Note on Broken Symmetry and Spin Waves

Lectures on Condensed Matter Physics

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Some thoughts on Broken Symmetry and Spin- Waves (in progress)

1 Section

The rotation by finite angle of ferromagnet ground state ($\sum_i S_i^z = NS$)

$$|\Psi(\theta)\rangle = e^{-i\theta \sum_i S_i^x} |\Psi\rangle \tag{1}$$

for a finite angle the exponent is of order N and this is not an infinitesimal rotation. But

$$a_0 = \frac{1}{\sqrt{2SN}} \sum_i S_i^+ \tag{2}$$

$$a_0^\dagger = \frac{1}{\sqrt{2SN}} \sum_i S_i^- \tag{3}$$

and $S_i^x = \left(S_i^+ + S_i\right)/2$

$$e^{-i\theta \sum_i S_i^x} = e^{-i\theta\sqrt{NS/2}\left(a_0 + a_0^\dagger\right)} = e^{\alpha a_0 - \alpha^* a_0^\dagger} \tag{4}$$

with

$$\alpha = -i\theta\sqrt{NS/2} \tag{5}$$

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But this a displacement operator generating a coherent state where

$$\langle\Psi(\theta)|\, a_0 \,|\Psi(\theta)\rangle = \alpha \tag{6}$$

and

$$\langle\Psi(\theta)|\, a_0^\dagger a_0 \,|\Psi(\theta)\rangle = |\alpha|^2 = \frac{NS\theta^2}{2} \tag{7}$$

The rotated state is a condensation of spin wave of momentum 0. Of course this costs no energy, because it is a linear combination of states of energy equal to the GS energy. If we compute the overlap

$$\langle\Psi(\theta)|\Psi(0)\rangle = \langle\Psi(0)|\, e^{i\theta\sum_i S_i^x} \,|\Psi(0)\rangle = \langle\Psi(0)|\, e^{\alpha a_0 - \alpha^* a_0^\dagger} \,|\Psi(0)\rangle \tag{8}$$

we can use the relation

$$\begin{aligned} e^{\alpha a_0 - \alpha^* a_0^\dagger} &= e^{-\alpha^* a_0^\dagger} e^{\alpha a_0} e^{-\frac{|\alpha|^2}{2}\left[a_0, a_0^\dagger\right]} \\ &= e^{-\frac{|\alpha|^2}{2}} e^{-\alpha^* a_0^\dagger} e^{\alpha a_0} \end{aligned} \tag{9}$$

and

$$\langle\Psi(\theta)|\Psi(0)\rangle = e^{-\frac{|\alpha|^2}{2}} \langle\Psi(0)|\, e^{-\alpha^* a_0^\dagger} e^{\alpha a_0} \,|\Psi(0)\rangle = e^{-\frac{NS\theta^2}{2}} \tag{10}$$

In the thermodynamic limit the overlap is zero for any finite θ. Local operators like have vanishing matrix elements

$$\begin{aligned} \langle\Psi(\theta)|\, \mathbf{S}_i\cdot\mathbf{S}_j \,|\Psi(0)\rangle &= e^{-\frac{|\alpha|^2}{2}} \langle\Psi(0)|\, e^{\alpha a_0} \mathbf{S}_i\cdot\mathbf{S}_j \,|\Psi(0)\rangle \\ &= e^{-\frac{|\alpha|^2}{2}} \langle\Psi(0)| \prod_k e^{i\theta S_k^x} \mathbf{S}_i\cdot\mathbf{S}_j \,|\Psi(0)\rangle \\ &= e^{-\frac{|\alpha|^2}{2}} \langle\Psi(0)|\, e^{i\theta\left(S_i^x+S_j^x\right)} \mathbf{S}_i\cdot\mathbf{S}_j e^{-i\theta\left(S_i^x+S_j^x\right)} e^{\alpha a_0} \,|\Psi(0)\rangle \\ &= e^{-\frac{|\alpha|^2}{2}} \langle\Psi(0)|\, e^{i\theta\left(S_i^x+S_j^x\right)} \mathbf{S}_i\cdot\mathbf{S}_j e^{-i\theta\left(S_i^x+S_j^x\right)} \,|\Psi(0)\rangle \\ &= e^{-\frac{NS\theta^2}{2}} \langle\Psi(0)|\, \mathbf{S}_i\cdot\mathbf{S}_j \,|\Psi(0)\rangle \end{aligned} \tag{11}$$

In the thermodynamic limit we again get zero. In the $N \to \infty$ limit states of different θ are essentially in different Hilbert spaces unconnected by local operators. Similar argument can be made for other local operators, not necessarily scalar, and the prefactor $\exp(-NS\theta^2/2)$ kills all such matrix elements.

2 The Anti ferromagnet

The infinite range anti ferromagnet is exactly solvable

$$\begin{aligned} \mathcal{H} &= \frac{J}{N} \sum_{i\in A; j\in B} \mathbf{S}_i\cdot\mathbf{S}_j \\ &= \frac{J}{N}\mathbf{S}_A\cdot\mathbf{S}_B = \frac{J}{2N}\left[(\mathbf{S}_A+\mathbf{S}_B)^2 - S_A^2 - S_B^2\right] \end{aligned} \tag{12}$$

In this form it is clear the minimum energy is obtained for a singlet $\mathbf{S}_A + \mathbf{S}_B = 0$ with maximum possible spin for each of the sub-lattices $S_{A(B)} = NS/2$.

$$E(S_T, S_A, S_B) = \frac{J}{2N}\left[S_T(S_T+1) - S_A(S_A+1) - S_B(S_B+1)\right] \tag{13}$$

and the GS energy is ($S_T = 0$)

$$\begin{aligned} E_0 &= -\frac{J}{2N}\left[2\frac{NS}{2}\left(\frac{NS}{2}+1\right)\right] \\ &= -\frac{JNS^2}{4}\left(1+\frac{2}{NS}\right) \end{aligned} \tag{14}$$

In the thermodynamic limit

$$\frac{E_0}{N} = -\frac{JS^2}{4} \tag{15}$$

which is exactly the Néel state energy. The Néel state, in the $N \to \infty$, limit is a linear combination of multiplet states of different S_T, all essentially degenerate with the true singlet ground state (as long as $S_T \sim \mathcal{O}(1)$ rather than $S_T \sim \mathcal{O}(N)$). For $N \gg 1$ this state is very long lived (infinitely so, for $N \to \infty$) and we can just as well assume it to be the GS with a broken symmetry. Anderson argued that a similar result holds for the AF short-range models that have Néel order.

The short range model a state with saturated sub-lattice magnetization is in fact one which is totally symmetric in the exchange of any two spins of the same sub-lattice; the maximum spin multiplet of $\mathbf{S}$

$$\mathbf{S}_A := \sum_{i\in A}\mathbf{S}_i \tag{16}$$

is totally symmetric under exchange of two spins (of the same sub-lattice). Hence,

$$\mathbf{S}_i \cdot \mathbf{S}_j\,|\Psi_0\rangle \qquad i\in A; j\in B \tag{17}$$

is independent of i, because the state is symmetrical in the exchange of any two spins in A. If the sub-lattice magnetization is saturated,

$$\sum_{<ij>} J\mathbf{S}_i\cdot\mathbf{S}_j\,|\Psi_0\rangle = \frac{J}{2}\sum_{<ij>}\left(\frac{1}{N_A}\sum_{i\in A}\mathbf{S}_i\right)\cdot\left(\frac{1}{N_B}\sum_{j\in B}\mathbf{S}_j\right) = \frac{JNz}{2N_AN_B}\mathbf{S}_A\cdot\mathbf{S}_B$$

The ground state of this model will again be a singlet but the quantum fluctuations are again negligeable because $\mathbf{S}_{A(B)}$ are essentially classical spins with quantum spin number $NS/2 \gg 1$. Nevertheless, linear spin-wave theory shows that the sub-lattice magnetization is *not* saturated.

2.1 Linear spin wave theory

The Néel state

$$S_i^z |\Psi_N\rangle = S |\Psi_N\rangle ; \qquad i \in A \tag{18}$$
$$S_i^z |\Psi_N\rangle = -S |\Psi_N\rangle ; \qquad i \in B \tag{19}$$

The Goldstone mode

$$R_x(\theta) = e^{-i\theta S_T^x} \approx 1 - i\theta \left(\sum_{i\in A} S_i^x + \sum_{j\in B} S_j^x \right) \tag{20}$$

and

$$\begin{aligned} R_x(\theta) |\Psi_N\rangle &= |\Psi_N\rangle - i\theta \left(\sum_{i\in A} S_i^x + \sum_{j\in B} S_j^x \right) |\Psi_N\rangle \\ &= |\Psi_N\rangle - i\theta \left(\sum_{i\in A} S_i^- + \sum_{j\in B} S_j^+ \right) |\Psi_N\rangle \end{aligned} \tag{21}$$

So the zero energy mode is

$$\left(\sum_{i\in A} S_i^- + \sum_{j\in B} S_j^+ \right) |\Psi_N\rangle \tag{22}$$

This suggest a Holstein-Primakoff transformation defined by spin deviations

$$|\{n_{iA}\}, \{n_{jB}\}\rangle \tag{23}$$

with

$$n_{iA} = S - M_i^z; \qquad n_{iA} = 0, \ldots, 2S$$
$$n_{jB} = S_j^z - (-S); \qquad n_{jB} = 0, \ldots, 2S$$

Using the *linearized* version of HP transformation

$$S_i^z = S - a_i^\dagger a_i; \qquad i \in A \tag{24}$$
$$S_j^z = b_j^\dagger b_j - S \qquad j \in B \tag{25}$$

and

$$a_i^\dagger = \frac{1}{\sqrt{2S}} S_i^- \qquad i \in A \tag{26}$$
$$b_j^\dagger = \frac{1}{\sqrt{2S}} S_j^\dagger; \qquad j \in B \tag{27}$$

which we now replace in Hamiltonian

$$\begin{aligned}\mathcal{H} &= \sum_{i\in A, j\in B} J_{ij}\left[S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right] \\ &= \sum_{i\in A, j\in B} J_{ij}\left[\left(S - a_i^\dagger a_i\right)\left(b_j^\dagger b_j - S\right) + S\left(a_i b_j + a_i^\dagger b_j^\dagger\right)\right] \\ &= -\frac{N\tilde{J}(0)}{2}S^2 + S\sum_{i\in A, j\in B} J_{ij}\left[a_i^\dagger a_i + b_j^\dagger b_j\right] + S\sum_{i\in A, j\in B} J_{ij}\left[a_i b_j + a_i^\dagger b_j^\dagger\right] \\ &= E_N + \tilde{J}(0)S\left(\sum_{i\in A} a_i^\dagger a_i + \sum_{j\in B} b_i^\dagger b_i\right) + S\sum_{i\in A, j\in B} J_{ij}\left[a_i b_j + a_i^\dagger b_j^\dagger\right] \qquad (28)\end{aligned}$$

The first term is the Néel reference state energy

$$\mathcal{H} = E_N + \tilde{J}(0)S\left(\sum_{i\in A} a_i^\dagger a_i + \sum_{j\in B} b_i^\dagger b_i\right) + S\sum_{i\in A, j\in B} J_{ij}\left[a_i b_j + a_i^\dagger b_j^\dagger\right] \qquad (29)$$

This a Boson Hamiltonian quadratic in second quantized operators that can be diagonalized exactly:

- Fourier transformations
- Bogoliubov-Valatin two-mode canonical quantization

2.2 Fourier Transformation

The FBZ is now that of each sub-lattice. (N is the number of sites in each sub-lattice)

$$a_i = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}\in FBZ} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} \qquad (30)$$

$$b_j = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}\in FBZ} b_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} \qquad (31)$$

$$\begin{aligned}\sum_{i\in A} a_i^\dagger a_i &= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \sum_{i\in A} e^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{R}_i} \\ &= \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \qquad (32)\end{aligned}$$

$$\sum_{i\in A} a_i^\dagger a_i = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \qquad (33)$$

$$\sum_{j\in B} b_j^\dagger b_j = \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \qquad (34)$$

$$
\begin{aligned}
\sum_{i\in A, j\in B} J_{ij}\left[a_i b_j + a_i^\dagger b_j^\dagger\right] &= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}} b_{\mathbf{k}'} \sum_{i\in A, j\in B} J_{ij} e^{i(\mathbf{k}\cdot\mathbf{R}_i + \mathbf{k}'\cdot\mathbf{R}_j)} \\
&+ \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}}^\dagger b_{\mathbf{k}'}^\dagger \sum_{i\in A, j\in B} J_{ij} e^{-i(\mathbf{k}\cdot\mathbf{R}_i - \mathbf{k}'\cdot\mathbf{R}_j)} \qquad (35)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i\in A, j\in B} J_{ij} e^{i(\mathbf{k}\cdot\mathbf{R}_i + \mathbf{k}'\cdot\mathbf{R}_j)} &= \sum_{i\in A, j\in B} J_{ij} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j) + i(\mathbf{k}'+\mathbf{k})\cdot\mathbf{R}_j} \\
&= N\tilde{J}(-\mathbf{k})\delta_{\mathbf{k}+\mathbf{k}',0} \qquad (36)
\end{aligned}
$$

After Fourier transform

$$
\mathcal{H} = E_N + S\sum_{\mathbf{k}\in FBZ}\left[\tilde{J}(0)\left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}\right) + \tilde{J}(\mathbf{k})\left(a_{\mathbf{k}} b_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger\right)\right] \qquad (37)
$$

2.2.1 Bogoliubov-Valatin two-mode canonical transformation

For each $\mathbf{k}$ we have a pair of coupled modes

$$
a_{\mathbf{k}}, b_{-\mathbf{k}} \qquad (38)
$$

Modes of different $\mathbf{k}$ commute and we can diagonalize separately each

$$
\mathcal{H}_{\mathbf{k}} = \mathrm{S}\left[\tilde{J}(0)\left(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}\right) + \tilde{J}(\mathbf{k})\left(a_{\mathbf{k}} b_{-\mathbf{k}} + a_{\mathbf{k}}^\dagger b_{\mathbf{k}}^\dagger\right)\right] \qquad (39)
$$

or simplifying notation

$$
\mathcal{H}_2 = \epsilon_0\left(a^\dagger a + b^\dagger b\right) + \Delta(ab + a^\dagger b^\dagger) \qquad (40)
$$

Results (Δ real) :

$$
\mathcal{H} = E_N + \tilde{J}(0)S\sum_{\mathbf{k}\in FBZ}\left[\sqrt{1-\left(\frac{\tilde{J}(\mathbf{k})}{\tilde{J}(0)}\right)^2} - 1\right] + \tilde{J}(0)S\sum_{\mathbf{k}\in FBZ}\sqrt{1-\left(\frac{\tilde{J}(\mathbf{k})}{\tilde{J}(0)}\right)^2}\left(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \beta_{-\mathbf{k}}^\dagger\beta_{-\mathbf{k}}\right) \qquad (41)
$$

where

$$
\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} + v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger \qquad (42)
$$

$$
\beta_{\mathbf{k}} = v_{\mathbf{k}} a_{\mathbf{k}}^\dagger + u_{\mathbf{k}} b_{-\mathbf{k}} \qquad (43)
$$

with

$$
u_{\mathbf{k}} := \sqrt{\frac{\epsilon_0 + E_{\mathbf{k}}}{2E_{\mathbf{k}}}}; \qquad E_{\mathbf{k}} = \sqrt{\epsilon_0^2 - \Delta_{\mathbf{k}}^2} \qquad (44)
$$

$$
v_{\mathbf{k}} = \sqrt{\frac{\epsilon_0 - E_{\mathbf{k}}}{2E_{\mathbf{k}}}}; \qquad (45)
$$

In version uses $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ to get

$$a_{\mathbf{k}} = u_{\mathbf{k}}\alpha_{\mathbf{k}} - v_{\mathbf{k}}\beta_{\mathbf{k}}^\dagger \tag{46}$$

$$b_{-\mathbf{k}}^\dagger = -v_{\mathbf{k}}\alpha_{\mathbf{k}} + u_{\mathbf{k}}\beta_{\mathbf{k}}^\dagger \tag{47}$$

Spin wwve dispersion at low $\mathbf{k}$

$$\begin{aligned}\hbar\omega_{\mathbf{k}} &= \tilde{J}(0)S\sqrt{1-\left(\frac{\tilde{J}(\mathbf{k})}{\tilde{J}(0)}\right)^2} = \tilde{J}(0)S\sqrt{1-\left(1-\frac{\hbar Dk^2}{\tilde{J}(0)}\right)^2} \\ &\approx \tilde{J}(0)S\sqrt{1-\left(1-2\frac{\hbar Dk^2}{\tilde{J}(0)}\right)} = S\sqrt{\tilde{J}(0)\hbar Dk^2} = v_s k \end{aligned} \tag{48}$$

Two linear dispersing modes.

$$v_s = S\sqrt{\tilde{J}(0)\hbar D} \tag{49}$$

The sub-lattice magnetization

$$\begin{aligned} M_A(T) &= S - \frac{1}{N}\sum_i a_i^\dagger a_i = S - \frac{1}{N}\sum_{\mathbf{k}}\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle \\ &= S - \frac{1}{N}\sum_{\mathbf{k}} u_{\mathbf{k}}^2\langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}\rangle + v_{\mathbf{k}}^2\langle b_{-\mathbf{k}} b_{-\mathbf{k}}^\dagger\rangle \\ &= S - \frac{1}{N}\sum_{\mathbf{k}} v_{\mathbf{k}}^2 - \frac{1}{N}\sum_{\mathbf{k}} u_{\mathbf{k}}^2\langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}\rangle + v_{\mathbf{k}}^2\langle b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}\rangle \\ &= S - \frac{1}{N}\sum_{\mathbf{k}} v_{\mathbf{k}}^2 - \frac{1}{N}\sum_{\mathbf{k}} \frac{\epsilon_0}{E_{\mathbf{k}}}\frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}}-1} \end{aligned} \tag{50}$$

Note that a lower bounded spectrum requires a non-negative real spin wave energy

$$E_{\mathbf{k}} = \tilde{J}(0)S\sqrt{1-\left(\frac{\tilde{J}(\mathbf{k})}{\tilde{J}(0)}\right)^2} \tag{51}$$

which is verified if

$$\frac{\tilde{J}(\mathbf{k})}{\tilde{J}(0)} \leq 1 \tag{52}$$

For J_{ij} this is verified

$$\begin{aligned}\tilde{J}(0) &= \sum_n J\left(\mathbf{R}_n\right) \\ \tilde{J}(\mathbf{k}) &= \sum_n J\left(\mathbf{R}_n\right)\cos\left(\mathbf{k}\cdot\mathbf{R}_n\right)\end{aligned} \tag{53}$$