MANY BODY PHYSICS: 621. Spring 2023

Exercise 2. (Due Apr 5.)

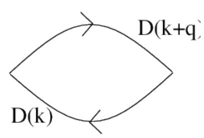
1. Use the method of complex contour integration to carry out the Matsubara sums in the following:

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

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

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

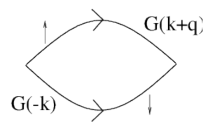
   (ii) The dynamic charge-susceptibility of a free Bose gas, i.e

   $\chi_c(q, i\nu_n) =$ 

   $$= T \sum_{i\nu_n} \int \frac{d^3k}{(2\pi)^3} D(q+k) D(k). \tag{2}$$

   Please analytically extend your final answer to real frequencies.

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

   $\chi_P(q, i\nu_n) =$ 

   $$= T \sum_{i\omega_r} \int \frac{d^3k}{(2\pi)^3} G(q+k) G(-k) \tag{3}$$

   where $G(k) \equiv G(\mathbf{k}, \mathbf{i}\omega_\mathbf{n}) = [\mathbf{i}\omega_\mathbf{n} - \epsilon_\mathbf{k}]^{-1}$. (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

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

   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

   $$\mathbf{M}_j = \mathbf{M} e^{i\mathbf{Q}\cdot\mathbf{R}_j} \tag{5}$$

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

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

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

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

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

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

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

$\epsilon_{\mathbf{k}} = -2t(c_x + c_y + c_z)$, $(c_l \equiv \cos k_l,\ l = x, y, z)$ 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 $\epsilon_{\mathbf{k+Q}} = -\epsilon_{\mathbf{k}}$. Show that the energy eigenvalues of the mean-field Hamiltonian have a BCS form

$$E_{\mathbf{k}\pm} = \pm \sqrt{\epsilon^2_{\mathbf{k}} + M^2} - \mu. \tag{9}$$

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

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

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

$$\frac{1}{2}\sum_{\mathbf{k},p=\pm1}\tanh\left(\frac{\sqrt{\epsilon_{\mathbf{k}}^2+M^2}-\mu p}{2T}\right)\frac{1}{\sqrt{\epsilon_{\mathbf{k}}^2+M^2}}=\frac{1}{I}. \tag{11}$$

(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

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

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

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

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

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

(a) Make a spectral decomposition, and show that

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

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

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

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 $S(\mathbf{q},\omega)$,

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

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

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

By carrying out a spectral decomposition, show that

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

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