

# TFY4210, Quantum theory of many-particle systems, 2016:

## Solution to tutorial 7

### 1. Bogoliubov transformation for bosons.

(a) Calculate  $[a_1, a_1^\dagger] = 1$ :

$$1 = [a_1, a_1^\dagger] = [ub_1 - vb_2^\dagger, ub_1^\dagger - vb_2] = u^2 \underbrace{[b_1, b_1^\dagger]}_1 + v^2 \underbrace{[b_2^\dagger, b_2]}_{-1} = u^2 - v^2. \quad (1)$$

(b) We have

$$\begin{aligned} a_1^\dagger a_1 &= (ub_1^\dagger - vb_2)(ub_1 - vb_2^\dagger) \\ &= u^2 b_1^\dagger b_1 + v^2 \underbrace{b_2 b_2^\dagger}_{b_2^\dagger b_2 + 1} - uv b_1^\dagger b_2^\dagger - uv b_2 b_1 \\ &= u^2 b_1^\dagger b_1 + v^2 b_2^\dagger b_2 - uv(b_1 b_2 + \text{h.c.}) + v^2. \end{aligned} \quad (2)$$

By the symmetry in the definitions, the result for  $a_2^\dagger a_2$  is obtained by letting  $1 \leftrightarrow 2$  in the final expression:

$$a_2^\dagger a_2 = u^2 b_2^\dagger b_2 + v^2 b_1^\dagger b_1 - uv(b_1 b_2 + \text{h.c.}) + v^2. \quad (3)$$

Thus

$$\varepsilon(a_1^\dagger a_1 + a_2^\dagger a_2) = \varepsilon(u^2 + v^2)(b_1^\dagger b_1 + b_2^\dagger b_2) - 2\varepsilon uv(b_1 b_2 + \text{h.c.}) + 2\varepsilon v^2. \quad (4)$$

Furthermore,

$$\begin{aligned} a_1 a_2 &= (ub_1 - vb_2^\dagger)(ub_2 - vb_1^\dagger) \\ &= u^2 b_1 b_2 + v^2 b_2^\dagger b_1^\dagger - uv(\underbrace{b_1 b_1^\dagger}_{b_1^\dagger b_1 + 1} + b_2^\dagger b_2) \\ &= u^2 b_1 b_2 + v^2 b_2^\dagger b_1^\dagger - uv(b_1^\dagger b_1 + b_2^\dagger b_2) - uv. \end{aligned} \quad (5)$$

Thus

$$\Delta(a_1 a_2 + \text{h.c.}) = \Delta(u^2 + v^2)(b_1 b_2 + \text{h.c.}) - 2\Delta uv(b_1^\dagger b_1 + b_2^\dagger b_2) - 2\Delta uv. \quad (6)$$

This gives

$$\begin{aligned} H &= \varepsilon(a_1^\dagger a_1 + a_2^\dagger a_2) + \Delta(a_1 a_2 + \text{h.c.}) \\ &= [\varepsilon(u^2 + v^2) - \Delta \cdot 2uv](b_1^\dagger b_1 + b_2^\dagger b_2) \\ &\quad + [\Delta(u^2 + v^2) - \varepsilon \cdot 2uv](b_1 b_2 + \text{h.c.}) \\ &\quad + (\varepsilon \cdot 2v^2 - \Delta \cdot 2uv). \end{aligned} \quad (7)$$

This expression is diagonal in  $b$ -bosons provided that the coefficient of  $(b_1 b_2 + \text{h.c.})$  vanishes, i.e.

$$\Delta(u^2 + v^2) = \varepsilon \cdot 2uv. \quad (8)$$

With  $u = \cosh \eta$ ,  $v = \sinh \eta$  this condition becomes

$$\Delta \cosh 2\eta = \varepsilon \sinh 2\eta, \quad (9)$$

i.e.

$$\tanh 2\eta = \frac{\Delta}{\varepsilon}. \quad (10)$$

With this choice of  $\eta$ ,  $H$  becomes

$$H = F(b_1^\dagger b_1 + b_2^\dagger b_2) + G \quad (11)$$

with

$$F = \varepsilon(u^2 + v^2) - \Delta \cdot 2uv, \quad (12)$$

$$G = \varepsilon \cdot 2v^2 - \Delta \cdot 2uv. \quad (13)$$

It remains to simplify the expressions for  $F$  and  $G$  so that they are given in terms of the model parameters  $\varepsilon$  and  $\Delta$  only. First consider

$$\begin{aligned} F &= \varepsilon \cosh 2\eta - \Delta \sinh 2\eta = \cosh 2\eta (\varepsilon - \Delta \tanh 2\eta) \\ &= \cosh 2\eta \left( \varepsilon - \Delta \cdot \frac{\Delta}{\varepsilon} \right) = \frac{\cosh 2\eta}{\varepsilon} (\varepsilon^2 - \Delta^2) \end{aligned} \quad (14)$$

Using the hyperbolic identity  $\cosh^2 x = (1 - \tanh^2 x)^{-1}$  we have

$$\cosh^2 2\eta = \frac{1}{1 - \tanh^2 2\eta} = \frac{1}{1 - \left(\frac{\Delta}{\varepsilon}\right)^2} = \frac{\varepsilon^2}{\varepsilon^2 - \Delta^2}. \quad (15)$$

Thus

$$\cosh 2\eta = \frac{\varepsilon}{\sqrt{\varepsilon^2 - \Delta^2}} \quad (16)$$

(only the positive root exists since the cosh function is positive for all arguments). Inserting this into (14) gives

$$F = \sqrt{\varepsilon^2 - \Delta^2}. \quad (17)$$

Next, we have

$$\begin{aligned} G &= \varepsilon(v^2 + v^2) - \Delta \cdot 2uv = \varepsilon(u^2 + v^2 - 1) - \Delta \cdot 2uv \\ &= \varepsilon(u^2 + v^2) - \Delta \cdot 2uv - \varepsilon = F - \varepsilon, \end{aligned} \quad (18)$$

i.e.

$$G = \sqrt{\varepsilon^2 - \Delta^2} - \varepsilon. \quad (19)$$

(c) Since Eq. (11) expresses  $H$  as a linear combination of the number operators for  $b_1$ -bosons and  $b_2$ -bosons, the eigenstates of  $H$  contain definite numbers of these bosons and can be labeled by these two numbers, which are both nonnegative integers. Thus let us write the eigenstates as  $|n_{b_1}, n_{b_2}\rangle$  where  $n_{b_1}$  is the number of  $b_1$ -bosons and  $n_{b_2}$  is the number of

$b_2$ -bosons. The associated energy eigenvalue of  $H$  is  $F(n_{b_1} + n_{b_2}) + G \equiv E(n_{b_1}, n_{b_2})$ .

Since  $\varepsilon$  and  $\Delta$  are positive with  $\varepsilon > \Delta$  it follows that  $F > 0$ . Thus the lowest energy is obtained for  $n_{b_1} = n_{b_2} = 0$ , corresponding to the eigenstate  $|n_{b_1} = 0, n_{b_2} = 0\rangle \equiv |\Psi_0\rangle$ , which is therefore the ground state of  $H$ . Since there are no  $b_1$  or  $b_2$ -bosons in  $|\Psi_0\rangle$ , acting on  $|\Psi_0\rangle$  with the annihilation operator  $b_1$  or the annihilation operator  $b_2$  will give 0:

$$b_i|\Psi_0\rangle = 0, \quad (i = 1, 2). \quad (20)$$

Another way of saying this is that  $|\Psi_0\rangle$  is the vacuum state of the  $b$ -bosons. The ground state energy is  $E(n_{b_1} = 0, n_{b_2} = 0) = G = \sqrt{\varepsilon^2 - \Delta^2} - \varepsilon$ .

(d) The first excited states have one  $b$ -boson, either of the  $b_1$ -type or of the  $b_2$ -type (both cost the same energy  $F$  to create). Thus the first excited states are  $|n_{b_1} = 1, n_{b_2} = 0\rangle$  and  $|n_{b_1} = 0, n_{b_2} = 1\rangle$  and their energy is  $E(n_{b_1} = 1, n_{b_2} = 0) = E(n_{b_1} = 0, n_{b_2} = 1) = F + G$ .<sup>1</sup>

(e) We have

$$a_1 = ub_1 - vb_2^\dagger \Rightarrow ua_1 = u^2b_1 - uvb_2^\dagger, \quad (21)$$

$$a_2^\dagger = ub_2^\dagger - vb_1 \Rightarrow va_2^\dagger = uvb_2^\dagger - v^2b_1. \quad (22)$$

Adding the two rightmost equations, the coefficients of  $b_2^\dagger$  cancel, while the total coefficient of  $b_1$  is seen to be  $u^2 - v^2$ , which equals 1. Thus

$$b_1 = ua_1 + va_2^\dagger. \quad (23)$$

(f) We want to show that the given expression for  $|\Psi_0\rangle$  satisfies

$$b_1|\Psi_0\rangle = 0. \quad (24)$$

Define  $\lambda = \tanh \eta$  and insert the expressions for  $b_1$  and  $|\Psi_0\rangle$  in terms of  $a$ -bosons. This gives

$$b|\Psi_0\rangle \propto (ua_1 + va_2^\dagger) \exp(-\lambda a_1^\dagger a_2^\dagger) |0\rangle. \quad (25)$$

Let us try to move  $a_1$  past the exponential so that we can use<sup>2</sup>  $a_1|0\rangle = 0$  to simplify things. However, note that  $a_1$  does not commute with the argument of the exponential. We can however write

$$\begin{aligned} a_1 \exp(-\lambda a_1^\dagger a_2^\dagger) |0\rangle &= \underbrace{\exp(-\lambda a_1^\dagger a_2^\dagger) \exp(\lambda a_1^\dagger a_2^\dagger)}_I a_1 \exp(-\lambda a_1^\dagger a_2^\dagger) |0\rangle \\ &= \exp(-\lambda a_1^\dagger a_2^\dagger) \underbrace{\exp(\lambda a_1^\dagger a_2^\dagger) a_1 \exp(-\lambda a_1^\dagger a_2^\dagger)}_{\text{use Baker-Hausdorff formula to calculate}} |0\rangle \end{aligned} \quad (26)$$

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<sup>1</sup>As a check of the correctness of the results in (c) and (d) for the energy of the ground state and the first excited states, note that for  $\Delta = 0$  these energies reduce to 0 and  $\varepsilon$ , respectively, which agrees with what one finds from the defining expression for  $H$  when  $\Delta = 0$  (the energies can then be deduced from direct inspection of this expression, as a Bogoliubov transformation is then unnecessary since in the absence of the  $\Delta$ -term  $H$  is in diagonal form from the outset).

<sup>2</sup>Note that we have defined the state denoted  $|0\rangle$  as the vacuum of the  $a$ -bosons while  $|\Psi_0\rangle$  is the vacuum of the  $b$ -bosons. Do not confuse these two vacuum states!

The first term on the rhs of the Baker-Hausdorff formula is just  $a_1$ . The second term is the commutator

$$[a_1, -\lambda a_1^\dagger a_2^\dagger] = -\lambda a_2^\dagger [a_1, a_1^\dagger] = -\lambda a_2^\dagger. \quad (27)$$

Since this expression commutes with  $-\lambda a_1^\dagger a_2^\dagger$ , all higher order terms in the Baker-Hausdorff expansion vanish. Thus

$$\exp(\lambda a_1^\dagger a_2^\dagger) a_1 \exp(-\lambda a_1^\dagger a_2^\dagger) = a_1 - \lambda a_2^\dagger \Rightarrow a_1 \exp(-\lambda a_1^\dagger a_2^\dagger) = \exp(-\lambda a_1^\dagger a_2^\dagger) (a_1 - \lambda a_2^\dagger). \quad (28)$$

Also using that  $a_2^\dagger \exp(-\lambda a_1^\dagger a_2^\dagger) = \exp(-\lambda a_1^\dagger a_2^\dagger) a_2^\dagger$  (which follows since  $a_2^\dagger$  commutes with the argument of the exponential) we get

$$\begin{aligned} (ua_1 + va_2^\dagger) \exp(-\lambda a_1^\dagger a_2^\dagger) |0\rangle &= ua_1 \exp(-\lambda a_1^\dagger a_2^\dagger) |0\rangle + va_2^\dagger \exp(-\lambda a_1^\dagger a_2^\dagger) |0\rangle \\ &= \exp(-\lambda a_1^\dagger a_2^\dagger) [u(a_1 - \lambda a_2^\dagger) + va_2^\dagger] |0\rangle \\ &= \exp(-\lambda a_1^\dagger a_2^\dagger) [-u\lambda + v] a_2^\dagger |0\rangle \\ &= 0 \end{aligned} \quad (29)$$

which concludes the proof. Here we used  $a_1 |0\rangle = 0$  (to get the penultimate line) before using

$$-u\lambda + v = -\cosh \eta \tanh \eta + \sinh \eta = 0. \quad (30)$$

## **2. Ferromagnetic Heisenberg model with a spin anisotropy revisited.**

For  $D \geq 0$  we found  $\Delta = 2SD$  (for details, see the solution to tutorial 6).

For  $D = 0$ ,  $\Delta = 0$ . This means that we have gapless magnons in this case ( $\omega_{\mathbf{k}} \rightarrow 0$  as  $\mathbf{k} \rightarrow 0$ ). Note that for  $D = 0$  the Hamiltonian  $H$  reduces to the Heisenberg model  $H_{\text{Heis}}$  which is invariant under identical rotations of all spins around an arbitrary axis by an arbitrary angle, which is a continuous symmetry. As the ground states break this continuous symmetry, Goldstone's theorem is applicable and thus predicts the existence of gapless magnons. So our result  $\Delta = 0$  for  $D = 0$  is also predicted by the Goldstone theorem.

For  $D > 0$ ,  $\Delta > 0$ . Thus the magnons are gapped. In this case the continuous symmetry of  $H$  is restricted to rotations by an arbitrary angle around the  $z$  axis only, as the term  $H_D$  is not invariant under arbitrary rotations around other axes. In this case there are only two ground states, one with spins ordering along the  $+z$  direction and the other with spins ordering along the  $-z$  direction, and these ground states are invariant under arbitrary rotations around the  $z$  axis. Hence this continuous symmetry is not broken by the ground states in this case. (The ground states merely break the *discrete* symmetry of  $H$  given by the transformation  $S_i^z \rightarrow -S_i^z$ ,  $S_i^+ \leftrightarrow S_i^-$  for all  $i$ .) Therefore Goldstone's theorem is not applicable in this case, and so the absence of gapless magnons is not a contradiction of Goldstone's theorem.

### 3. The total $S^z$ operator for the antiferromagnetic Heisenberg model.

(a) We have

$$\begin{aligned} S^z &= \sum_j S_j^z = \sum_{j \in A} S_j^z + \sum_{j \in B} S_j^z = \sum_{j \in A} (S - a_j^\dagger a_j) + \sum_{j \in B} (-S + b_j^\dagger b_j) \\ &= \sum_{j \in B} b_j^\dagger b_j - \sum_{j \in A} a_j^\dagger a_j. \end{aligned} \quad (31)$$

Fourier transforming to operators  $b_{\mathbf{k}}$ ,

$$b_j = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_j} b_{\mathbf{k}} \quad (32)$$

where  $N/2$  is the number of sites on the B (and A) sublattice and the sum goes over the magnetic Brillouin zone, gives

$$\sum_{j \in B} b_j^\dagger b_j = \sum_{\mathbf{k}, \mathbf{k}'} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \underbrace{\frac{2}{N} \sum_{j \in B} e^{-i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}_j}}_{\delta_{\mathbf{k}, \mathbf{k}'}} = \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \quad (33)$$

and similarly,  $\sum_{j \in A} a_j^\dagger a_j = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ , thus giving

$$S^z = \sum_{\mathbf{k}} (b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - a_{\mathbf{k}}^\dagger a_{\mathbf{k}}). \quad (34)$$

Now introduce the Bogoliubov transformation to  $\alpha$  and  $\beta$  operators:

$$a_{\mathbf{k}} = u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \beta_{-\mathbf{k}}^\dagger, \quad (35)$$

$$b_{\mathbf{k}} = u_{\mathbf{k}} \beta_{\mathbf{k}} + v_{\mathbf{k}} \alpha_{-\mathbf{k}}^\dagger. \quad (36)$$

This gives (using also the bosonic commutation relations and that the coefficient functions  $u_{\mathbf{k}}$  and  $v_{\mathbf{k}}$  are real)

$$\begin{aligned} S^z &= \sum_{\mathbf{k}} [(u_{\mathbf{k}} \beta_{\mathbf{k}}^\dagger + v_{\mathbf{k}} \alpha_{-\mathbf{k}})(u_{\mathbf{k}} \beta_{\mathbf{k}} + v_{\mathbf{k}} \alpha_{-\mathbf{k}}^\dagger) - (u_{\mathbf{k}} \alpha_{\mathbf{k}}^\dagger + v_{\mathbf{k}} \beta_{-\mathbf{k}})(u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \beta_{-\mathbf{k}}^\dagger)] \\ &= \sum_{\mathbf{k}} [u_{\mathbf{k}}^2 \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} - v_{\mathbf{k}}^2 (\beta_{-\mathbf{k}}^\dagger \beta_{-\mathbf{k}} + 1) - u_{\mathbf{k}}^2 \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + v_{\mathbf{k}}^2 (\alpha_{-\mathbf{k}}^\dagger \alpha_{-\mathbf{k}} + 1) \\ &\quad + u_{\mathbf{k}} v_{\mathbf{k}} (\alpha_{-\mathbf{k}} \beta_{\mathbf{k}} - \alpha_{\mathbf{k}} \beta_{-\mathbf{k}} + \text{h.c.})] \end{aligned} \quad (37)$$

Let us change summation variable from  $\mathbf{k}$  to  $-\mathbf{k}$  in the first term on the last line (if you prefer, first define  $\mathbf{k}' = -\mathbf{k}$ , rewrite the sum as a sum over  $\mathbf{k}'$  (which goes over exactly the same set of wavevectors as the sum over  $\mathbf{k}$  since the magnetic Brillouin zone has inversion symmetry about the origin) and then rename  $\mathbf{k}'$  as  $\mathbf{k}$ ) and use  $u_{-\mathbf{k}} = u_{\mathbf{k}}$ ,  $v_{-\mathbf{k}} = v_{\mathbf{k}}$ . After doing the sum the first and second term on the last line then cancel, and thus the contribution

from the h.c. on the same line also vanishes. Furthermore, we use  $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$  to simplify the first line, giving

$$S^z = \sum_{\mathbf{k}} [\beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} - \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}]. \quad (38)$$

(b) The Hamiltonian can be written as a sum of  $N$  independent harmonic oscillator Hamiltonians (for each of the  $N/2$   $\mathbf{k}$ -vectors in the magnetic Brillouin zone there are two oscillators, one of  $\alpha$  type and one of  $\beta$  type):

$$H = E_0 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} [\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}] \equiv E_0 + \sum_{\mathbf{k}} \omega_{\mathbf{k}} [\hat{n}_{\alpha_{\mathbf{k}}} + \hat{n}_{\beta_{\mathbf{k}}}] \quad (39)$$

where  $\hat{n}_{\alpha_{\mathbf{k}}} = \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}$  and  $\hat{n}_{\beta_{\mathbf{k}}} = \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}$  are the respective number operators. The eigenstates  $|\Psi\rangle$  of  $H$  are therefore eigenstates of these number operators and can be written

$$|\Psi(\{n_{\alpha_{\mathbf{k}}}, n_{\beta_{\mathbf{k}}}\})\rangle \propto \prod_{\mathbf{k}} \left[ (\alpha_{\mathbf{k}}^\dagger)^{n_{\alpha_{\mathbf{k}}}} (\beta_{\mathbf{k}}^\dagger)^{n_{\beta_{\mathbf{k}}}} \right] |G\rangle \quad (40)$$

where the product goes over all wavevectors in the magnetic Brillouin zone,  $n_{\alpha_{\mathbf{k}}}$  and  $n_{\beta_{\mathbf{k}}}$  denote the number of magnons in the various oscillators, and  $|G\rangle$  is the vacuum state of the  $\alpha$ - and  $\beta$ -bosons and thus also the ground state of  $H$  (the use of  $\propto$  instead of an equality sign is due to the omission of normalization factors; for these, see e.g. the discussion of second quantization for bosons in Sec. 2.2 in the lecture notes on second quantization).

As Eq. (38) expresses  $S^z$  entirely in terms of the above-mentioned number operators, the eigenstates of  $H$  are also eigenstates of  $S^z$ . The associated eigenvalues are  $\sum_{\mathbf{k}} (n_{\beta_{\mathbf{k}}} - n_{\alpha_{\mathbf{k}}})$ , as seen by acting with  $S^z$  on  $|\Psi\rangle$ :

$$S^z |\Psi\rangle = \sum_{\mathbf{k}} (\hat{n}_{\beta_{\mathbf{k}}} - \hat{n}_{\alpha_{\mathbf{k}}}) |\Psi\rangle = \sum_{\mathbf{k}} (n_{\beta_{\mathbf{k}}} - n_{\alpha_{\mathbf{k}}}) |\Psi\rangle. \quad (41)$$