• PROPERTIES OF THE HEISENBERG MODEL

* Let's come back now to the half-filled case. As we saw in pages ㊵ and ㊶, in the strong-coupling regime $U >> t$, we may reduce the Hubbard Hamiltonian to a ferromagnetic or antiferromagnetic Heisenberg model, depending whether we have bosons or fermions.

· The Heisenberg model is crucial for quantum magnetism, and it is hence quite instructive to have a look to its basic properties, since while doing so we will learn some interesting concepts.

Recall that the Heisenberg model is of the form:

$$\hat{H} = J \sum_{\langle ij \rangle} \overline{S}_i \cdot \overline{S}_j$$

where $J > 0$ for antiferromagnets

$J < 0$ for ferromagnets.

· The Hamiltonian is rotationally invariant since it commutes with all three components of the total spin

$$\vec{S}_{tot} = \sum_i \overline{S}_i$$

Thus the eigenstates are labelled by

$$|\psi\rangle = |S_{tot}, M\rangle \quad \text{with } M = -S_{tot}, \dots, S_{tot}$$

$$S_{tot} \leq \underset{\substack{\uparrow \\ \text{number of} \\ \text{sites}}}{N} S \leftarrow \text{spin (in this case } 1/2\text{)}$$

(but we will keep it general)

M is the eigenvalue of the total magnetization

$$S^z_{tot} = \sum_i S_i^z$$

and $\hat{S}^2_{tot} = S_{tot}(S_{tot}+1)$ as always.

· Note also that since the model is translationally invariant, the lattice momentum K is also a good quantum number. We will use this fact in a moment when introducing spin-wave theory.

- For the ferromagnetic case, the ferromagnetic state

↑ ↑ ↑ ↑ ....

is an eigenstate of the Hamiltonian. This is easy to see, because this state is $|S, M=S\rangle$, and M is a good quantum number. This state is obviously also the ground state of the system. Note however that the ferromagnetic state breaks the rotational symmetry of the Hamiltonian.

We could have e.g. ↓↓↓... or ↗↗... or ↘↘... and so on. (actually and infinite degenerate multiplet).

We have here an example of spontaneous symmetry breaking, in which the ground state does not have the symmetry of the Hamiltonian. This has relevant consequences e.g. for the excitation spectrum as we will discuss later.

- For the antiferromagnetic case the situation is far more complicated.

Let's introduce some useful concepts:

- The staggered magnetization operator on sublattices A and B (Note: as previously we implicitly assume a bipartite lattice here) is defined as:

$$S^{stagg} = \sum_{i \in A} S_i^z - \sum_{i \in B} S_i^z$$

- The Ising configurations form the basis set

$$|\phi_\alpha\rangle = |S, m_1^\alpha\rangle_1 \otimes |S, m_2^\alpha\rangle_2 \otimes \dots \otimes |S, m_N^\alpha\rangle_N$$

where $|S, m_i\rangle_i$ denotes an eigenstate of $\vec{S}_i^{\,2}, S_i^z$ with eigenvalues $S(S+1)$ and m_i respectively.

- The Néel state is then

$$|\psi^{Néel}\rangle = \prod_i |S, \eta_i S\rangle_i \quad \text{with} \quad \eta_i = \begin{cases} 1 & i \in A \\ -1 & i \in B \end{cases}$$

i.e. the state

$$\begin{matrix} & \vdots & \\ \dots & \uparrow \downarrow \uparrow \downarrow \uparrow & \dots \\ & \downarrow \uparrow \downarrow \uparrow \downarrow & \\ & \vdots & \end{matrix}$$

* The Néel state maximizes S^{stagg} and it represents our intuitive picture about and antiferromagnet. This state, however, is <u>not an eigenstate</u> of $\hat{H}$, due to the <u>spin flip</u> terms

$$S_i^+ S_j^- \,|\ldots \underset{\overset{\uparrow}{i}}{S}, \underset{\overset{\uparrow}{j}}{-S}, +S, -S \ldots\rangle = |\ldots S, \underset{\overset{\uparrow}{i}}{-S+1}, \underset{\overset{\uparrow}{j}}{S-1}, S, \ldots\rangle$$

* One can show that the ground state of an antiferromagnetic Heisenberg model on a finite bipartite lattice is a <u>global singlet</u>, i.e.

$$\vec{S}_{tot}\,|\Psi_0\rangle = 0$$

(<u>Note</u>: This is the so-called <u>Marshall's theorem</u>. For a proof of this theorem see e.g. Auerbach's book.)

[<u>Note(II)</u>: Spontaneous symmetry breaking into a Néel state is however still possible in the strict thermodynamic limit ($N \to \infty$). Note that a Néel state is a superposition of an infinite number of states with different total spin, but all with $S^z_{tot} = 0$. Those states become for $N \to \infty$ degenerate with the singlet ground state of finite chains.]

* <u>HOLSTEIN - PRIMAKOFF SPIN REPRESENTATION</u>

* To study the properties of the Heisenberg model it is convenient to consider the case of <u>large spin S</u>. In the limit $S \to \infty$ one reaches the <u>classical limit</u>, this is easy to see if we define the <u>unit vectors</u>

$\vec{S}_i / S \equiv \vec{s}_i$, then

- $[S_i^\alpha, S_j^\beta] = i\,\delta_{ij}\,\varepsilon_{\alpha\beta\gamma}\,\dfrac{S_i^\gamma}{S} \xrightarrow[S\to\infty]{} 0$
- $\vec{s}_i^{\,2} = \vec{S}_i^{\,2}/S^2 = S(S+1)/S^2 \xrightarrow[S\to\infty]{} 1$

} the operators $\hat{\vec{s}}_i$ behave hence as simple vectors $\vec{s}_i$, i.e. they are <u>classical</u>.

* The classical Hamiltonian for antiferromagnets is minimized by the <u>Néel state</u> (we choose the z-axis as the direction of the classical spins). One can then study the effects of <u>quantum fluctuations</u> arising from the finiteness of S, which will introduce deviations from the classical state.

* In order to carry out that task, <u>Holstein and Primakoff</u> introduced a <u>boson operator</u> b which represents the 3 spin component operators as

$$\left.\begin{aligned} S_i^+ &= \sqrt{2S - b_i^+ b_i}\; b_i \\ S_i^- &= b_i^+ \sqrt{2S - b_i^+ b_i} \\ S_i^z &= S - b_i^+ b_i \end{aligned}\right\} \text{Holstein-Primakoff (HP) transformation}$$

- One may easily check that the spin commutation relations are fulfilled:

$$\begin{aligned} [S_i^z, S_i^-] &= - b_i^+ b_i\, b_i^+ \sqrt{2S - b_i^+ b_i} + b_i^+ \sqrt{2S - b_i^+ b_i}\; b_i^+ b_i \\ &= - b_i^+ (1 + b_i^+ b_i) \sqrt{2S - b_i^+ b_i} + b_i^+ b_i^+ b_i \sqrt{2S - b_i^+ b_i} \\ &= - b_i^+ \sqrt{2S - b_i^+ b_i} = - S_i^- \end{aligned}$$

and similarly $[S_i^z, S_i^+) = S_i^+$

Also

$$\begin{aligned} [S_i^+, S_i^-] &= \sqrt{2S - b_i^+ b_i}\; b_i b_i^+ \sqrt{2S - b_i^+ b_i} - b_i^+ (2S - b_i^+ b_i) b_i \\ &= \sqrt{2S - b_i^+ b_i}\; (1 + b_i^+ b_i) \sqrt{2S - b_i^+ b_i} - b_i^+ (2S - b_i^+ b_i) b_i \\ &= (1 + b_i^+ b_i)(2S - b_i^+ b_i) - b_i^+ (2S - b_i^+ b_i) b_i = 2 S_i^z \end{aligned}$$

- The Fock space of b is of course unconstrained from above. The <u>physical subspace</u> is spanned by the states $(\hat{n}_b = b^+ b)$

$$\{|n_b\rangle\}_S = \{\underset{\substack{\Updownarrow \\ |S_i^z = S\rangle}}{|0\rangle}, |1\rangle, \dots, \underset{\substack{\Updownarrow \\ |S_i^z = -S\rangle}}{|2S\rangle}\}$$

Note that the spin operators do not connect the physical to the unphysical subspaces:

$$\langle 2S+1 | S_i^- | 2S \rangle = 0 \nearrow \text{ since } S_i^- |2S\rangle = b_i^+ \sqrt{2S - b_i^+ b_i}\, |2S\rangle = 0$$

- Hence, if we expect that fluctuations around the classical state are not strong, we may consider the density of HP bosons at each site small and we do not have to take special care about the unphysical states.
- One may then expand:

$$\sqrt{2S - n_b} \simeq \sqrt{2S} \left\{ 1 - \frac{n_b}{4S} - \frac{n_b^2}{32 S^2} \cdots \right\}$$

* SPIN WAVE THEORY FOR THE FERROMAGNET

- We consider first the ferromagnetic case

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

Assuming small fluctuations around the classical state $(\uparrow\uparrow \dots \uparrow\uparrow \dots)$ we employ:

$$\left.\begin{aligned} S_i^+ &\simeq \sqrt{2S}\, b_i \\ S_i^- &\simeq b_i^+ \sqrt{2S} \end{aligned}\right\} \longrightarrow S_i^+ S_j^- = 2S\, b_i b_j^+$$

$$S_i^z = S - b_i^+ b_i \longrightarrow S_i^z S_j^z = S^2 - S(b_j^+ b_i + b_i^+ b_i)$$

Then:

$$\hat{H} \simeq -N|J|zS^2/2 - \frac{J}{2} \sum_{\vec{j},\vec{\delta}} \left[-2S\, b_{\vec{j}}^+ b_{\vec{j}} + S\, b_{\vec{j}}^+ b_{\vec{j}+\vec{\delta}} + S\, b_{\vec{j}+\vec{\delta}}^+ b_{\vec{j}} \right]$$

where $z \equiv$ coordination number

$\vec{\delta} \equiv$ nearest neighbors $(z = \sum_{\vec{\delta}})$

$N \equiv$ number of sites

We introduce the Fourier transform $b_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{j}} e^{i\vec{k}\cdot\vec{j}}\, b_{\vec{j}}$

to get

$$\hat{H} \simeq -N|J|zS^2/2 + \underbrace{\sum_{\vec{k}} \varepsilon(\vec{k})\, b_{\vec{k}}^+ b_{\vec{k}}} \longrightarrow \text{Non-interacting spin waves with dispersion}$$

where:

$$\varepsilon(\vec{k}) = S|J|z \left[1 - \frac{1}{z} \sum_{\langle ij \rangle} e^{i(\vec{j}-\vec{i})\cdot\vec{k}} \right] = S|J|z(1 - \gamma_{\vec{k}})$$

[Note: for a cubic lattice $\gamma_{\vec{k}} = \frac{2}{z}(\cos k_x + \cos k_y + \cos k_z)$

- At zero temperature $(T=0) \longrightarrow \langle b_{\vec{k}}^+ b_{\vec{k}} \rangle = 0$ and one recovers the classical energy:

$$E_0 = -S^2 |J| N z/2$$

The ground state is not shifted, because the ferromagnetic state is an eigenstate of $\hat{H}$ as already mentioned. This will be different for the antiferromagnetic case, as we will see in a moment.

· The low-momentum limit of the dispersion law is:

$$\epsilon(\vec{k}) \sim S|J||\vec{k}|^2 \rightarrow \text{i.e. quadratic and gapless.}$$

This is the gapless Goldstone mode, which is a consequence of the broken symmetry of the ferromagnetic ground state.

[Note: If the Hamiltonian has some continuous symmetry that is spontaneously broken then the system admits excitations with $\epsilon_{\vec{k}\to 0} \to 0$.] → Goldstone theorem.

· The Goldstone mode dominates the low-T and low-k correlations of the ferromagnet

The correction to the magnetization at finite T is given by:

$$\Delta m_0 = \frac{1}{N}\langle S^z_{tot}\rangle - \underset{\substack{\uparrow \\ \text{purely} \\ \text{ferro}}}{S} = -\langle n_i\rangle = -\frac{1}{N}\sum_{\vec{k}} n_{\vec{k}}$$

where $n_{\vec{k}} = \dfrac{1}{e^{\epsilon(\vec{k})/T}-1}$ is the Bose-Einstein occupation.

· The asymptotic low-T behaviour is found by introducing an infrared cutoff k_0. We choose an additional small but finite $\bar{k} > k_0$ (for which $\epsilon(k) \sim S|J|k^2$ holds). such that $\epsilon(\bar{k}) \ll k_B T \ll |J|S$

We may then break up the sum into:

$$\Delta m_0 \approx \underbrace{-\int_{k_0}^{\bar{k}} \frac{dk\, k^{d-1}}{(2\pi)^d}\frac{T}{JSk^2}}_{\downarrow} - \underbrace{\frac{1}{N}\sum_{|\vec{k}|>\bar{k}} \frac{1}{e^{\epsilon(\vec{k})/T}-1}}_{\text{This is finite}}$$

This term presents a divergence at low k_0 and finite T for dimensions $d = 1, 2$

$$\hookrightarrow \Delta m_0 \propto \left\{ \begin{array}{ll} -t/k_0 + \cdots & \text{for 1D} \\ t \log k_0 + \cdots & \text{for 2D} \end{array} \right\} \quad \text{where } t = T/JS$$

- This is a very important result. The magnetization correction Δm_0 diverges for vanishing k_0 in 1D and 2D, and hence our initial assumption of small spin fluctuations is wrong. Thus spin-wave theory fails in low dimensions. This is a consequence of a general theorem due to Mermin and Wagner which states that continuous symmetries (in this case SU(2) symmetry) cannot be broken in low $d<3$ for finite T.

- In 3D there are no infrared divergences. The leading T-dependence of Δm can be readily calculated:

$$\Delta m_0^{d=3} = -\int_{k_0}^{\bar{k}} \frac{dk\, k^2}{2\pi^2} \sum_{n=1}^{\infty} e^{-nk^2/t} \left(1+\mathcal{O}(t)\right)$$

$$\simeq -\frac{1}{8}\left(\frac{t}{\pi}\right)^{3/2} \sum_{n=1}^{\infty} n^{-3/2} = -\frac{1}{8}\left(\frac{t}{\pi}\right)^{3/2} \zeta(3/2)$$

↑ Riemann zeta ($\zeta(s)=\sum_{n=1}^{\infty} n^{-s}$)

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* SPIN WAVE THEORY FOR THE ANTIFERROMAGNET

- Let's consider now the antiferromagnetic case. We choose the classical Néel state to be in z-direction for the sublattice A and $-z$ for B.
- It is convenient to invert the quantization axis on sublattice B by a unitary transformation

$$\left.\begin{aligned} \tilde{S}_j^z &= -S_j^z \\ \tilde{S}_j^x &= S_j^x \\ \tilde{S}_j^y &= -S_j^y \end{aligned}\right\} \rightarrow \tilde{S}_j^- = S_j^+, \quad \tilde{S}_j^+ = S_j^-$$

(Note: It's easy to see that the spin commutations are not affected by this)

The Hamiltonian becomes then:

$$H = -|J| \sum_{\substack{\langle ij\rangle \\ i\in A}} S_i^z \tilde{S}_j^z + \frac{1}{2}|J| \sum_{\substack{\langle ij\rangle \\ i\in A}} \left(S_i^+ \tilde{S}_j + S_i^- \tilde{S}_j^-\right)$$

(Note: The Néel state looks for the $S, \tilde{S}$ spins as the ferro state ???..)

- Introducing the HP bosons as in p. ⑥③ we get

$$\hat{H} \simeq -JzS^2N/2 + JSz \sum_{\vec{j}\in A,B} b^+_{\vec{j}} b_{\vec{j}} + \frac{JS}{2} \sum_{\vec{j}\in A,B} \sum_{\vec{\delta}} \left(b^+_{\vec{j}} b^+_{\vec{j}+\vec{\delta}} + b_{\vec{j}} b_{\vec{j}+\vec{\delta}} \right)$$

Introducing the Fourier transform:

$$\hat{H} \cong -S^2 JNz/2 + JSz \sum_{\vec{k}} \left(b^+_{\vec{k}} b_{\vec{k}} + \frac{\gamma_{\vec{k}}}{2} \left(b^+_{\vec{k}} b^+_{-\vec{k}} + b_{\vec{k}} b_{-\vec{k}} \right) \right)$$

Note that contrary to the ferromagnetic case now the quadratic Hamiltonian contains both _normal_ (b^+b) _and anomalous_ (b^+b^+, bb) terms.

- We can diagonalize the Hamiltonian by means of a _Bogoliubov transformation_. We define a spin wave operator $\alpha_{\vec{k}}$ such that

$$\left.\begin{aligned} \alpha_{\vec{k}} &= \cosh\theta_{\vec{k}}\, b_{\vec{k}} - \sinh\theta_{\vec{k}}\, b^+_{-\vec{k}} \\ b_{\vec{k}} &= \cosh\theta_{\vec{k}}\, \alpha_{\vec{k}} + \sinh\theta_{\vec{k}}\, \alpha^+_{-\vec{k}} \end{aligned}\right\}$$

. where $\theta_{\vec{k}}$ are real and even in $\vec{k} \Leftrightarrow -\vec{k}$

. The α's are also bosons.

- choosing $\tanh 2\theta_{\vec{k}} = -\gamma_{\vec{k}}$ yields:

$$\hat{H} = -S^2 JNz/2 - JSzN/2 + \sum_{\vec{k}} \varepsilon(\vec{k}) \left[\alpha^+_{\vec{k}} \alpha_{\vec{k}} + 1/2 \right]$$

with $\varepsilon(\vec{k}) = JSz\sqrt{1-\gamma^2_{\vec{k}}}$ → _spin-wave dispersion_

. We see that unlike the case of the ferromagnet, the ground state energy is reduced by quantum fluctuations:

[The ground state is given by the vacuum of the α bosons]

$$E_0 = \underbrace{-S^2 JNz/2}_{\text{classical energy}} \underbrace{- \frac{1}{2} \sum_{\vec{k}} JSz \left(-\sqrt{1-\gamma^2_{\vec{k}}} + 1 \right)}_{\text{quantum fluctuations reduce the energy of the antiferromagnet}}$$

↪ This is of course because the Néel state is not an eigenstate.

[Note: For a 3D cubic lattice $E_0 \cong -\frac{NJS^2z}{2} \left(1 + 0.097/S \right)$]

- In the spin language the ground state admixes configurations with arbitrary number of spin flips relative to the Néel state. This reduces the staggered magnetization even at $T=0$, as we will see now.

- Note that the spin-wave dispersion is linear for $|\vec k| \to 0$

$$\epsilon_{\vec k} \simeq \underbrace{JS\sqrt{2z}}_{\hookrightarrow \text{ sound velocity}}\, |\vec k| \qquad \left(\begin{array}{l}\text{contrary to the FM case which}\\ \text{presented a quadratic dispersion}\end{array}\right)$$

let's have a look now to the correction to the staggered magnetization

$$\Delta m_0^s = \frac{1}{N}\left\langle \sum_{\vec r} e^{i\vec\pi\cdot\vec r} S^z_{\vec r}\right\rangle - S = -\frac{1}{N}\left\langle \sum_{\vec r} b^\dagger_{\vec r} b_{\vec r}\right\rangle = -\frac{1}{N}\sum_{\vec k}\langle b^\dagger_{\vec k} b_{\vec k}\rangle$$

$$= -\frac{1}{N}\sum_{\vec k}\left[\cosh^2\frac{\theta_{\vec k}}{2}\langle \alpha^\dagger_{\vec k}\alpha_{\vec k}\rangle + \sinh^2\frac{\theta_{\vec k}}{2}\langle \alpha_{-\vec k}\alpha^\dagger_{-\vec k}\rangle\right]$$

$$= -\frac{1}{N}\sum_{\vec k}\left[n_{\vec k}\left(\cosh^2\frac{\theta_{\vec k}}{2} + \sinh^2\frac{\theta_{\vec k}}{2}\right) + \sinh^2\frac{\theta_{\vec k}}{2}\right)\right]$$

$$= -\frac{1}{N}\sum_{\vec k}\left[n_{\vec k}\cosh\theta_{\vec k} + \frac{1}{2}\left(\cosh\theta_{\vec k} - 1\right)\right]$$

$$= \underbrace{-\frac{1}{N}\sum_{\vec k}\frac{1}{e^{\epsilon(\vec k)/T}-1}\,\frac{1}{\sqrt{1-\gamma_{\vec k}^2}}}_{\substack{\text{finite-}T\text{ correction}\\ (\Delta m_0^{s,TH})}} + \underbrace{\frac{1}{2N}\sum_{\vec k}\left(1-\frac{1}{\sqrt{1-\gamma_{\vec k}^2}}\right)}_{\substack{\text{effect of quantum fluctuations}\\ (\Delta m_0^{s,Q})}}$$

- We may now proceed as for the FM case to analyze the corrections of the staggered magnetization and in particular their infrared divergences for $|\vec k| \to 0$.

One obtains that

$$\Delta m_0^{s,TH} \sim \int dk\, k^{d-1}\frac{T}{k^2} \qquad \text{(as for the FM case)}$$

$$\Delta m_0^{s,Q} \sim \int dk\, k^{d-1}\frac{1}{k}$$

- One sees that as for the FM case the thermal correction stays finite in 3D but diverges in 2D and 1D (again the Mermin-Wagner theorem)
- The quantum correction is finite in 2D and 3D but diverges logarithmically in 1D
Spin-wave theory fails for an AFM in 1D even at $T=0$ (!!)