Exam solution, spring 2016
TFY4210 Quantum theory of many-particle systems

Problem 1

(a) The Hamiltonian $H_{\rm Heis}$ is invariant under global spin rotations ("global" means that all spins are rotated in the same way). Such an invariance of a Hamiltonian is by definition a **symmetry**.

Global spin rotations are continuous transformations, as the rotation angle (about any axis) is arbitrary and thus the possible angles form a continuous set. Therefore this symmetry is called a **continuous** symmetry.

The Hamiltonian $H_{\rm Heis}$ has ferromagnetic order in the ground state. In a ground state of $H_{\rm Heis}$ all spins point in the same direction (which can be any direction). Rotating all spins in this ground state gives a *different* ground state, i.e. with the spins ordered along a different direction. Thus, unlike the Hamiltonian, the ground state is *not* invariant under global spin rotations. One therefore says that the ground state **breaks** the continuous spin rotation symmetry of $H_{\rm Heis}$.

(b) While $H_{\rm Heis}$ has no preference for the ordering direction, H_D will prefer ordering along the z axis, as any ordering with nonzero spin components in the x and/or y directions would give a greater energy for $D > 0$.[1] Thus we expect H_D to reduce the set of possible ordering directions down to only two possibilities: the $+\hat{\boldsymbol{z}}$ or $-\hat{\boldsymbol{z}}$ directions.

Using Eqs. (18) and (19) in the formula set gives (to avoid unnecessary clutter we drop the site index j for the moment)

$$\begin{aligned}(\hat{S}^x)^2 + (\hat{S}^y)^2 &= \frac{1}{4}(\hat{S}^+ + \hat{S}^-)^2 - \frac{1}{4}(\hat{S}^+ - \hat{S}^-)^2 \\ &= \frac{1}{4}\left[(\hat{S}^+)^2 + (\hat{S}^-)^2 + \hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+ - (\hat{S}^+)^2 - (\hat{S}^-)^2 + \hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+\right] \\ &= \frac{1}{2}(\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+). \qquad (1)\end{aligned}$$

As discussed above, the possible ordering directions are $+\hat{\boldsymbol{z}}$ or $-\hat{\boldsymbol{z}}$. In the following spin-wave theory analysis we assume ordering in the $+\hat{\boldsymbol{z}}$ direction, as then we can use the standard version of the Holstein-Primakoff (HP) expressions for the spin operators. We also treat the square roots in the HP expressions to lowest order in $1/S$, giving $\hat{S}^+ \approx \sqrt{2S}a$, $\hat{S}^- \approx \sqrt{2S}a^\dagger$ (higher order terms can be seen to give boson-boson interactions, which we are told to neglect here). Thus

$$(\hat{S}^x)^2 + (\hat{S}^y)^2 = \frac{1}{2}(2S)(aa^\dagger + a^\dagger a) = S(2a^\dagger a + 1), \qquad (2)$$

[1] This reasoning about H_D is based on thinking about the spins in a simplified way, as classical objects, which would seem like a reasonable thing to do in order to get some qualitative insight, also since the spin-wave theory to be later employed is a semiclassical theory, being essentially a $1/S$ expansion with $S \to \infty$ corresponding to the limit of classical spins.

where we used $[a, a^\dagger] = 1$ in the last transition. Adding the site index j to the operators, we get

$$H_D = DS\sum_j (2a_j^\dagger a_j + 1) = NSD + 2SD\sum_j a_j^\dagger a_j. \tag{3}$$

We now introduce the Fourier transformation (23) in the formula set to get

$$\sum_j a_j^\dagger a_j = \frac{1}{N}\sum_j \sum_{\boldsymbol{k}} \sum_{\boldsymbol{k}'} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_j} e^{i\boldsymbol{k}'\cdot\boldsymbol{r}_j} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}'} = \sum_{\boldsymbol{k},\boldsymbol{k}'} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}'} \underbrace{\frac{1}{N}\sum_j e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}_j}}_{\delta_{\boldsymbol{k},\boldsymbol{k}'}} = \sum_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}, \tag{4}$$

where we used Eq. (24) in the formula set. (The wavevector sums run over the first Brillouin zone.) This gives

$$H_D = NSD + 2SD\sum_{\boldsymbol{k}} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}}, \tag{5}$$

which is in the form of Eq. (4) in the exam text, with $C = NSD$ and $\Delta = 2SD$.

(c) The magnon dispersion of H_{tot} is $\omega_{\boldsymbol{k}}^{\text{tot}} = \omega_{\boldsymbol{k}} + \Delta$. The minimum value of the function $\omega_{\boldsymbol{k}} = 2JS(2 - \cos k_x - \cos k_y)$ is 0 (this happens at $\boldsymbol{k} = 0$). Therefore Δ is the smallest value of the magnon energy $\omega_{\boldsymbol{k}}^{\text{tot}}$, i.e. Δ is the **energy gap** of H_{tot}.

Goldstone's theorem says that a broken continuous symmetry implies gapless magnons. Thus the crucial qualitative distinction is between gapped and gapless magnons. Since the magnon gap $\Delta = 2SD$ is nonzero for $D > 0$ and zero for $D = 0$, these are the two cases to consider:

- $\underline{D > 0}$: Since Δ is nonzero, we can conclude from the Goldstone theorem that there is no broken continuous symmetry in this case.[2] This conclusion is consistent with the symmetry properties for $D > 0$: The only continuous symmetry of H_{tot} is due to rotations around the z axis, and the ground state does not break this symmetry since its order is along $\hat{\boldsymbol{z}}$ (under such rotations the ground state is invariant (up to an overall phase, which has no physical significance)).

- $\underline{D = 0}$: In this case Δ is zero, and there is also a broken continuous symmetry as discussed in (a). By the Goldstone theorem, the former property is implied by the latter. So the picture is consistent also in this case.

(d) We expect the rotated state $U|G\rangle$ to be a ground state for $D = 0$, since then the ordering can be in any direction. For $D > 0$ the order is in the $+\hat{\boldsymbol{z}}$ or $-\hat{\boldsymbol{z}}$ direction, so we do not expect $U|G\rangle$ to be a ground state then.

[2] Because if we assume a broken continuous symmetry in this case, Goldstone's theorem would imply gapless magnons, which would contradict the fact that $\Delta > 0$, so our assumption must be wrong. (Incidentally, the general rule of logic used here is: A $\Rightarrow$ B (i.e., A implies B) in turn implies that (not B) $\Rightarrow$ (not A) (i.e., the negation of B implies the negation of A). In our situation, A = broken continuous symmetry, B = gapless magnons.

The state $|G\rangle$ is the ground state corresponding to order in the assumed ordering direction $+\hat{\boldsymbol{z}}$. Since $a_{\boldsymbol{k}}|G\rangle = 0$ for all $\boldsymbol{k}$, the ground state energy is $E_0^{\rm tot}$, as seen from

$$H_{\rm tot}|G\rangle = (E_0^{\rm tot} + \sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}}^{\rm tot} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}})|G\rangle = E_0^{\rm tot}|G\rangle. \tag{6}$$

Thus, if (and only if) $U|G\rangle$ is also a ground state, it will satisfy the same eigenvalue equation, i.e. with the eigenvalue $E_0^{\rm tot}$:

$$H_{\rm tot}(U|G\rangle) = E_0^{\rm tot}(U|G\rangle) \qquad \text{(condition for } U|G\rangle \text{ being a ground state)} \tag{7}$$

The strategy is thus to calculate the lhs and see whether it reduces to the rhs.

The operator U producing a global spin rotation by angle θ around the x axis is

$$U = \prod_j U_j, \quad \text{where} \quad U_j = e^{-i\hat{S}_j^x \theta}, \tag{8}$$

since $\hat{S}_j^x$ is the generator for rotations of the spin at site j around the x axis. The order of the U_j operators in the product doesn't matter since spin operators for different sites commute. For the same reason,[3] we can rewrite U as

$$U = e^{-i(\sum_j \hat{S}_j^x)\theta} = e^{-i\hat{S}^x\theta}. \tag{9}$$

Thus we see that the total generator involved is $\hat{S}^x = \sum_j \hat{S}_j^x$, the sum of the generators for the individual spins. Using the standard approximate HP expressions as in (b), $\hat{S}^x$ can be rewritten as

$$\hat{S}^x = \sum_j \hat{S}_j^x = \frac{1}{2}\sum_j (\hat{S}_j^+ + \hat{S}_j^-) = \frac{1}{2}\sqrt{2S}\sum_j (a_j + a_j^\dagger) = \sqrt{\frac{SN}{2}}(a_{\boldsymbol{k}=0} + a_{\boldsymbol{k}=0}^\dagger), \tag{10}$$

where in the last transition we used that $a_{\boldsymbol{k}=\boldsymbol{0}} = N^{-1/2}\sum_j a_j$, which follows from the inverse transformation of Eq. (23) in the formula set. Specializing now to an infinitesimal transformation with rotation angle $d\theta$, U can be approximated as

$$U \approx 1 - i\hat{S}^x d\theta = 1 - id\theta\sqrt{\frac{SN}{2}}(a_{\boldsymbol{k}=0} + a_{\boldsymbol{k}=0}^\dagger), \tag{11}$$

and therefore, since $a_{\boldsymbol{k}=0}|G\rangle = 0$,

$$U|G\rangle = |G\rangle - id\theta\sqrt{\frac{SN}{2}}a_{\boldsymbol{k}=\boldsymbol{0}}^\dagger|G\rangle. \tag{12}$$

Thus $U|G\rangle$ is a linear combination of the ground state $|G\rangle$ and the state $a_{\boldsymbol{k}=0}^\dagger|G\rangle$ having one magnon with wavevector $\boldsymbol{k} = 0$. We find

$$\begin{aligned} H_{\rm tot}(U|G\rangle) &= H_{\rm tot}|G\rangle - id\theta\sqrt{\frac{SN}{2}}H_{\rm tot}a_{\boldsymbol{k}=\boldsymbol{0}}^\dagger|G\rangle = E_0^{\rm tot}|G\rangle - id\theta\sqrt{\frac{SN}{2}}(E_0^{\rm tot} + \omega_{\boldsymbol{k}=0}^{\rm tot})a_{\boldsymbol{k}=\boldsymbol{0}}^\dagger|G\rangle \\ &= E_0^{\rm tot}(U|G\rangle) - i\Delta d\theta\sqrt{\frac{SN}{2}}a_{\boldsymbol{k}=\boldsymbol{0}}^\dagger|G\rangle. \end{aligned} \tag{13}$$

[3] That is, we use that if $[A, B] = 0$, then $e^A e^B = e^{A+B}$.

This reduces to the rhs of (7) only if $\Delta = 0$, which happens if $D = 0$. This confirms our expectations stated at the beginning.

Problem 2

(a) We get

$$\hat{n}_j^2 = c_j^\dagger c_j c_j^\dagger c_j = c_j^\dagger (1 - c_j^\dagger c_j) c_j = \hat{n}_j - (c_j^\dagger)^2 c_j^2, \tag{14}$$

where we used Eq. (10) in the formula set for $j = j'$. Using Eq. (11) in the formula set for $j = j'$ gives $2c_j^2 = 2(c_j^\dagger)^2 = 0$, so $c_j^2 = (c_j^\dagger)^2 = 0$ (this is a mathematical statement of the Pauli principle). Inserting this into (14) gives $\hat{n}_j^2 = \hat{n}_j$.

As each factor in $\hat{O}_j$ commutes with c_j and $c_j^\dagger$, $\hat{O}_j$ does as well. Thus

$$[\hat{S}_j^+, \hat{S}_j^-] = \hat{O}_j c_j^\dagger \hat{O}_j c_j - \hat{O}_j c_j \hat{O}_j c_j^\dagger = \hat{O}_j^2 (c_j^\dagger c_j - c_j c_j^\dagger) = \hat{O}_j^2 (2\hat{n}_j - 1). \tag{15}$$

As all factors in $\hat{O}_j$ commute with each other, we get $\hat{O}_j^2 = \prod_{i=1}^{j-1} (1 - 2\hat{n}_i)^2$. Here $(1-2\hat{n}_i)^2 = 1 - 4\hat{n}_i + 4\hat{n}_i^2 = 1$, where we used $\hat{n}_i^2 = \hat{n}_i$. Thus $\hat{O}_j^2 = 1$. It follows that $[\hat{S}_j^+, \hat{S}_j^-] = 2\hat{n}_j - 1 = 2\hat{S}_j^z$.

(b) We have

$$\begin{aligned} \hat{S}_j^+ \hat{S}_{j+1}^- &= \hat{O}_j c_j^\dagger \hat{O}_{j+1} c_{j+1} = c_j^\dagger \hat{O}_j \hat{O}_{j+1} c_{j+1} = c_j^\dagger (1 - 2\hat{n}_j) c_{j+1} \\ &= c_j^\dagger c_{j+1} - 2 \underbrace{c_j^\dagger c_j^\dagger}_{0} c_j c_{j+1} = c_j^\dagger c_{j+1}. \end{aligned} \tag{16}$$

(We used $\hat{O}_j \hat{O}_{j+1} = \left[\prod_{i=1}^{j-1} (1 - 2\hat{n}_i)^2\right] (1 - 2\hat{n}_j) = 1 - 2\hat{n}_j$.) This gives[4]

$$H = -\sum_{j=1}^{N} \left[\frac{J_\perp}{2} (c_j^\dagger c_{j+1} + \text{h.c.}) + J_z \left(\hat{n}_j - \frac{1}{2}\right) \left(\hat{n}_{j+1} - \frac{1}{2}\right) \right]. \tag{17}$$

(c) For $J_z = 0$,[5] H reduces to

$$H = -\frac{J_\perp}{2} \sum_j (c_j^\dagger c_{j+1} + \text{h.c.}). \tag{18}$$

The Fourier transformation $c_j = N^{-1/2} \sum_k e^{ikj} c_k$ is used to trade the N operators c_j for N operators c_k. The periodic boundary condition $c_{N+1} = c_1$ can be seen to imply $e^{ikN} = 1$, which gives $k = 2\pi m/N$, where m is an integer. The inverse transformation $c_k = N^{-1/2} \sum_j e^{-ikj} c_j$ shows that $c_k = c_{k+2\pi}$, so two wavevectors differing by an integer multiple of 2π are equivalent. The simplest way to pick N inequivalent wavevectors is to pick N successive values of

[4] As noted in the exam text, we simply assume that also the fermions satisfy periodic boundary conditions; this is good enough for our purposes here.

[5] For $J_z \neq 0$, the term $J_z \sum_j \hat{n}_j \hat{n}_{j+1}$, representing interactions between fermions on nearest-neighbour sites, makes the problem very complicated to analyze.

the integer m. A standard choice is $m = -N/2, \ldots, N/2-1$ (N assumed even here) which gives $k \in [-\pi, \pi\rangle$, an interval called the first Brillouin zone (1BZ).

Using the Fourier transformation gives

$$\sum_j c_j^\dagger c_{j+1} = \frac{1}{N}\sum_j \sum_{k,k'} e^{-ikj} e^{ik'(j+1)} c_k^\dagger c_{k'} = \sum_{k,k'} c_k^\dagger c_{k'} e^{ik'} \underbrace{\frac{1}{N}\sum_j e^{-i(k-k')j}}_{\delta_{k,k'}} = \sum_k e^{ik} c_k^\dagger c_k, \quad (19)$$

where we used Eq. (24) in the formula set. Thus

$$H = -\frac{J_\perp}{2}\left(\sum_k e^{ik} c_k^\dagger c_k + \text{h.c.}\right) = -\frac{J_\perp}{2}\sum_k (e^{ik} + e^{-ik}) c_k^\dagger c_k = -J_\perp \sum_k \cos k \; c_k^\dagger c_k, \quad (20)$$

which is in the form $H = \sum_k \varepsilon_k c_k^\dagger c_k$ with $\varepsilon_k = -J_\perp \cos k$.

(d) Given the form of H as a weighted sum of number operators $\hat{n}_k = c_k^\dagger c_k$, the eigenstates of H have a definite number of fermions n_k for each $k \in$ 1BZ. Due to the Pauli principle, n_k can only be 0 or 1. The ground state is the eigenstate with minimum energy.[6] The minimum energy is obtained by having all k with $\varepsilon_k < 0$ occupied by a fermion, and all k with $\varepsilon_k > 0$ unoccupied.[7] Since $J_\perp > 0$, this means that all wavevectors with $|k| < \pi/2$ are occupied while all those with $|k| > \pi/2$ are not.[8] The ground state $|G\rangle$ can therefore be expressed as

$$|G\rangle = \left(\prod_{\substack{k \\ |k|<\pi/2}} c_k^\dagger\right)|0\rangle \quad (21)$$

where $|0\rangle$ is the vacuum state with no fermions. The ground state energy is

$$E_0 = \sum_{\substack{k \\ |k|<\pi/2}} \varepsilon_k. \quad (22)$$

We take the limit $N \to \infty$ and rewrite the sum as an integral, using $\sum_k \to (N/2\pi)\int dk$. This gives the ground state energy per site

$$e_0 \equiv \lim_{N\to\infty} \frac{E_0}{N} = (-J_\perp)\frac{1}{2\pi}\int_{-\pi/2}^{\pi/2} dk \; \cos k = -\frac{J_\perp}{2\pi}\sin k\Big|_{-\pi/2}^{\pi/2} = -\frac{J_\perp}{\pi}. \quad (23)$$

[6] In some problems the total number of fermions is fixed to some definite value. In such a situation, one would have to find the ground state as the minimum-energy state among the subset of states with the appropriate fermion number. However, the problem considered here is not of this type. The original model is a spin model, for which the total S^z of the states can vary between $-N/2$ (all spins down) to $N/2$ (all spins up). From the Jordan-Wigner expression for $\hat{S}_j^z$ one sees that the corresponding states in the fermion description have a fermion number that can vary between 0 and N.

[7] As noted in the exam text, we ignore possible ground state degeneracy issues here. These occur if $k = \pm\pi/2$ are among the allowed wavevectors, which happens only if $N = 4M$ with M some integer. Since $\varepsilon_k = 0$ for these two wavevectors, the total energy is the same regardless of whether they are occupied or not, thus giving a 4-fold degenerate ground state.

[8] Thus the system has a Fermi wavevector given by $k_F = \pi/2$.

(e) From the Jordan-Wigner transformation it follows that $\langle \hat{S}_j^z \rangle = \langle \hat{n}_j \rangle - 1/2$. Using the Fourier transformation gives

$$\langle \hat{n}_j \rangle = \langle c_j^\dagger c_j \rangle = \frac{1}{N} \sum_{k,k'} e^{-i(k-k')j} \langle c_k^\dagger c_{k'} \rangle. \tag{24}$$

For the ground state expectation value, $\langle c_k^\dagger c_{k'} \rangle = \langle G | c_k^\dagger c_{k'} | G \rangle$, with $|G\rangle$ the Fermi sea (21). For this to be nonzero, a necessary (but not sufficient) condition is that $k = k'$, since otherwise the state $c_k^\dagger c_{k'} |G\rangle$ cannot have the same occupation numbers as $|G\rangle$ and is therefore orthogonal to it. Thus $\langle \hat{n}_j \rangle$ is seen to be independent of j and given by

$$\langle \hat{n}_j \rangle = \frac{1}{N} \sum_k \langle c_k^\dagger c_k \rangle = \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} dk = \frac{1}{2}, \tag{25}$$

where in the last step we rewrote the sum as an integral. More simply, one can just stick with the sum and note that the number of fermions/occupied wavevectors in the ground state is $N/2$, giving $\langle \hat{n}_j \rangle = \frac{1}{N} \cdot \frac{N}{2} = \frac{1}{2}$. Thus $\langle \hat{S}_j^z \rangle = 1/2 - 1/2 = 0$.

Problem 3

(a) We use the wavevector (momentum) basis which diagonalizes the momentum operator $\hat{\boldsymbol{p}}$.[9] (Since we set $\hbar = 1$, we have $\boldsymbol{p} = \boldsymbol{k}$.) The single-particle wavefunctions in this basis are plane waves:

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{L^3}} \, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \quad (= \langle \boldsymbol{r} | \boldsymbol{k} \rangle) \tag{26}$$

The periodic boundary conditions give, for the x direction, that $\phi_{\boldsymbol{k}}(\boldsymbol{r} + L\hat{\boldsymbol{e}}_x) = \phi_{\boldsymbol{k}}(\boldsymbol{r}) \Rightarrow e^{ik_x L} = 1 \Rightarrow k_x = 2\pi n_x / L$ where n_x is an arbitrary integer. Using the same reasoning for the y and z directions, we find that the allowed wavevectors are given by

$$\boldsymbol{k} = \frac{2\pi}{L}(n_x, n_y, n_z) \quad \text{where } n_x, n_y, n_z \text{ can take any integer values.} \tag{27}$$

Since H_0 is a single-particle operator, we use Eqs. (29)-(30) in the formula set to calculate its second-quantized expression, with $\alpha \to \boldsymbol{k}$, $\beta \to \boldsymbol{k}'$. This gives

$$H_0 = \sum_{\boldsymbol{k},\boldsymbol{k}'} \langle \boldsymbol{k} | \frac{\hat{\boldsymbol{p}}^2}{2m} | \boldsymbol{k}' \rangle c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}'} \tag{28}$$

where the operator $c_{\boldsymbol{k}}^\dagger$ creates an electron in the plane-wave state (26).[10] The matrix element is

$$\langle \boldsymbol{k} | \frac{\hat{\boldsymbol{p}}^2}{2m} | \boldsymbol{k}' \rangle = \frac{\boldsymbol{k}'^2}{2m} \langle \boldsymbol{k} | \boldsymbol{k}' \rangle = \frac{\boldsymbol{k}^2}{2m} \delta_{\boldsymbol{k},\boldsymbol{k}'}. \tag{29}$$

[9] Normally one should in addition consider a basis for the electron's spin degree of freedom, but here you are told to neglect the spin.

[10] Although the same notation $c_{\boldsymbol{k}}^\dagger$ is used in lattice problems (see e.g. Problem 2), the meaning is not the same, as in that case the state created is not a plane wave state but a Bloch state. Also, in lattice problems the $\boldsymbol{k}$-vectors have a finite range (they lie inside the 1BZ), while here (see (27)) the range of the $\boldsymbol{k}$-vectors is unrestricted (because this is a continuum problem, so the Hilbert space is infinite-dimensional even for a finite system size).

Alternatively, the matrix element can be calculated from Eq. (30) in the formula set as

$$\int d^3r\, \frac{1}{\sqrt{L^3}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \frac{(-\nabla^2)}{2m} \frac{1}{\sqrt{L^3}} e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} = -\frac{(i\boldsymbol{k}')^2}{2m} \underbrace{\frac{1}{L^3}\int d^3r\, e^{-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}_{\delta_{\boldsymbol{k},\boldsymbol{k}'}} = \frac{\boldsymbol{k}^2}{2m}\delta_{\boldsymbol{k},\boldsymbol{k}'}. \tag{30}$$

This gives $H_0 = \sum_{\boldsymbol{k}} \frac{\boldsymbol{k}^2}{2m} c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}}$. To incorporate working in the grand canonical ensemble characterized by a chemical potential μ, we subtract μ from the energy of each particle,[11] thus giving (with some (conventional) abuse of notation, as we continue to use the same symbol H_0 for the modified expression)

$$H_0 = \sum_{\boldsymbol{k}} \left(\frac{\boldsymbol{k}^2}{2m} - \mu \right) c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}}. \tag{31}$$

We can thus identify $\varepsilon_{\boldsymbol{k}} = \boldsymbol{k}^2/(2m)$.

(b) To find $c_{\boldsymbol{k}}(\tau)$, one can differentiate the definition $c_{\boldsymbol{k}}(\tau) = e^{H_0\tau} c_{\boldsymbol{k}} e^{-H_0\tau}$ with respect to time, which gives

$$\frac{dc_{\boldsymbol{k}}(\tau)}{d\tau} = e^{H_0\tau}[H_0, c_{\boldsymbol{k}}]e^{-H_0\tau} = \sum_{\boldsymbol{k}'} \xi_{\boldsymbol{k}'} e^{H_0\tau} \underbrace{[\hat{n}_{\boldsymbol{k}'}, c_{\boldsymbol{k}}]}_{-c_{\boldsymbol{k}}\delta_{\boldsymbol{k},\boldsymbol{k}'}} e^{-H_0\tau} = -\xi_{\boldsymbol{k}} c_{\boldsymbol{k}}(\tau), \tag{32}$$

where we used Eq. (27) in the formula set. The solution of the differential equation (which also satisfies $c_{\boldsymbol{k}}(0) = c_{\boldsymbol{k}}$) is $c_{\boldsymbol{k}}(\tau) = e^{-\xi_{\boldsymbol{k}}\tau} c_{\boldsymbol{k}}$. As the τ-integral goes from 0 to β, it is sufficient to consider the $\tau > 0$ part of $\mathcal{G}(\boldsymbol{k}, \tau)$:

$$\mathcal{G}(\boldsymbol{k}, \tau > 0) = -\langle c_{\boldsymbol{k}}(\tau) c_{\boldsymbol{k}}^\dagger(0)\rangle = -e^{-\xi_{\boldsymbol{k}}\tau}\langle c_{\boldsymbol{k}} c_{\boldsymbol{k}}^\dagger\rangle = -e^{-\xi_{\boldsymbol{k}}\tau}(1-\langle c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}}\rangle) = -e^{-\xi_{\boldsymbol{k}}\tau}(1-n_F(\xi_{\boldsymbol{k}})), \tag{33}$$

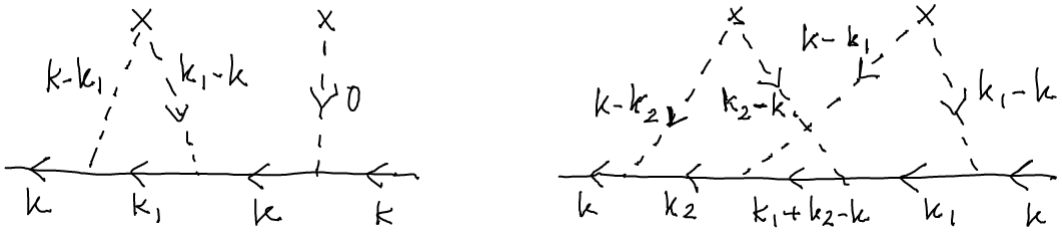
where we used the equal-time anticommutation relations and the noninteracting nature of H_0 (the latter fact giving the Fermi-Dirac distribution in the final expression). Thus

$$\begin{aligned} \mathcal{G}(\boldsymbol{k}, ip_m) &= \int_0^\beta d\tau\, e^{ip_m\tau}\mathcal{G}(\boldsymbol{k}, \tau > 0) = -(1 - n_F(\xi_{\boldsymbol{k}})) \int_0^\beta d\tau\, e^{(ip_m - \xi_{\boldsymbol{k}})\tau} \\ &= -\frac{(1 - n_F(\xi_{\boldsymbol{k}}))\left[e^{(ip_m-\xi_{\boldsymbol{k}})\beta} - 1\right]}{ip_m - \xi_{\boldsymbol{k}}} = \ldots = \frac{1}{ip_m - \xi_{\boldsymbol{k}}}, \end{aligned} \tag{34}$$

where $e^{ip_m\beta} = -1$ and Eq. (33) in the formula set are used to arrive at the final expression. The retarded Green function is obtained as ($\eta = 0^+$)

$$G^R(\boldsymbol{k}, \omega) = \mathcal{G}(\boldsymbol{k}, ip_m)\Big|_{ip_m \to \omega + i\eta} = \frac{1}{\omega - \xi_{\boldsymbol{k}} + i\eta}. \tag{35}$$

[11] That is, we subtract $\mu\hat{N}$ from H_0, where $\hat{N}$ is the total number operator, which, using the momentum basis, is given by $\hat{N} = \sum_{\boldsymbol{k}} c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}}$.



(c) The expressions for the left and right diagrams are, respectively (see the figures above for the wavevector labeling):

$$N^2 U(0)[\mathcal{G}(\boldsymbol{k})]^3 \sum_{\boldsymbol{k}_1} U(\boldsymbol{k}_1 - \boldsymbol{k}) U(\boldsymbol{k} - \boldsymbol{k}_1) \mathcal{G}(\boldsymbol{k}_1), \tag{36}$$

$$N^2 [\mathcal{G}(\boldsymbol{k})]^2 \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2} U(\boldsymbol{k}_1 - \boldsymbol{k}) U(\boldsymbol{k} - \boldsymbol{k}_1) U(\boldsymbol{k}_2 - \boldsymbol{k}) U(\boldsymbol{k} - \boldsymbol{k}_2) \mathcal{G}(\boldsymbol{k}_1) \mathcal{G}(\boldsymbol{k}_2) \mathcal{G}(\boldsymbol{k}_1 + \boldsymbol{k}_2 - \boldsymbol{k}) \tag{37}$$

(here $\mathcal{G}(\boldsymbol{k})$ is short for the noninteracting Matsubara Green function $\mathcal{G}(\boldsymbol{k}, ip_m)$ calculated in (b)). A diagram that does not fall into two separate pieces by cutting a single internal electron line is called irreducible. Otherwise the diagram is called reducible. Inspection shows that the left diagram is reducible (falls into two pieces by cutting the internal electron line with wavevector $\boldsymbol{k}$) and the right diagram is irreducible.

(d) Each irreducible diagram in the Feynman expansion for $\mathcal{G}(\boldsymbol{k}, ip_m)$ gives rise to a self-energy diagram, obtained by removing the two external electron lines. (The mathematical expression for the self-energy diagram is similarly obtained from that of the irreducible diagram by removing the two factors of $\mathcal{G}(\boldsymbol{k})$ associated with the external lines.) For example, the irreducible diagram shown above has the self-energy diagram shown to the left.

The self-energy $\Sigma(\boldsymbol{k}, ip_m)$ is the sum of all self-energy diagrams.

(e) We rewrite $\bar{G}^R(\boldsymbol{k}, \omega)$ as

$$\bar{G}^R(\boldsymbol{k}, \omega) = \frac{1}{\omega - \xi_{\boldsymbol{k}} - \Sigma_r^R(\boldsymbol{k}, \omega) - i\Sigma_i^R(\boldsymbol{k}, \omega)} = \frac{\omega - \xi_{\boldsymbol{k}} - \Sigma_r^R(\boldsymbol{k}, \omega) + i\Sigma_i^R(\boldsymbol{k}, \omega)}{(\omega - \xi_{\boldsymbol{k}} - \Sigma_r^R(\boldsymbol{k}, \omega))^2 + (\Sigma_i^R(\boldsymbol{k}, \omega))^2}. \tag{38}$$

Thus

$$A(\boldsymbol{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma_i^R(\boldsymbol{k}, \omega)}{(\omega - \xi_{\boldsymbol{k}} - \Sigma_r^R(\boldsymbol{k}, \omega))^2 + (\Sigma_i^R(\boldsymbol{k}, \omega))^2}. \tag{39}$$

By using that for fermions, $A(\boldsymbol{k}, \omega) \geq 0$ always, it follows that the sign of $\Sigma_i^R(\boldsymbol{k}, \omega)$ must be negative.