Quantum Magnets as "superfluids"

Consider a spin-S quantum spin system with the Hamiltonian $H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j$ where $\langle ij\rangle$ denotes nearest neighbors on some lattice. For simplicity, consider a square or a cubic lattice. When $J<0$, the spins have the tendency to point all in the same direction at sufficienty low temperatures and the corresponding spontaneous symmetry broken phase is called a ferromagnet :

$$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \\ \uparrow & \uparrow & \uparrow & \uparrow \end{array} .$$

In contrast, when $J>0$, spins have the tendency to anti-align with their nearest neighbor and the corresponding phase is called antiferromagnet: $\begin{array}{cccc} \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \end{array}$. Intersetingly, these phases can be understood as BEC/superfluids by representing spin operators in terms of fictitious bosons.

One such representation is the following, which is well-suited in the limit of large spin $S \gg 1$:

$$S_x + i S_y = S^+ = \sqrt{2S - n_b}\; b$$
$$S^z = S - n_b$$

where $n_b = b^+ b$ and one restricts $0 \leqslant n_b \lessapprox S$. This representation is useful when the spontaneous breaking of the spin-rotation SU(2) symmetry is assumed to occur along z-axis with $\langle S^z \rangle \simeq S$ i.e. $n_b/S \ll 1$. Therefore, this is a large-S (semiclassical) expansion.

Let's consider ferro and anti-ferro cases.

This representation goes by the name 'Holstein- Primakov (H-P) bosons'.

Ferromagnet using HP bosons:

$$H = -|J| \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

Since in the SSB phase, all spins point along the same direction, the details of lattice (e.g. bipartite vs not) do not matter. Using HP bosons,

$$H = -|J| \sum_{\langle ij \rangle} \left[S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + h.c.) \right]$$

$$= -|J| \sum_{\langle ij \rangle} \Big[(S - b^\dagger_i b_i)(S - b^\dagger_j b_j)$$

$$+ \frac{1}{2} \left(\sqrt{2S - b^\dagger_i b_i}\, b_i\, b^\dagger_j \sqrt{2S - b^\dagger_j b_j} + h.c. \right) \Big]$$

Expanding $\sqrt{2S - b^\dagger b}$ in the limit $S \gg b^\dagger b$ as $\sqrt{2S} \left[1 - \frac{b^\dagger b}{2S} \right]^{1/2} \simeq \sqrt{2S} \left[1 - \frac{b^\dagger b}{4S} + \dots \right]$

and keeping the terms upto $O(S^0)$ in H, one finds,

$$H = H_0 + H_1 + H_2$$

where $H_0 = -S^2 |J| \frac{NZ}{2} = O(S^2)$

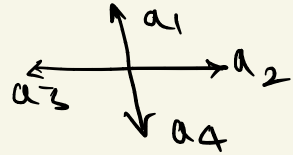
$$H_1 = S|J| \left[Z \sum_i b^+_i b_i - \sum_{\langle ij \rangle} (b^+_i b_j + h.c.) \right]$$

$$= \frac{S|J|Z}{N} \sum_k b^+_k b_k \left(1 - \frac{1}{Z} \sum_{\vec{a}_r} e^{i\vec{k}.\vec{a}_r}\right)$$
$$= O(S).$$

where Z is the coordination number and the sum over $\vec{a}_r$ in H_1 corresponds to sum over nearest neighbor bonds of any given lattice site. e.g. on the square lattice, $\frac{1}{Z} \sum_{\vec{a}_r} e^{i\vec{k}.\vec{a}_r} \equiv \gamma_k$

$$= \frac{1}{4} \left(e^{ik_x} + e^{ik_y} + e^{-ik_x} + e^{-ik_y}\right)$$

$$= \frac{\cos(k_x) + \cos(k_y)}{2}$$



Finally, H_2 is the interaction term between the bosons at $O(1)$ [there are higher order interaction terms and non-interaction terms as well].

$$H_2 = \frac{|J|}{4} \sum_{\langle ij \rangle} [b_i^\dagger b_j^\dagger (b_i - b_j)^2 + h.c.]$$

Retaining only $H_0 + H_1$,

$$H \simeq -S^2 |J| \frac{Nz}{2} + \sum_k \omega_k b_k^\dagger b_k$$

where $\omega_k = S|J|z \left(1 - \frac{1}{z} \sum_{\vec{a}_r} e^{i\vec{k}\cdot\vec{a}_r}\right)$

$\simeq c\, k^2$ at small k

where $c \simeq S|J|z$.

Therefore, the Goldstone modes of the SSB have dispersion $\omega_k \sim k^2$.

Exactly at $T=0$, these modes are unoccupied and therefore the ground state has no fluctuations. This is because the order parameter $\sum_i S_i^z$ commutes with the Hamiltonian. Note that H_0 precisely corresponds to the ground state energy of a classical ferromagnet.

At $T>0$, the Goldstone modes would be occupied with Bose distribution $n_B(k) = \frac{1}{e^{\beta\omega_k}-1}$ and the question of the stability of the ferromagnet is identical to the question of stability of a non-relativistic BEC at $T > 0$. The leading order correction to the ground state order parameter ($= S$) is given as

$$\langle S^z(T)\rangle - \langle S^z(T=0)\rangle$$

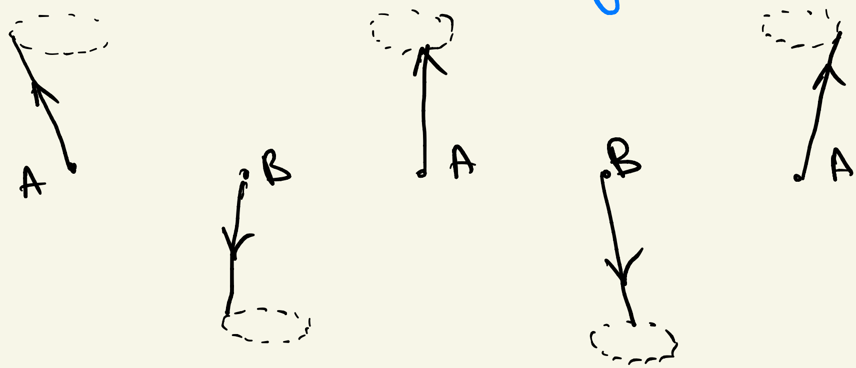
$$= S - \langle b^+_i b_i\rangle - S$$

$$= -\frac{1}{N} \sum_k \langle b^+_k b_k\rangle$$

$$= -\frac{1}{(2\pi)^d} \int_0^{\wedge} \frac{d^d k}{e^{\beta c k^2} - 1}$$

The integral converges only in $d > 2$ $\Rightarrow$ ferromagnet is unstable against the thermal fluctuations in $d = 1$ and $d = 2$. In $d = 2$, if instead of SU(2) symmetric H, one had only a U(1) symmetric H (e.g. due to an easy-plane anisotropy) then the system would allow for vortices leading to a finite T transition between a phase with power-law correlations for ferromagnetic order parameter, and a phase with exponentially decaying correlations (BKT transition).

Antiferromagnet using HP bosons:



We restrict ourselves to a bipartite lattice. The spins point along $+\hat{z}$ direction the A sublattice and $-\hat{z}$ direction on the B sublattice.

Since the order parameter is $(-)^{(x+y)}\langle S(x,y)\rangle$, one can perform a unitary transformation so that H is expressed in terms of operators that vary smoothly in space.

On B sublattice, lets define

$$\tilde{S}^z = -S^z, \quad \tilde{S}^x = S^x, \quad \tilde{S}^y = -S^y$$

so that the commutation relations $[S^\alpha, S^\beta] = i\varepsilon_{\alpha\beta\gamma} S^\gamma$ are obeyed by $\tilde{S}$ variables. Note that $S^+ = S^x + iS^y$ $= \tilde{S}^x - i\tilde{S}^y = \tilde{S}^-$. Therefore,

$$H = |J| \sum_{\substack{\langle ij\rangle \\ i\in A \\ j\in B}} \left[S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + h.c) \right]$$

$$= |J| \sum_{\langle ij\rangle} \left[-S_i^z \tilde{S}_j^z + \frac{1}{2}(S_i^+ \tilde{S}_j^+ + h.c) \right]$$

Now we simply use the standard HP bosons on both sublattices,

$$S^+ \text{ or } \tilde{S}^+ = \sqrt{2S - n_b}\, b$$

$$S^z \text{ or } \tilde{S}^z = S - n_b$$

Substituting this representation and again keeping the first few terms, one finds,

$$H = H_0 + H_1 + H_2 + \ldots$$

where $H_0 = -S^2 |J| \frac{N z}{2}$

$$H_1 = |J| S z \sum_k \left[b_k^\dagger b_k + \frac{\gamma_k}{2} \left(b_k^\dagger b_{-k}^\dagger + h.c. \right) \right]$$

where $\gamma_k = \frac{1}{z} \sum_{a_r} e^{i \vec{k} \cdot \vec{a}_r}$ as before.

and $H_2 = -\frac{|J|}{4} \sum_{(ij)} \left[b_i^\dagger (b_j^\dagger + b_i)^2 b_j + h.c. \right]$

The crucial point to note is that $b_k^\dagger$ / b_k do not diagonalize H_1 due to the terms $(b_k^\dagger b_{-k}^\dagger + h.c.)$.

This is a consequence of the fact that unlike a FM, where the classical ground state is the quantum ground state, for an AFM, the quantum (i.e. actual) ground state is not the product state $|\uparrow \downarrow \uparrow \ldots\rangle$, but instead it contains quantum fluctuations.

This is because the order parameter $(-)^r \langle S(r) \rangle$, <u>does not</u> commute with H.

To diagonalize H_1, we employ the Bogolibor transformation, similar the case for a superfluid.

$$b_k = \cosh(\theta_k)\,\alpha_k + \sinh(\theta_k)\,\alpha^{+}_{-k}$$

where α_k are standard boson operators, $[\alpha_k, \alpha^{+}_{k'}] = \delta_{kk'}$ etc.

$$\Rightarrow \quad H_1 = |J| S Z_1 \sum_k \Big[\big(\cosh(2\theta_k)$$

$$+ \gamma_k \sinh(2\theta_k) \big) \alpha^{+}_k \alpha_k$$

$$+ \frac{1}{2} \big(\sinh(2\theta_k) + \gamma_k \cosh(2\theta_k) \big) \left(\alpha^{+}_k \alpha^{+}_{-k} + h.c. \right)$$

$$+ \sinh^2\theta_k + \frac{\gamma_k}{2} \sinh(2\theta_k) \Big]$$

One choose θ_k so that the terms $\alpha^{+}_k \alpha^{+}_{-k}$ vanish.

$$\Rightarrow \quad \tanh(2\theta_k) = -\gamma_k .$$

Using this, H_1 becomes,

$$H_1 = \sum_k \omega_k \left(\alpha^+_k \alpha_k + \frac{1}{2}\right) - \frac{JzNS}{2}$$

where $\omega_k = |J| S z \sqrt{1 - \gamma_k^2}$

ω_k vanishes at two k-points :

$\vec{k} = \vec{0}$ and $\vec{k} = (\pi, \pi, \ldots \pi) \equiv \vec{Q}$ on

a cubic lattice in d-dimensions.

For $|k|$ small, $\gamma_k \simeq 1 - \frac{k^2}{z}$

on a cubic lattice in d- dimensions

with $z = 2d$.

$$\Rightarrow \quad \omega_k \simeq JS\sqrt{2z}\; |k|$$

$$= c\,|k|.$$

Similarly, when $\vec{k} \simeq \vec{Q}$,

$$\omega_k \simeq J S \sqrt{2z}\, |\vec{k} - \vec{Q}|$$

Let us calculate the ground state energy and order parameter.

<u>Energy</u>: In the ground state, the modes α_k are unoccupied.

$\Rightarrow \quad \alpha_k |0\rangle = 0$

$\Rightarrow$ g.s. energy $E_{g\text{-}s} = E_{cl}$ (= classical energy) $+ \sum_k \frac{\omega_k}{2} - \frac{JSzN}{2}$

$$= E_{cl} + \frac{1}{2} \sum_{\vec{k}} |J| S z \left(\sqrt{1-\gamma^2} - 1 \right)$$

where $E_{cl} = H_0 = -\dfrac{S^2 J N z}{2}$.

Since $\sqrt{1-y^2} < 1$

$\Rightarrow \quad E_{g.s.} < E_{cl}$

$\Rightarrow$ Quantum fluctuations lower the energy compared to the classical ground state.

Order parameter:

Classically, at $T=0$, the order parameter is just S. Quantum fluctuations cause it to reduce by an amount

$$\Delta m = \frac{1}{N} \sum_{\vec{r}} e^{i\vec{Q}\cdot\vec{r}} \langle S^z_{\vec{r}} \rangle - S$$

$$= \frac{1}{N} \sum_{\vec{r}} [S - n_b(\vec{r})] - S$$

$$= - \int \frac{d^d k}{(2\pi)^d} \langle b^\dagger_k b_k \rangle$$

$$= \frac{1}{2} - \int \frac{d^d k}{(2\pi)^d} \frac{(n_B(k) + \frac{1}{2})}{\sqrt{1 - \gamma_k^2}}$$

The integral behaves as

$$-\int \frac{d^d k}{k\,(e^{\beta k} - 1)} + \frac{1}{2} \int \frac{d^d k}{k}$$

Therefore, it diverges at $T \geq 0$ in $d = 1$, and at $T > 0$ in $d = 2$. It is finite at $T > 0$ in $d \geq 3$.

Thus, quantum fluctuations destroy AFM ordering at $T \geq 0$ in $d = 1$ and at $T > 0$ in $d = 2$, as expected from Mermin - Wagner theorem.

One may summarize the results as,

	Ferromagnet	Antiferromagnet
$T = 0$	Stable in any d. $[m, H] = 0$. Classical g.s. = Quantum g.s.	Stable only in $d > 1$. $[m, H] \neq 0$. Classical g.s. $\neq$ Quantum g.s.
$T \geq 0$	Stable only in $d > 2$. $\omega_{Goldstone} \sim k^2$.	Stable only in $d > 2$. $\omega_{Goldstone} \sim k$.