |x_n\rangle$$

or

$$(-J)(C_{n-1} - 2C_n + C_{n+1}) = EC_n$$

Let us take as a trial function

$$C_{n} = e^{ikx_{n}}$$
(Bloch state)  
$$(-J)(e^{ik(x_{n}-a)} - 2e^{ikx_{n}} + e^{ik(x_{n}+a)}) = Ee^{ikx_{n}}$$
$$E = 2J[1 - \cos(ka)]$$
(energy dispersion)

The difference energy solutions correspond to "waves" of down spin-called "spin waves." For  $ka \ll 1$ , *E* is approximated by

$$E = 2A\frac{k^2a^2}{2} = Ak^2a^2$$