MANY BODY PHYSICS: 621. Spring 2022

Solution to Exercise 2.

1. (a) Let us first write the density in terms of the Boson propagator.

$$\rho(T) = \frac{N}{V} = V^{-1} \sum_{\mathbf{k}} \langle b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \rangle = -V^{-1} \sum_{\mathbf{k}} \underbrace{\left(-\langle T b_{\mathbf{k}}(0^{-}) b_{\mathbf{k}}^{\dagger}(0) \rangle \right)}_{\left(-\langle T b_{\mathbf{k}}(0^{-}) b_{\mathbf{k}}^{\dagger}(0) \rangle \right)}$$
$$= -\frac{1}{V} \sum_{\mathbf{k}} T \sum_{i\nu_{n}} \frac{1}{i\nu_{n} - \omega_{\mathbf{k}}} e^{i\nu_{n}O^{+}}$$
(1)

Now the Matsubara sum can be re-written as an anticlockwise contour integral C_1 around the imaginary axis

$$\langle \hat{n}_{\mathbf{k}} \rangle = -T \sum_{i\nu_n} \frac{1}{i\nu_n - \omega_{\mathbf{k}}} e^{i\nu_n O^+} = - \oint_{C_1} \frac{dz}{2\pi i} n(z) \frac{1}{z - \omega_{\mathbf{k}}} e^{z0^+}.$$
 (2)

The convergence factor e^{z0^+} decays for negative real z = -|x| while n(z) decays for positive real z = |x|, so the contour integral at infinity vanishes and we can accordingly add null contours to distort the contour into C_2 , running clockwise around the pole in the Green's function at $z = \omega_k$. (Note that had we chosen instead of n(z), n(z) + 1, which has the same pole structure, we would not have been able to distort the contour, because this function does not decay for positive real z). This then gives

$$\langle \hat{n}_{\mathbf{k}} \rangle = -\oint_{C_2} \frac{dz}{2\pi i} n(z) \frac{1}{z - \omega_{\mathbf{k}}} = \oint_{\tilde{C}_2} \frac{dz}{2\pi i} n(z) \frac{1}{z - \omega_{\mathbf{k}}} = n(\omega_{\mathbf{k}})$$
(3)

so that

$$\rho(T) = \frac{1}{V} \sum_{\mathbf{k}} n(\omega_{\mathbf{k}}) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta(E_{\mathbf{k}}-\mu)} - 1}.$$
(4)

Here, we have taken the thermodynamic limit, assuming that n_k remains finite. When Bose Einstein condensation occurs, $\mu \to 0$, so that the occupancy $n_{k=0} \sim O(V) = n_0$ becomes macroscopic. In this case we must write

$$\rho(T) = n_0 + \int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta E_{\mathbf{k}}} - 1}.$$
(5)

(b) The Feynman diagram for the dynamic charge susceptibility is given by

$$\chi_c(q, i\nu_n) = \int \frac{d^3k}{(2\pi)^3} \overline{T\sum_{i\nu_r} D(\mathbf{q} + \mathbf{k}, i\nu_n + i\nu_r) D(\mathbf{k}, i\nu_n)}$$



We rewrite the Matsubara sum as a Contour integral, replacing $iv_n \rightarrow z$, along the countour C_1 enclosing the poles of n(z) at $z = iv_n$, which runs anticlockwise around the imaginary axis. We distort this countour into a contour C_2 that runs clockwise around the poles of the Greens functions at $z = \omega_k$ and $z = \omega_{k+q} - iv_n$,

$$I = \oint_{C_1} \frac{dz}{2\pi i} n(z) \, [\dots] == \oint_{C_2} \frac{dz}{2\pi i} n(z) \, [\dots] = - \oint_{C_2} \frac{dz}{2\pi i} n(z) \, [\dots]$$
(6)

This then gives

$$I = -\oint_{C_2} \frac{dz}{2\pi i} n(z) \left[\left(\frac{1}{i\nu_n + z - \omega_{\mathbf{k}+\mathbf{q}}} \right) \left(\frac{1}{z - \omega_{\mathbf{k}}} \right) \right]$$
(7)

so that

$$I = -\left(\frac{n(\omega_{\mathbf{k}+\mathbf{q}} - i\nu_n) - n(\omega_{\mathbf{k}})}{\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}} - i\nu_n}\right) = \frac{n(\omega_{\mathbf{k}+\mathbf{q}}) - n(\omega_{\mathbf{k}})}{i\nu_n - (\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}})}$$
(8)

where we have used the fact that $n(\omega_{\mathbf{k}+\mathbf{q}}-i\nu_n) = n(\omega_{\mathbf{k}+\mathbf{q}})$. Thus the charge susceptibility of the Bose gas is given by

$$\chi_c(\mathbf{q}, i\nu_n) = \int \frac{d^3k}{(2\pi)^3} \left(\frac{n(\omega_{\mathbf{k}+\mathbf{q}}) - n(\omega_{\mathbf{k}})}{i\nu_n - (\omega_{\mathbf{k}+\mathbf{q}} - \omega_{\mathbf{k}})} \right).$$
(9)

which is a kind of Bosonic Lindhardt function.

(c) The pair susceptibility diagram is written

$$\chi_P(q, i\nu_n) = \int \frac{d^3k}{(2\pi)^3} T \sum_{i\omega_r} G(\mathbf{q} + \mathbf{k}, i\nu_n + i\omega_r) G(-\mathbf{k}, -i\omega_r).$$
(10)

There is no minus sign infront, because there is no fermion loop in the diagram. We replace $i\omega_r \rightarrow z$ and carry out the out the Matsubara sum as a contour integral around the poles of the Fermi function (C_2). We then distort the contour around the poles in the Green's functions, as follows

$$\begin{array}{c|c} -\underline{\mathbf{1}} \times \\ \hline \mathbf{1} & & \\ \hline \mathbf{1} &$$



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so that

$$\chi_P(\mathbf{q}, i\nu_n) = \int \frac{d^3k}{(2\pi)^3} \left[\frac{f(\epsilon_{\mathbf{k}+\mathbf{q}}) + f(\epsilon_{\mathbf{k}}) - 1}{i\nu_n - (\epsilon_{\mathbf{k}+\mathbf{q}} + \epsilon_{\mathbf{k}})} \right].$$
 (12)

If we set $q = (\mathbf{q}, i\nu_n) = 0$, the static pair susceptibility is then given by

$$\chi_P = \int \frac{d^3k}{(2\pi)^3} \left[\frac{1 - 2f(\epsilon_{\mathbf{k}})}{2\epsilon_{\mathbf{k}}} \right] = \int \frac{d^3k}{(2\pi)^3} \left[\frac{\tanh(\beta\epsilon_{\mathbf{k}}/2)}{2\epsilon_{\mathbf{k}}} \right]$$
(13)

We can replace the summation over momentum by an integral over the density of states $N(\epsilon)$, so that

$$\chi_P = \int d\epsilon N(\epsilon) \left[\frac{\tanh(\beta\epsilon/2)}{2\epsilon} \right]$$
(14)

To obtain a finite result we must introduce a cut-off on the energy integral, which in conventional superconductors is the Debye energy. As $T \rightarrow 0$, there is still an infra-red divergence in the integral. To study this, we can approximate the density of states by its value N(0) near the Fermi energy, so that

$$\chi_P \sim N(0) \int_{-\Lambda}^{\Lambda} d\epsilon \left[\frac{\tanh(\beta \epsilon/2)}{2\epsilon} \right] = N(0) \int_{0}^{\Lambda} d\epsilon \left[\frac{\tanh(\beta \epsilon/2)}{\epsilon} \right]$$
(15)

Now for $\epsilon \gtrsim k_B T$, $\tanh(\beta \epsilon/2) \sim 1$, which gives rise to a logarithmic divergence in the integral, which is cut-off at $\epsilon \sim k_B T$, so that

$$\chi_P \sim N(0) \int_{k_B T}^{\Lambda} d\epsilon \frac{1}{\epsilon} \sim N(0) \ln \left[\frac{\Lambda}{k_B T}\right].$$
(16)

The pair susceptibility of a Fermi liquid is thus logarithmically divergent in the temperature. This means that an arbitrarily small attractive pairing interaction g innevitably gives rise to a Cooper pair instability at sufficiently low temperature.

2. (a) We begin by formulating the partition function as a path integral

$$Z = \int \mathcal{D}[c^{\dagger}, c] e^{-S}$$
(17)

.

where

$$S = \int_{0}^{\beta} d\tau \left[\sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} \left(\partial_{\tau} + \epsilon_{\mathbf{k}} - \mu \right) c_{\mathbf{k}\sigma} - \frac{I}{2} \sum_{j} \left(c_{j\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} c_{j\beta} \right)^{2} \right]$$
(18)

Next we make the Hubbard-Stratonovich transformation

$$-\frac{I}{2}\sum_{j}(c_{j}^{\dagger}\vec{\sigma}c_{j})^{2}\longrightarrow\vec{M}_{j}\cdot(c_{j}^{\dagger}\vec{\sigma}c_{j})+\frac{\vec{M}_{j}^{2}}{2I},$$
(19)

so that the partition function can be written

$$Z = \int \mathcal{D}[\vec{M}, c^{\dagger}, c] e^{-S[c^{\dagger}, c, \vec{M}]}$$
(20)

where

$$S[c^{\dagger}, c, \vec{M}] = \int_{0}^{\beta} d\tau \left[\sum_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}\sigma} \left(\partial_{\tau} + \epsilon_{\mathbf{k}} - \mu \right) c_{\mathbf{k}\sigma} + \sum_{j} \left(\vec{M}_{j} \cdot \left(c^{\dagger}_{j} \vec{\sigma} c_{j} \right) + \frac{\vec{M}_{j}^{2}}{2I} \right) \right]$$
(21)

Now let us look for saddle point (mean-field) solutions where $\vec{M}_j = \vec{M}e^{i\mathbf{Q}\cdot\mathbf{R}}$. The magnetic field term can be cast in momentum space as follows

$$\vec{M}_{j} \cdot (c_{j}^{\dagger} \vec{\sigma} c_{j}) = \vec{M} \cdot \sum_{j} e^{i\mathbf{Q} \cdot \mathbf{R}_{j}} (c_{j}^{\dagger} \vec{\sigma} c_{j}) = \sum_{\mathbf{k}} \vec{M} \cdot (c_{\mathbf{k}+\mathbf{Q}}^{\dagger} \vec{\sigma} c_{\mathbf{k}})$$
$$= \sum_{\mathbf{k} \in (1/2)} \vec{M} \cdot (c_{\mathbf{k}+\mathbf{Q}}^{\dagger} \vec{\sigma} c_{\mathbf{k}} + \mathrm{H.c})$$
(22)

Now the kinetic term can be written

$$H_{0} = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} = \sum_{\mathbf{k} \in \frac{1}{2} \mathbf{BZ}} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k} \in \frac{1}{2} \mathbf{BZ}} (\epsilon_{\mathbf{k}+\mathbf{Q}} - \mu) c_{\mathbf{k}+\mathbf{Q}\sigma}^{\dagger} c_{\mathbf{k}+\mathbf{Q}\sigma}$$
(23)

so if we introduce the four-spinor

$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \\ c_{\mathbf{k}+\mathbf{Q}} \\ c_{\mathbf{k}+\mathbf{Q}} \end{pmatrix}, \qquad (24)$$

we can combine (23) and (22) into a single matrix equation

$$H = \sum_{\mathbf{k} \in \frac{1}{2}BZ} \psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \psi_{\mathbf{k}}$$
(25)

where

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & \mathbf{M} \cdot \vec{\sigma} \\ \mathbf{M} \cdot \vec{\sigma} & \epsilon_{\mathbf{k}+\mathbf{Q}} - \mu \end{pmatrix}.$$
 (26)

The action associated with the mean-field theory is

$$S_{MF} = \int_{0}^{\beta} d\tau \left[\sum_{\mathbf{k} \in \frac{1}{2}BZ} \psi_{\mathbf{k}}^{\dagger} \left(\partial_{\tau} + \mathcal{H}(\mathbf{k}) \right) \psi_{\mathbf{k}} + \frac{N_{s} \vec{M}^{2}}{2I} \right]$$
(27)

where N_s is the number of sites in the crystal.

(b) From the action, we can read-off the inverse Greens function of the ψ_k field as

$$\mathcal{G}^{-1}(\mathbf{k},\omega) = (\omega - \mathcal{H}(\mathbf{k})). \tag{28}$$

The energy eigenvalues of the mean-field Hamiltonian are determined by the zeros of the determinant of the inverse Greens function, i.e

$$0 = \det\left[\mathcal{G}^{-1}\right] = \det\left(\begin{matrix} \omega - \epsilon_{\mathbf{k}} + \mu & -\mathbf{M} \cdot \vec{\sigma} \\ -\mathbf{M} \cdot \vec{\sigma} & \omega + \epsilon_{\mathbf{k}} + \mu \end{matrix}\right) = \left[(\omega + \mu)^2 - \epsilon_{\mathbf{k}}^2 - (\vec{M})^2\right]^2, \quad (29)$$

where we have used the particle-hole symmetry $\epsilon_{k+Q} = -\epsilon_k$. The zeros of the determinant then determine the eigenvalues

$$E_{\mathbf{k}p} = p\omega_{\mathbf{k}} - \mu, \qquad (p = \pm) \tag{30}$$

where $\omega_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + M^2}$. Each of these eigenvalues has a two-fold spin degeneracy

(c) Using the one-particle Eigenvalues, the total free energy is

$$F = \sum_{\mathbf{k} \in \frac{1}{2}BZ, p=\pm 1} -2T \ln \left[1 + e^{-\beta(p\omega_{\mathbf{k}} - \mu)} \right] + \frac{N_s M^2}{2I}$$
(31)

Writing

$$\sum_{p=\pm 1} \ln\left[1 + e^{-\beta(-\mu + p\omega_{\mathbf{k}})}\right] = \sum_{p} \ln\left[2\cosh\left(\frac{\beta}{2}(p\omega_{\mathbf{k}} - \mu)\right)\right] + \beta\mu$$
(32)

we then obtain

$$F = \sum_{\mathbf{k}, p=\pm 1} -T \ln\left[2\cosh\left(\frac{\beta E_{\mathbf{k}p}}{2}\right)\right] + \mathcal{N}_s\left(\frac{M^2}{2I} - \mu\right)$$
(33)

where we have absorbed the factor of two by re-extending the summation to the full Brillouin zone.

(d) Taking the derivative of the free energy with respect to M, we obtain

$$\frac{\partial F}{\partial M} = -\frac{1}{2} \sum_{p} \int_{\mathbf{k}} \tanh\left(\frac{\beta(\omega_{\mathbf{k}} - p\mu)}{2}\right) \frac{M}{\omega_{\mathbf{k}}} + \frac{M}{I}$$
(34)

giving us the gap equation

$$\frac{1}{I} = \frac{1}{2} \sum_{p} \int_{\mathbf{k}} \tanh\left(\frac{(\sqrt{\epsilon_{\mathbf{k}}^2 + M^2 - p\mu})}{2T}\right) \frac{1}{\sqrt{\epsilon_{\mathbf{k}}^2 + M^2}}$$
(35)



FIG. 1: 3D Plot of phase diagram for the spin density wave, calculated parametrically. Notice that the backwards curvature of the phase boundary at finite μ indicates that at low temperature, the phase transition becomes first order.

(e) At half filling, $\mu = 0$. Setting M = 0 in the gap equation gives us the equation for T_c

$$\frac{1}{I} = \int_{\mathbf{k}} \tanh\left(\frac{\epsilon_{\mathbf{k}}}{2T_c}\right) \frac{1}{\epsilon_{\mathbf{k}}} = \chi_{\mathcal{Q}}(T_c)$$
(36)

which is identical for the equation for T_c in a BCS superconductor. By replacing the momentum sum by an energy integral, and approximating the density of states by its value at the Fermi energy N(0), we see that spin density wave susceptibility χ_Q is logarithmically divergent in temperature

$$\chi_{Q}(T) \sim 2N(0) \int_{T}^{\Lambda} \frac{d\epsilon}{\epsilon} \sim 2N(0) \ln\left(\frac{\Lambda}{T}\right)$$
 (37)

which diverges as $T \to 0$. The SDW instability at $I\chi(T)$ will thus occur for arbitrarily small I, with transition temperature given by $T_c \sim \Lambda e^{-1/(2N(0)I)}$.

At finite μ the critical value for I_c will become finite. We can calculate the phase

diagram by computing the critical coupling constant as a function of T_c and μ ,

$$\frac{1}{I(\mu, T_c)} = \int \frac{d^3k}{(2\pi)^3} \frac{\sum_{\pm} \tanh\left[(|\epsilon_{\mathbf{k}}| \pm \mu)/2T_c\right]}{|\epsilon_{\mathbf{k}}|}$$
(38)

where $\epsilon_{\mathbf{k}} = -2t(c_x + c_y + c_z)$. It is easiest to do this calculation by approximating the density of states as a constant. If you wish to do the calculation for the true 3D density of states, it is useful to first calculate the density of states and represent it as an interpolation function, and to calculate

$$\frac{1}{I(\mu, T_c)} = \int_{-6t}^{6t} d\epsilon N(\epsilon) \frac{\sum_{\pm} \tanh\left[(|\epsilon| \pm \mu)/2T_c\right]}{2|\epsilon|}$$
(39)

A 3D plot of the phase diagram obtained using this procedure is shown in Fig. 1.

3. (a) We begin by using a complete basis of energy eigenstates, such that

$$\begin{split} H \left| \lambda \right\rangle &= E_{\lambda} \left| \lambda \right\rangle, \\ \sum_{\lambda} \left| \lambda \right\rangle \left\langle \lambda \right| &= 1, \\ \left\langle \lambda \left| S_{\mathbf{q}}^{\pm}(t) \right| \zeta \right\rangle &= \left\langle \lambda \left| e^{iHt} S_{\mathbf{q}}^{\pm} e^{-iHt} \right| \zeta \right\rangle = e^{-i(E_{\zeta} - E_{\lambda})t} \left\langle \lambda \left| S_{\mathbf{q}}^{\pm} \right| \zeta \right\rangle \end{split}$$

The dynamic spin susceptibility is then given by

$$\begin{split} \chi_{R}(\mathbf{q},t) &= i \langle \left[S_{\mathbf{q}}^{-}(t), S_{-\mathbf{q}}^{+}(0) \right) \right] \rangle \theta(t-t') \\ &= i \sum_{\lambda,\zeta} e^{-\beta(E_{\lambda}-F)} \left\{ \left\langle \lambda \left| S_{\mathbf{q}}^{-}(t) \right| \zeta \right\rangle \left\langle \zeta \left| S_{-\mathbf{q}}^{+}(0) \right| \lambda \right\rangle - \left\langle \lambda \left| S_{-\mathbf{q}}^{+}(0) \right| \zeta \right\rangle \left\langle \zeta \left| S_{\mathbf{q}}^{-}(t) \right| \lambda \right\rangle \right\} \theta(t) \\ &= i \sum_{\lambda,\zeta} e^{\beta F} (e^{-\beta E_{\lambda}} - e^{-\beta E_{\zeta}}) \left| \left\langle \zeta \left| S_{-\mathbf{q}}^{+} \right| \lambda \right\rangle \right|^{2} e^{-i(E_{\zeta}-E_{\lambda})t} \theta(t), \end{split}$$

where we have used the identity $\langle \lambda | S_{\mathbf{q}}^{-} | \zeta \rangle = \langle \zeta | S_{-\mathbf{q}}^{+} | \lambda \rangle^{*}$. Now, by introducing the spectral function

$$\chi''(\mathbf{q},\omega) = \pi(1-e^{-\beta\omega})\sum_{\lambda,\zeta} p_{\lambda} \left| \left\langle \zeta \left| S_{-\mathbf{q}}^{+} \right| \lambda \right\rangle \right|^{2} \delta[\omega - (E_{\zeta} - E_{\lambda})], \tag{40}$$

where $p_{\lambda} = e^{-\beta(E_{\lambda}-F)}$ is the probability of being in the initial state $|\lambda\rangle$, we see that the retarded response function can be written,

$$\chi_R(\mathbf{q},t) = i\theta(t) \int \frac{d\omega'}{\pi} e^{-i\omega' t} \chi''(\mathbf{q},\omega').$$
(41)

(b) Fourier transforming this result,

$$\chi_R(\mathbf{q},\omega) = \int_0^\infty dt \chi_R(\mathbf{q},t) e^{i\omega t} e^{-\delta t} = i \int \frac{d\omega'}{\pi} \chi''(\mathbf{q},\omega') \int_0^\infty dt e^{i(\omega-\omega'+i\delta)t}, \qquad (42)$$

where we have inverted the order of the frequency and time integrations. Now using

$$i \int_0^\infty dt e^{i(\omega - \omega' + i\delta)t} = \frac{1}{\omega' - \omega - i\delta},\tag{43}$$

we obtain the "Kramers-Krönig" relation

$$\chi_R(\mathbf{q},\omega) = \int \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\delta} \chi''(\mathbf{q},\omega').$$
(44)

 $\frac{\mathbf{x} \mathbf{x} \mathbf{x} \mathbf{x} \mathbf{x}}{\mathbf{z} \mathbf{z}} = \mathbf{u}^{\prime} - i\mathbf{s} \quad (\mathbf{c})$ $\frac{\mathbf{e}_{\mathbf{z}} \mathbf{u}^{\prime} - i\mathbf{s}}{\mathbf{z} \mathbf{z}} = \mathbf{u}^{\prime} - i\mathbf{s} \quad (\mathbf{c})$

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 $\chi_{R}(z)$

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$$S(\mathbf{q}, t) = \langle S_{\mathbf{q}}^{-}(t)S_{-\mathbf{q}}^{+}(0) \rangle$$

=
$$\sum_{\lambda,\zeta} e^{-\beta(E_{\lambda}-F)} \langle \lambda | S_{\mathbf{q}}^{-}(t) | \zeta \rangle \langle \zeta | S_{-\mathbf{q}}^{+}(0) | \lambda \rangle$$

=
$$\sum_{\lambda,\zeta} e^{-\beta(E_{\lambda}-F)} | \langle \zeta | S_{-\mathbf{q}}^{+} | \lambda \rangle |^{2} e^{-i(E_{\zeta}-E_{\lambda})t}$$
(45)

If we now Fourier transform this expression, the frequency dependent correlation function can be written

$$S(\mathbf{q},\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} S(\mathbf{q},t)$$

=
$$\sum_{\lambda,\zeta} p_{\lambda} \left| \left\langle \zeta \left| S_{-\mathbf{q}}^{+} \right| \lambda \right\rangle \right|^{2} 2\pi \delta(E_{\zeta} - E_{\lambda} - \omega).$$
(46)

Now using (40), we can write this as

$$S(\mathbf{q},\omega) = \frac{2}{1 - e^{-\beta\omega}} \chi''(\mathbf{q},\omega) = 2[1 + n(\omega)]\chi''(\mathbf{q},\omega).$$
(47)