

MANY BODY PHYSICS: 621. Spring 2022

Exercise 2. (Due Weds 23 Mar.)

1. Use the method of complex contour integration to carry out the Matsubara sums in the following:

(i) Derive the density of a spinless Bose Gas at finite temperature from the boson propagator $D(k) \equiv D(\mathbf{k}, i\nu_n) = [i\nu_n - \omega_{\mathbf{k}}]^{-1}$, where $\omega_{\mathbf{k}} = E_{\mathbf{k}} - \mu$ is the energy of a boson, measured relative to the chemical potential.

$$\rho(T) = \frac{N}{V} = V^{-1} \sum_{\mathbf{k}} \langle T b_{\mathbf{k}}(0^-) b_{\mathbf{k}}^\dagger(0) \rangle = -(\beta V)^{-1} \sum_{i\nu_n, \mathbf{k}} D(k) e^{i\nu_n 0^+}. \quad (1)$$

How do you need to modify your answer to take account of Bose Einstein condensation?

(ii) The dynamic charge-susceptibility of a free Bose gas, i.e

$$\chi_c(q, i\nu_n) = \begin{array}{c} \text{D(k+q)} \\ \curvearrowright \\ \text{D(k)} \\ \curvearrowleft \end{array} = T \sum_{i\nu_n} \int \frac{d^3k}{(2\pi)^3} D(q+k) D(k). \quad (2)$$

Please analytically extend your final answer to real frequencies.

(iii) The “pair-susceptibility” of a spin-1/2 free Fermi gas, i.e.

$$\chi_P(q, i\nu_n) = \begin{array}{c} \uparrow \text{G(k+q)} \\ \curvearrowright \\ \text{G(-k)} \downarrow \end{array} = T \sum_{i\nu_n} \int \frac{d^3k}{(2\pi)^3} G(q+k) G(-k) \quad (3)$$

where $G(k) \equiv G(\mathbf{k}, i\omega_n) = [i\omega_n - \epsilon_{\mathbf{k}}]^{-1}$. (Note the direction of the arrows: why is there no minus sign for the Fermion loop?) Show that the static pair susceptibility, $\chi_P(0)$ is given by

$$\chi_P = \int \frac{d^3k}{(2\pi)^3} \frac{\tanh[\beta\epsilon_{\mathbf{k}}/2]}{2\epsilon_{\mathbf{k}}} \quad (4)$$

Can you see that this quantity diverges at low temperatures? How does it diverge, and why ?

2. Mean field theory for antiferromagnetic Spin Density Wave

Using a path integral approach, develop the mean-field theory for a three dimensional tight-binding cubic lattice with commensurate antiferromagnetic order parameter

$$\mathbf{M}_j = \mathbf{M} e^{i\mathbf{Q} \cdot \mathbf{R}_j} \quad (5)$$

where $\mathbf{Q} = (\pi, \pi, \pi)$. The Hamiltonian for this model is given by

$$H = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} - \frac{I}{2} \sum_j (\vec{\sigma}_j)^2 \quad (6)$$

where $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y + \cos k_z)$ and $\vec{\sigma}_j \equiv c_{j\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{j\beta}$ is the spin density at site j .

(a) Show that the mean-field free energy can be written in the form

$$H_{MF} = \sum_{\mathbf{k} \in \frac{1}{2}BZ} \psi_{\mathbf{k}}^\dagger \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & \mathbf{M} \cdot \vec{\sigma} \\ \mathbf{M} \cdot \vec{\sigma} & \epsilon_{\mathbf{k}+\mathbf{Q}} - \mu \end{pmatrix} \psi_{\mathbf{k}} + \mathcal{N}_s \frac{M^2}{2I} \quad (7)$$

where $M = |\mathbf{M}|$ is the magnitude of the staggered magnetization, \mathcal{N}_s is the number of sites in the lattice, $\psi_{\mathbf{k}}$ denotes the four-component spinor

$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \\ c_{\mathbf{k}+\mathbf{Q}\uparrow} \\ c_{\mathbf{k}+\mathbf{Q}\downarrow} \end{pmatrix}, \quad (8)$$

$\epsilon_{\mathbf{k}} = -2t(c_x + c_y + c_z)$, ($c_l \equiv \cos k_l$, $l = x, y, z$) is the kinetic part of the energy and the summation is restricted to the magnetic Brillouin zone. (Half of the crystal Brillouin zone.)

(b) On a tight binding lattice the kinetic energy has the “nesting” property that $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$. Show that the energy eigenvalues of the mean-field Hamiltonian have a BCS form

$$E_{\mathbf{k}\pm} = \pm \sqrt{\epsilon_{\mathbf{k}}^2 + M^2} - \mu. \quad (9)$$

corresponding to an excitation spectrum with gap M . Notice that the gap is offset by an amount μ . Over half the Brillouin zone, each of these eigenvalues is doubly degenerate.

(c) Show that the mean-field free energy takes the form

$$F = \sum_{\mathbf{k}, p=\pm 1} -T \ln \left[2 \cosh \left(\frac{\beta E_{\mathbf{k}p}}{2} \right) \right] + \mathcal{N}_s \left(\frac{M^2}{2I} - \mu \right), \quad (10)$$

where the momentum sum is over the full Brillouin zone.

(d) By minimizing the free energy with respect to M , show that the gap equation for M is given by

$$\frac{1}{2} \sum_{\mathbf{k}, p=\pm 1} \tanh \left(\frac{\sqrt{\epsilon_{\mathbf{k}}^2 + M^2} - \mu p}{2T} \right) \frac{1}{\sqrt{\epsilon_{\mathbf{k}}^2 + M^2}} = \frac{1}{I}. \quad (11)$$

(e) Show that at half filling, the nesting guarantees that a transition to a spin-density wave will occur for arbitrarily small interaction strength I . What do you think will happen at a finite doping ($\mu \neq 0$)?

3. Spectral decomposition. The dynamic spin susceptibility of a magnetic system, is defined as

$$\chi(\mathbf{q}, t_1 - t_2) = i \langle [S^-(\mathbf{q}, t_1), S^+(-\mathbf{q}, t_2)] \rangle \theta(t_1 - t_2) \quad (12)$$

where $S^\pm(\mathbf{q}) = S_x(\mathbf{q}) \pm iS_y(\mathbf{q})$ are the raising and lowering operators at wavevector \mathbf{q} ,

$$S^\pm(\mathbf{q}) = \int d^3 e^{-i\mathbf{q}\cdot\mathbf{x}} S^\pm(\mathbf{x}) \quad (13)$$

so that $S^-(\mathbf{q}) = [S^+(-\mathbf{q})]^\dagger$. The dynamic spin susceptibility determines the response of the magnetization at wavevector \mathbf{q} to an applied magnetic field

$$M(\mathbf{q}, t) = (g\mu_B)^2 \int \chi(\mathbf{q}, t - t') B(\mathbf{q}, t') dt'. \quad (14)$$

(a) Make a spectral decomposition, and show that

$$\chi(\mathbf{q}, t) = i\theta(t) \int \frac{d\omega}{\pi} \chi''(\mathbf{q}, \omega) e^{i\omega t} \quad (15)$$

where $\chi''(\mathbf{q}, \omega)$ (often called the “power-spectrum” of spin fluctuations) is

$$\chi''(\mathbf{q}, \omega) = (1 - e^{-\beta\omega}) \sum_{\lambda, \zeta} e^{-\beta(E_\lambda - F)} |\langle \zeta | S^+(-\mathbf{q}) | \lambda \rangle|^2 \pi \delta[\omega - (E_\zeta - E_\lambda)] \quad (16)$$

and F is the Free energy.

(b) Fourier transform (15) to obtain a simple integral transform which relates $\chi(\mathbf{q}, \omega)$ and $\chi''(\mathbf{q}, \omega)$. The correct result is a “Kramers Kronig” transformation.

(c) How is $\chi(\mathbf{q}, t)$ related to the imaginary time response function $\chi(\mathbf{q}, \tau) = \langle S^-(\mathbf{q}, \tau), S^+(-\mathbf{q}, 0) \rangle$?

- (d) In neutron scattering experiments, the inelastic scattering cross-section is directly proportional to a spectral function called $S(\mathbf{q}, \omega)$,

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S(\mathbf{q}, \omega) \quad (17)$$

where $S(\mathbf{q}, \omega)$ is the Fourier transform of a correlation function:

$$S(\mathbf{q}, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S^-(\mathbf{q}, t) S^+(-\mathbf{q}, 0) \rangle \quad (18)$$

By carrying out a spectral decomposition, show that

$$S(\mathbf{q}, \omega) = (1 + n(\omega)) \chi''(\mathbf{q}, \omega) \quad (19)$$

This relationship, plus the one you derived in (d) can be used to completely measure the dynamical spin susceptibility via inelastic neutron scattering.