TFY 4210 exam 2014

Solution sketch

Problem 1 (a) Single-particle operator

$\Rightarrow$ In second quantization,

$$H = \sum_{\alpha\beta} \langle\alpha|\hat{h}|\beta\rangle \, c_\alpha^\dagger c_\beta$$

where $\langle\alpha|\hat{h}|\beta\rangle = \int dx \; \phi_\alpha^*(x)\, \hat{h}(x)\, \phi_\beta(x)$

No spin $\Rightarrow$ $x \to$ spatial coordinate (called z here)

$$\hat{h} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}$$

Momentum basis: $\alpha \to k$,
with eigenfunctions

$$\phi_k(z) = \frac{1}{\sqrt{L}} e^{ikz} \qquad \text{(plane waves)}$$

$$\Rightarrow \langle\alpha|\hat{h}|\beta\rangle = \langle k|\hat{h}|k'\rangle$$

$$= \int_0^L dz \, \frac{1}{\sqrt{L}} e^{-ikz} \left(-\frac{\hbar^2}{2m}\right) \underbrace{\frac{\partial^2}{\partial z^2} e^{ik'z}}_{(ik')^2 e^{ik'z}} \cdot \frac{1}{\sqrt{L}}$$

$$= \frac{\hbar^2 (k')^2}{2m} \underbrace{\frac{1}{L}\int_0^L dz\, e^{-i(k-k')z}}_{\delta_{kk'}} = \frac{\hbar^2 k^2}{2m}\delta_{kk'}$$

$$\Rightarrow \quad H = \sum_{kk'} \langle k|\hat{h}|k'\rangle c_k^\dagger c_{k'}$$

$$= \sum_{kk'} \frac{\hbar^2 k^2}{2m} \delta_{kk'} c_k^\dagger c_{k'} = \sum_{k} \frac{\hbar^2 k^2}{2m} c_k^\dagger c_k$$

$$\equiv \underline{\underline{\sum_k \varepsilon_k c_k^\dagger c_k}} \quad \Rightarrow \quad \underline{\underline{\varepsilon_k = \frac{\hbar^2 k^2}{2m}}}$$

(b)

1. $$H|\ell\rangle = \sum_{k'} \xi_{k'} \hat{n}_{k'} \prod_{k \in S_\ell} c_k^\dagger |0\rangle$$

Consider a particular k' in the sum.
If $k' \notin S_\ell$, $\hat{n}_{k'}$ can be commuted past all $c_k^\dagger$ operators (using $[\hat{n}_{k'}, c_k^\dagger] = 0$) and then gives $\hat{n}_{k'}|0\rangle = 0$, so no contribution.

If $k' \in S_\ell$, $\hat{n}_{k'}$ can be commuted past all $c_k^\dagger$ operator with $k \neq k'$ until it stands to the immediate left of $c_{k'}^\dagger$. Then use

$$n_{k'} c_{k'}^\dagger = c_{k'}^\dagger n_{k'} + c_{k'}^\dagger$$

$n_{k'}$ can be commuted further to the right using $[n_{k'}, c_k^\dagger] = 0$ and then giving $n_{k'}|0\rangle = 0$, ~~so~~ no contribution. So we are left with the second term $c_{k'}^\dagger$.

$$\Rightarrow \quad n_{k'}|\ell\rangle = |\ell\rangle \quad \text{if} \quad k' \in S_\ell$$
$$n_{k'}|\ell\rangle = 0 \quad \text{if} \quad k' \notin S_\ell$$

$\Rightarrow \; H|l\rangle = \sum_{k \in S_l} \xi_k |l\rangle = E_l |l\rangle$

$\Rightarrow \; |l\rangle$ is an eigenstate of H with eigenvalue

$$E_l = \sum_{k \in S_l} \xi_k$$

2. The ground state is obtained by occupying all k-states having $\xi_k < 0$ with one fermion (no more are allowed due to the Pauli principle) and leaving all k-states having $\xi_k > 0$ unoccupied.

$\Rightarrow$ ground state is $|G\rangle \equiv \prod_{\substack{k \\ \text{s.t. } \xi_k < 0}} c_k^\dagger |0\rangle$

ground state energy is $E_0 = \sum_{\substack{k \text{ s.t.} \\ \xi_k < 0}} \xi_k$

("s.t" $\hat{=}$ "such that")

(c)

1. $$\int_{-\infty}^{\infty} d\omega \, A(\nu,\omega) = \frac{1}{Z} \sum_{l,m} |\langle m | c_\nu^\dagger | l \rangle|^2 \cdot \left(e^{-\beta E_l} + e^{-\beta E_m}\right) \cdot \underbrace{\int_{-\infty}^{\infty} d\omega \, \delta(\omega + E_l - E_m)}_{=1}$$

$$= \frac{1}{Z} \sum_{l,m} |\langle m | c_v^\dagger | l \rangle|^2 \left(e^{-\beta E_l} + e^{-\beta E_m} \right)$$

$$= \frac{1}{Z} \sum_{l,m} \Big[\langle l | c_v | m \rangle \langle m | c_v^\dagger | l \rangle \, e^{-\beta E_l}$$
$$+ \langle m | c_v^\dagger | l \rangle \langle l | c_v | m \rangle \, e^{-\beta E_m} \Big]$$

use $\sum_m |m\rangle\langle m| = I$ in first line and
$\sum_l |l\rangle\langle l| = I$ in second line

$$\Rightarrow \int_{-\infty}^{\infty} d\omega \, A(v,\omega) = \frac{1}{Z} \Big[\sum_l \langle l | c_v c_v^\dagger | l \rangle e^{-\beta E_l}$$
$$+ \sum_l \langle l | c_v^\dagger c_v | l \rangle e^{-\beta E_l} \Big]$$

(where we changed $m \to l$ in second line)

$$= \frac{1}{Z} \sum_l e^{-\beta E_l} \langle l | \underbrace{\left(c_v c_v^\dagger + c_v^\dagger c_v \right)}_{=1} | l \rangle$$

$$\overset{\text{use } \langle l | l \rangle = 1}{=} \frac{1}{Z} \underbrace{\sum_l e^{-\beta E_l}}_{Z} = \underline{\underline{1}}$$

2. $$A(k,\omega) = \frac{1}{Z} \sum_{l,m} |\langle m | c_k^\dagger | l \rangle|^2$$
$$\cdot \left(e^{-\beta E_l} + e^{-\beta E_m} \right) \cdot \delta(\omega + E_l - E_m)$$

Because of the Pauli principle, $\langle m | c_k^\dagger | l \rangle$ is nonzero only if $k \notin S_l$ and $k \in S_m$.

Furthermore, m is determined when $c_k^\dagger |l\rangle$ is given: $S_m = S_l \underset{\substack{\text{union}\\\text{symbol}}}{\underset{\uparrow}{\cup}} \{k\}$

Then $|\langle m| c_k^\dagger |l\rangle|^2 = 1$ (and 0 otherwise)

$$\Rightarrow A(k,\omega) = \frac{1}{Z} \sum_{\substack{l \\ \text{s.t. } k \text{ is} \\ \text{empty}}} 1 \cdot \left(e^{-\beta E_l} + e^{-\beta E_m} \right) \delta(\omega + E_l - E_m)$$

$E_m = E_l + \xi_k$ (since $S_m = S_l \cup \{k\}$)

$$\Rightarrow A(k,\omega) = \frac{1}{Z} \sum_{\substack{l \\ \text{s.t. } k \text{ is} \\ \text{empty}}} \left(e^{-\beta E_l} + e^{-\beta (E_l + \xi_k)} \right) \cdot \underbrace{\delta(\omega - \xi_k)}_{\substack{\text{indep. of } l, \\ \text{so take outside sum}}}$$

$$= \delta(\omega - \xi_k) \frac{1}{Z} \sum_{\substack{l \\ \text{s.t. } k \text{ is} \\ \text{empty}}} \left(e^{-\beta E_l} + e^{-\beta (E_l + \xi_k)} \right)$$

The sum over l runs over all states with k unoccupied. But $E_l + \xi_k$ is the energy of the state that only differs from l by having k occupied.

$$\Rightarrow \sum_{\substack{l \\ \text{s.t. } k \text{ is} \\ \text{empty}}} \left(e^{-\beta E_l} + e^{-\beta (E_l + \xi_k)} \right) = \sum_{\substack{(\underline{\text{all}} \text{ states}) \\ l}} e^{-\beta E_l} = Z$$

$$\Rightarrow \underline{\underline{A(k,\omega) = \delta(\omega - \xi_k)}}$$

Problem 2.

Both terms in H have exactly the same form, they just differ in the values of the relative position vectors $\vec{r}_j - \vec{r}_i$. In the first term ($\propto J$) they are $\hat{x}$ and $\hat{y}$. In the second term ($\propto J'$) they are $\hat{x}+\hat{y}$ and $-\hat{x}+\hat{y}$.

As the calculation of each term can be done from the solution of Problem 2a in the 2013 exam, I will refer to that solution here for convenience.

The first term in H, $-J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j$,

is obtained from that solution by setting

$$J_z = J_\perp = J \qquad (\text{and } \vec{\delta} = \hat{x}, \hat{y})$$

This gives (Eq. (29)-(31))

$$-J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j = E_0^{(J)} + \sum_{\vec{k}} \omega_{\vec{k}}^{(J)} a_k^\dagger a_k$$

with
$$E_0^{(J)} = -2JNS^2$$
$$\omega_k^{(J)} = 2SJ\left[2 - \cos k_x - \cos k_y\right]$$

The second term in H, $-J'\sum_{\langle\langle ij\rangle\rangle} \vec{S}_i \cdot \vec{S}_j$,

is obtained from that solution by setting

$$J_z = J_\perp = J' \quad \text{and} \quad \vec{\delta} = \hat{x}+\hat{y}, -\hat{x}+\hat{y}$$

This gives

$$-J' \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j = E_0^{(J')} + \sum_{\vec{k}} \omega_k^{(J')} a_k^\dagger a_k$$

with $E_0^{(J')} = -2J' N S^2$

$$\omega_k^{(J')} = 2SJ' [2 - \cos(k_x + k_y) - \cos(-k_x + k_y)]$$

$$= 4SJ' [1 - \cos k_x \cos k_y]$$

Adding the two terms thus gives

$$E_0 = E_0^{(J)} + E_0^{(J')} = \underline{\underline{-2(J+J') N S^2}}$$

$$\omega_k = \omega_k^{(J)} + \omega_k^{(J')} = \underline{\underline{2SJ[2 - \cos k_x - \cos k_y] + 4SJ'[1 - \cos k_x \cos k_y]}}$$

(b).

1. As $\vec{k} \to 0$, $\cos k_x \to 1$ and $\cos k_y \to 1$
$\Rightarrow \omega_{\vec{k}} \to 0 \Rightarrow$ gapless magnons

2. Both terms in H have full spin rotation symmetry (symmetry under arbitrary global spin rotations). The ground state is ferromagnetically ordered and breaks this continuous symmetry. By Goldstone's theorem the system should then have gapless excitations (the magnons). So the answer in (b) 1. is consistent with these arguments/results based on symmetry.

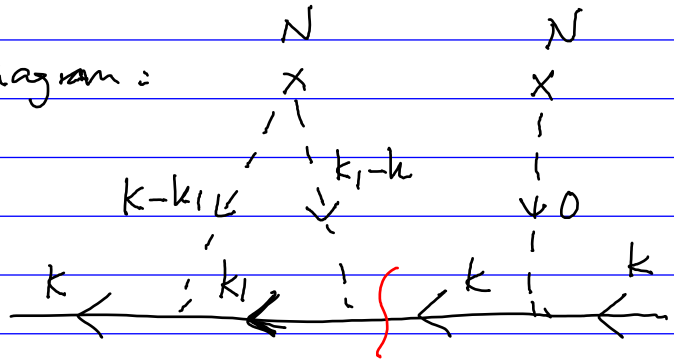
3. A term leading to a reduced symmetry of H, such that the resulting ground state now only breaks a discrete (as opposed to continuous) symmetry. For example the spin anisotropy term

$$-D\sum_j \left(S_j^z\right)^2$$

(cf. Tutorial 6 (Problem 2) and Tutorial 7 (Problem 2)).

Problem 3.

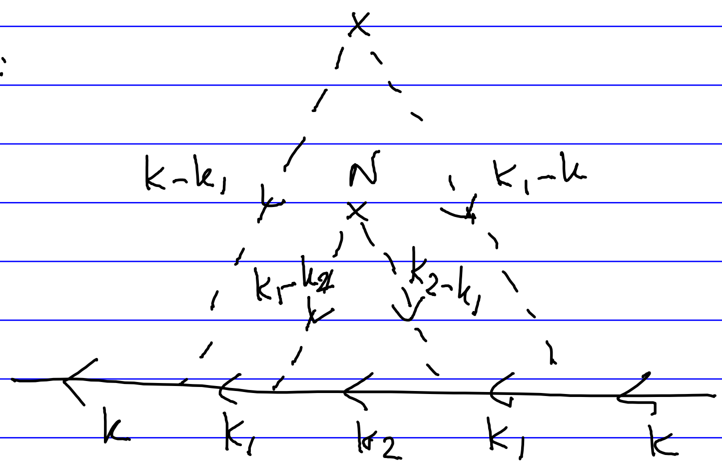
(a)(1+2). First diagram:



$$= N^2 [\mathcal{G}^{(0)}(k)]^3\, U(0) \sum_{\vec{k}_1} U(\vec{k}_1-\vec{k})\, U(\vec{k}-\vec{k}_1)\, \mathcal{G}^{(0)}(\vec{k}_1)$$

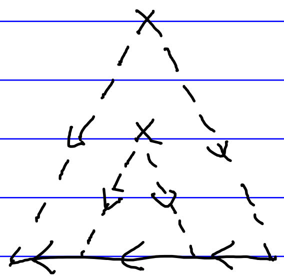
Reducible, i.e. can be cut in two pieces by cutting a single internal electron line (the one crossed by the red line shown)

Second diagram:

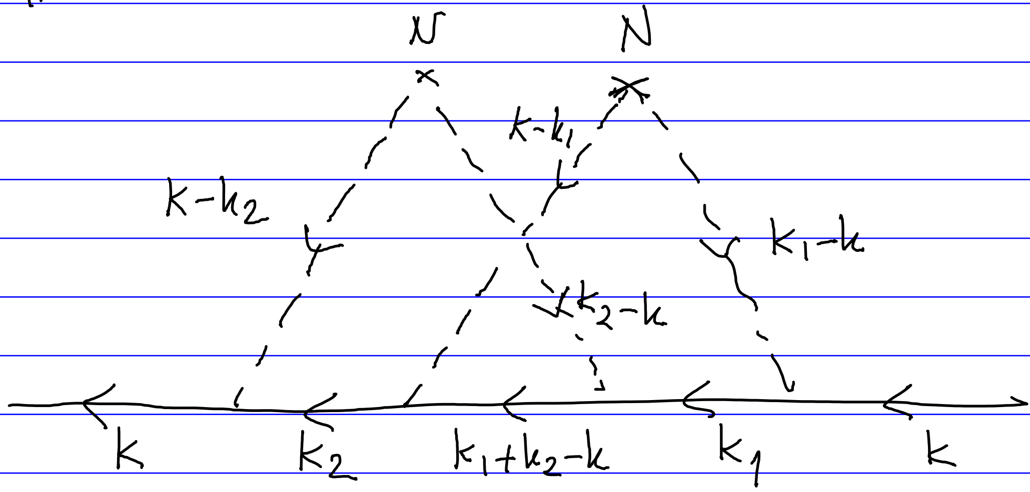


$$= N^2 [g^{(0)}(k)]^2 \sum_{k_1} U(k_1-k)\, U(k-k_1) [g^{(0)}(k_1)]^2 \cdot \sum_{k_2} U(k_1-k_2)\, U(k_2-k_1)\, g^{(0)}(k_2)$$

Irreducible. The self-energy diagram is



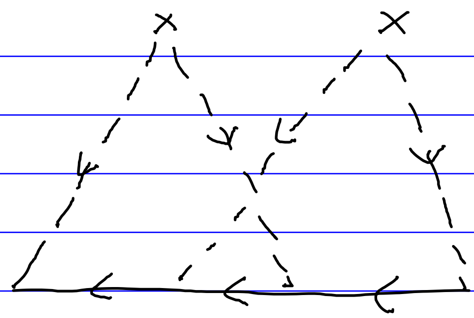
Third diagram:



$$\left(= N^2 [g^{(0)}(k)]^2 \sum_{k_1,k_2} U(k_1-k)\, U(k-k_1)\, U(k_2-k)\, U(k-k_2)\, g^{(0)}(k_1)\, g^{(0)}(k_2)\, g^{(0)}(k_1+k_2-k) \right)$$

Irreducible.

Self-energy diagram:



(b) An arbitrary term in $\bar{\mathcal{G}}(k)$ can be written

$$\mathcal{G}^{(0)}(k)\,\Sigma^{(i)}(k)\,\mathcal{G}^{(0)}(k)\,\Sigma^{(j)}(k)\,\mathcal{G}^{(0)}(k)\cdots\mathcal{G}^{(0)}(k)\,\Sigma^{(l)}(k)\,\mathcal{G}^{(0)}(k)$$

where the number of self-energy factors $\Sigma^{(i)}(k)$ can be $0,1,2,\ldots$ This gives

$$\mathcal{G}^{(0)}(k) = \mathcal{G}^{(0)}(k) + \sum_i \mathcal{G}^{(0)}(k)\Sigma^{(i)}(k)\mathcal{G}^{(0)}(k)$$

$$+\sum_{i,j} \mathcal{G}^{(0)}(k)\Sigma^{(i)}(k)\mathcal{G}^{(0)}(k)\Sigma^{(j)}(k)\mathcal{G}^{(0)}(k) + \cdots = \mathcal{G}^{(0)}(k)$$

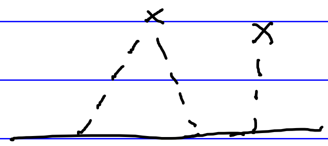
$$+\ \mathcal{G}^{(0)}(k)\Sigma(k)\mathcal{G}^{(0)}(k) + \mathcal{G}^{(0)}(k)\Sigma(k)\mathcal{G}^{(0)}(k)\Sigma(k)\mathcal{G}^{(0)}(k)+\cdots$$

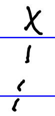
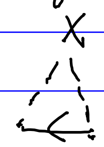
$$= \mathcal{G}^{(0)}(k) + \mathcal{G}^{(0)}(k)\Sigma(k)\underbrace{\left[\mathcal{G}^{(0)}(k) + \mathcal{G}^{(0)}(k)\Sigma(k)\mathcal{G}^{(0)}(k)+\cdots\right]}_{\bar{\mathcal{G}}(k)}$$

ie. $\bar{\mathcal{G}}(k) = \mathcal{G}^{(0)}(k) + \mathcal{G}^{(0)}(k)\Sigma(k)\bar{\mathcal{G}}(k)$

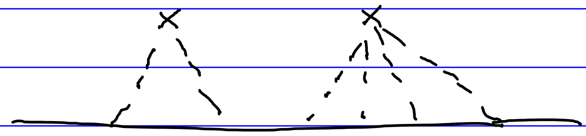
$$\Rightarrow\quad \underline{\underline{\bar{\mathcal{G}}(k)}} = \frac{\mathcal{G}^{(0)}(k)}{1-\Sigma(k)\mathcal{G}^{(0)}(k)} = \underline{\underline{\frac{1}{\left(\mathcal{G}^{(0)}(k)\right)^{-1} - \Sigma(k)}}}$$

(c)

1. The first diagram,  ,

can be written as products of $\mathcal{G}^{(0)}(k)$ factors and self-energy diagrams in Σ_{FB}, namely  and  . So this diagram is included in the diagrammatic expansion of $\bar{\mathcal{G}}_{FB}$.

The other two diagrams have self-energy factors that are not in $\overline{\Sigma}_{FB}$, hence they are not included in $\mathcal{G}_{FB}$.

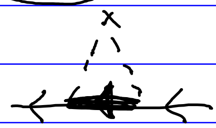
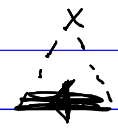
2. For example 

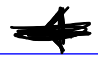
(d) The first diagram is included, because it was already included in $\mathcal{G}_{FB}$ (just replace $\mathcal{G}_{SCB}$ by $\mathcal{G}^{(0)}$ to get the diagram)

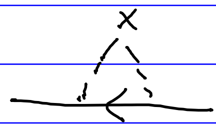
The second diagram is also included, because it contains a "nesting" of self-energy diagrams in Σ_{FB}. To see that it is included, consider

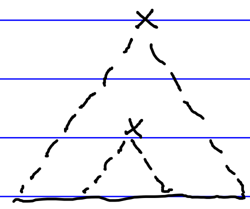
$$\overline{\mathcal{G}}_{SCB} = \mathcal{G}^{(0)} + \mathcal{G}^{(0)} \Sigma_{SCB} \mathcal{G}_{SCB}$$

$$= \mathcal{G}^{(0)} + \underbrace{\mathcal{G}^{(0)} \Sigma_{SCB} \mathcal{G}^{(0)}}_{\text{contains}} + \cdots$$

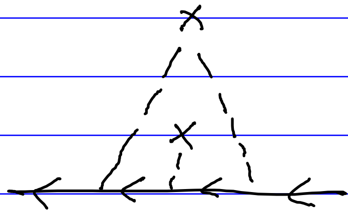
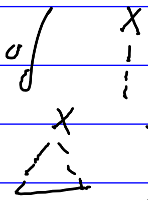
 since Σ_{SCB} contains 

But  $= \overline{\mathcal{G}}_{SCB} = \mathcal{G}^{(0)} + \underbrace{\mathcal{G}^{(0)} \Sigma_{SCB} \mathcal{G}^{(0)}}_{\text{contains}} + \cdots$



so $\overline{\mathcal{G}}_{SCB}$ contains 

On the other hand, we can never get crossed interaction lines, as in the third diagram, from this procedure. So the third diagram is not included.

2. For example  (nesting of  inside)

The level of nesting can be arbitrarily large, for example the following diagram is included: