TFY 4210 / FY 8302

Exam June 1, 2022

1a) The K-term favors spin-ordering along the z-axis in spin-space. It breaks the rotational invariance of the Heisenberg-model down to an Ising-symmetry, making it easy for the spins to order along the z-axis

1b) With $K=0$, using the Holstein-Primakoff transformation, and introducing F-transformed operators, we have

$$H = E_0 - 2JSz\sum_q \left(a_q^+ a_q + b_q^+ b_q\right) - 2JS\sum_q \gamma(q)\left(a_q b_q + b_q^+ a_q^+\right)$$

in the notation used in the lecture notes.

If we used the H-P transformation on the $-K\sum_i S_{iz}^2$ term, we get

$$-K\sum_i S_{iz}^2 = -KNS^2$$

$$+\,2KS\sum_q \left(a_q^+ a_q + b_q^+ b_q\right)$$

Adding this to the H, we get

$$H = E_0 - KNS^2$$

$$-\left(2JSz - 2KS\right)\sum_q \left(a_q^+ a_q + b_q^+ b_q\right)$$

$$-\,2JS\sum_q \gamma(q)\left(a_q b_q + b_q^+ b_q\right)$$

$$= -2JSz'\sum_q \left(a_q^+ a_q + b_q^+ b_q\right)$$

$$-\,2JS\sum_q \gamma(q)\left(a_q b_q + b_q^+ a_q^+\right)$$

This H has exactly the same form as for $K=0$, only with $z \to z' = z + \frac{K}{|J|}$. Therefore, applying what we found for $K=0$:

$$\underline{\underline{\omega_q = 2|J|S\left(\left(z+\frac{K}{J}\right)^2 - \gamma_q^2\right)^{1/2}}}$$

<u>1c)</u> Add an external magnetic field to the problem

$$-h\sum_{i\in A}\left(S - a_i^+ a_i\right) - h\sum_{i\in B}\left(-S + b_i^+ b_i\right)$$

$$= \underbrace{-hSN + hSN}_{=0}$$

$$+ h\sum_i \left(a_i^+ a_i - b_i^+ b_i\right)$$

i now runs over $\Diamond$ - lattice instead of $\square$ - lattice

Fourier - transform:

$$h\sum_q \left(a_q^+ a_q - b_q^+ b_q\right)$$

Next, use Bogoliubov - transf. to express this in terms of $A_q^+ A_q$, $B_q^+ B_q$.

Using the Bogoliubov-transform, we have

$$a_q^+ a_q - b_q^+ b_q$$

$$= (u_q A_q^+ - v_q B_q)(u_q A_q - v_q B_q^+)$$

$$- (-v_q A_q + u_q B_q^+)(-v_q A_q^+ + u_q B_q)$$

$$= u_q^2 A_q^+ A_q - u_q v_q A_q^+ B_q^+ - v_q u_q B_q A_q + v_q^2 B_q B_q^+$$

$$- [v_q^2 A_q A_q^+ - u_q v_q A_q - u_q v_q B_q^+ A_q^+ + u_q^2 B_q^+ B_q]$$

$$= (u_q^2 - v_q^2) A_q^+ A_q - (u_q^2 - v_q^2) B_q^+ B_q$$

$$= \underline{\underline{A_q^+ A_q - B_q^+ B_q}}$$

<u>1d)</u> $$H = \tilde{E}_0 + \sum_q \omega_q (A_q^+ A_q + B_q^+ B_q) + h \sum_q (A_q^+ A_q - B_q^+ B_q)$$

$$= \tilde{E}_0 + \sum_q \omega_q^+ A_q^+ A_q + \omega_q^- B_q^+ B_q$$

$$\omega_q^{\pm} = \omega_q \pm h$$

Thus, an applied magnetic field splits the magnon-modes that were degenerate in zero magnetic field.

(c) ω_q increases monotonically with q. Hence, it is minimum at $q = 0$

$$\omega^{-} = \omega_q - h$$

If $\omega^{-} < 0$, our starting point with small spin-fluctuations around an ordered Néel state with spins „up" <u>and</u> „down" along the z-axis, breaks down, since we can gain energy by producing B-magnons even in the ground state.

$q \to 0 \qquad \omega_q^- = 0 \implies$

$$2|J|S\left(\left(z+\frac{K}{|J|}\right)^2 - z^2\right)^{1/2} - h = 0$$

$$\underline{\underline{h_{max} = 2|J|S\left(\left(z+\frac{K}{|J|}\right)^2 - z^2\right)^{1/2}}}$$

1e) When $h > h_{max}$, the „down" spins will be twisted along the z-axis and prefer to point „up". Thus, our starting assumption of an ordered state with equally many „up" and „down", plus small fluctuations, will break down.

2a) $$H = -t \sum_{\langle ij \rangle} a_i^+ a_j + \frac{U}{2} \sum_i n_i (n_i - 1)$$

$(t, U) > 0$

First term: Hopping term of bosons on the lattice, i.e. kinetic energy

Second term: Onsite repulsion-term which tends to suppress multiple occupancy on each lattice site.

2b) Introducing Fourier-transformed operators, the kinetic energy term becomes

$$-t \sum_{\langle ij \rangle} a_i^+ a_j = \sum_k \varepsilon_k a_k^+ a_k$$

with $$\underline{\underline{\varepsilon_k = -t \sum_{\vec{\delta}} e^{i \vec{k} \cdot \vec{\delta}}}}$$

where $\vec{\delta}$ are the vectors that connect a site $\underline{i}$ to its nearest neighbors j

$$\frac{U}{2}\sum_i n_i(n_i-1) = \frac{U}{2}\sum_i (n_i n_i - n_i)$$

$$= \frac{U}{2}\sum_i (a_i^+ a_i a_i^+ a_i - a_i^+ a_i)$$

$$= \frac{U}{2}\sum_i a_i^+ a_i^+ a_i a_i + a_i^+ a_i - a_i^+ a_i)$$

$$= \frac{U}{2}\sum_i a_i^+ a_i^+ a_i a_i$$

$$= \frac{U}{2}\frac{1}{N^2}\sum_i \sum_{k_1 \cdots k_4} a_{k_1}^+ a_{k_2}^+ a_{k_3} a_{k_4} e^{-i(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\cdot \vec{r}_i}$$

$$= \frac{U}{2N}\sum_{k_1 \cdots k_4} a_{k_1}^+ a_{k_2}^+ a_{k_3} a_{k_4}\, \delta_{k_1+k_2,\, k_3+k_4}$$

$$U_{k_1 k_2 k_3 k_4} = \frac{U}{N}$$

2c) The model we have from 2b) is precisely the Bose-Hubbard model we have considered in the lectures. We may therefore use the results from there:

N_0: # particles in the ground state

$$N = N_0 + \sum_{k\neq 0} V_k^2 + \sum_{k\neq 0} \frac{u_k^2 + V_k^2}{e^{\beta E_k} - 1}$$

Condensate fraction

$$\frac{N_0}{N} = 1 - \frac{1}{N}\sum_{k\neq 0} V_k^2 - \frac{1}{N}\sum_{k\neq 0} \frac{u_k^2 + V_k^2}{e^{\beta E_k} - 1} \quad (**)$$

$$V_k^2 = \frac{1}{2}\left(-1 + \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - \varepsilon_2^2}}\right) = -1 + u_k^2$$

$$E_k = \sqrt{\varepsilon_k(\varepsilon_k + Un)} \quad (*)$$

$$\varepsilon_1 = \varepsilon_k + Un \; , \quad \varepsilon_2 = Un$$

$$n = \frac{N}{N_L}$$

NB!! In deriving the expression (*) for E_k, ε_k means the energy measured with respect to the lowest possible energy!

We had from 2b $\varepsilon_k = -t\sum_{\delta} e^{i\vec{k}\cdot\vec{\delta}}$

Lowest possible energy: at $\vec{k} = 0$.

$\varepsilon_0 = -zt$

E_k measured relative to ε_0:

$$E_k - \varepsilon_0 = zt - t\sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}}$$

Small $\vec{k}$:

$E_k \simeq A^2 k^2$ relative to minimum!

The expression for $\frac{N_0}{N}$ applies

in the limit where $N_0 \gg N_{>0}$

such that $N = N_0 + N_{>0}$

$N^2 \simeq N_0^2 + 2 N_0 N_{>0}$

Here $N_{>0}$ is the # particles outside

the $k=0$ condensate.

<u>2d)</u> Thermal correction to $\frac{N_0}{N}$

is represented by the term

$$-\frac{1}{N}\sum_{\vec{k}\neq 0}\frac{(u_k^2+v_k^2)}{e^{\beta E_k}-1}$$

where we <u>must</u> compute all energies

as measured relative to the minimum

Convert the sum to an integral

$$-\frac{1}{(2\pi)^d}\,\Omega_d \int_0^\infty dk\; k^{d-1}\,\frac{\tilde{A}/k}{e^{\beta c k}-1}$$

where we have used that

$$U_k^2+V_k^2 \approx \sqrt{\frac{U n}{2}}\;\frac{1}{\beta k} = \frac{\tilde{A}}{k}$$

Ω_d: Solid angle in d dimensions

$E_k \simeq c k$

at low k. At low T, only small k contribute to the integral. $\beta = \frac{1}{k_B T}$

$x \equiv \beta c k$

Thermal correction:

$$-\frac{\Omega_d}{(2\pi)^d}\,\tilde{A}\left(\frac{1}{\beta c}\right)^{d-1}\int_0^\infty dx\,\frac{x^{d-2}}{e^x-1}$$

$$\int_0^\infty dx\,\frac{x^{d-2}}{e^x-1} = \zeta(d-1)\,\Gamma(d-1)$$

$\zeta(x)$: Riemann ζ-function

$\Gamma(x)$: Gamma-function.

Thermal corrections: $\sim T^{d-1}$

2e) If the thermal corrections to $\frac{N_0}{N}$ diverge at arbitrarily low T, BEC will not take place.

The Riemann ζ-function diverges when its argument ≤ 1

This happens when $d-1 \leq 1$ in this case, i.e. $d \leq 2$

$d > 2$ for BEC to take place in the Bose Hubbard model