Statistical Physics & Condensed Matter Theory I: Exercise

1 Hubbard model

Let us consider the one-dimensional Hubbard model,

$$H = -t \sum_{\sigma} \sum_{j=1}^{N} \left(a^{\dagger}_{j\sigma} a_{j+1\sigma} + a^{\dagger}_{j+1\sigma} a_{j\sigma} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$$

where $a_{j\sigma}, a^{\dagger}_{j\sigma}$ are fermionic annihilation and creation operators obeying the anticommutation relations $\{a_{j\sigma}, a^{\dagger}_{j'\sigma'}\} \equiv a_{j\sigma} a^{\dagger}_{j'\sigma'} + a^{\dagger}_{j'\sigma'} a_{j\sigma} = \delta_{jj'} \delta_{\sigma\sigma'}$, $n_{j\sigma} \equiv a^{\dagger}_{j\sigma} a_{j\sigma}$ are the on-site number operators, and we adopt periodic boundary conditions $a_{j+N.\sigma} \equiv a_{j\sigma}$.

a)

Write the Hamiltonian in momentum space.

b)

Let us focus first on the free case $U = 0$. The coherent state path integral representation of the partition function $Z^{(0)}$ and free effective action[1] of the free system are

$$\mathcal{Z}^{(0)} = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S_0[\bar{\psi}, \psi]}, \qquad S_0[\bar{\psi}, \psi] = \sum_{kn\sigma} \bar{\psi}_{kn\sigma} \left[-i\omega_n + \xi_k \right] \psi_{kn\sigma}$$

in which $\xi_k \equiv \varepsilon_k - \mu = -2t \cos k - \mu$. Explicitly perform the necessary Grassmann integrations to show that the free energy $\mathcal{F}^{(0)} = -T \ln \mathcal{Z}^{(0)}$ of the noninteracting system is given by [2]

$$\mathcal{F}^{(0)} = -T \sum_{k\sigma} \ln \left[1 + e^{-\beta \xi_k} \right].$$

c)

Show that the $T \to 0$ limit of $\mathcal{F}^{(0)}$ is given by $2 \sum_k \xi_k \theta(-\xi_k)$ where $\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}$ is the Heaviside function. Taking $-2t < \mu < 2t$, define a Fermi momentum k_F. Taking the thermodynamic limit $N \to \infty$, calculate explicitly the free energy density $f^{(0)} = \mathcal{F}^{(0)}/N$, expressing your answer in terms of k_F. What is $f^{(0)}$ for $\mu < -2t$ and $\mu > 2t$?

d)

By directly performing the Grassmann integrations, show that the free ($U = 0$) Green's function is

$$\mathcal{G}^{(0)}_{k,n} \equiv \langle \bar{\psi}_{kn\sigma} \psi_{kn\sigma} \rangle_0 = \frac{1}{i\omega_n - \xi_k} \quad \text{where we denote} \quad \langle (...) \rangle_0 = \frac{1}{\mathcal{Z}^{(0)}} \int \mathcal{D}(\bar{\psi}, \psi)(...) e^{-S_0[\bar{\psi}, \psi]}.$$

[1] Here and in this whole exercise, we always write the momentum k and Matsubara frequency index n separately.
[2] Hint: the Matsubara sum can be performed using the formula given in 'Useful formulas'.

e)

Consider now the partition function of the interacting ($U \neq 0$) system. Show that the first-order correction to the free energy is given by

$$\mathcal{F}^{(1)} = T\langle S_{int}\rangle_0$$

where

$$S_{int}[\bar{\psi}, \psi] = \frac{UT}{N}\sum_{kk'q}\sum_{nn'm}\bar{\psi}_{k+q,n+m,\uparrow}\bar{\psi}_{k'-q,n'-m,\downarrow}\psi_{k',n',\downarrow}\psi_{k,n,\uparrow}.$$

f)

Calculate the first order in U correction to the free energy. Are both terms (Hartree and Fock; see 'Useful formulas') nonzero ? Give an explicit expression for $f^{(1)} = \mathcal{F}^{(1)}/N$ in the limit $T \to 0$ and thermodynamic limit in terms of the Fermi momentum k_F.

g)

Again, by direct calculation, show that up to and including terms of order U/t, the Green's function of the interacting system can be written[3]

$$\mathcal{G}_{k,n} \equiv \langle\bar{\psi}_{kn\sigma}\psi_{kn\sigma}\rangle = \frac{1}{i\omega_n - \xi_k - \Sigma_{k,n}}$$

where $\Sigma_{k,n}$ is called the *self-energy*. Give an expression for it to first order in U.

h)

We have seen in class that in the limit $U \to \infty$ (infinite repulsion), the half-filled Hubbard model becomes the Heisenberg model with exchange $J = 4t^2/U$. Without going into explicit calculations, can you say what kind of model the $U \to -\infty$ (infinite attraction) limit yields at a generic (not necessarily half) filling (assume for simplicity equal total numbers of spin-up and spin-down electrons) ?

[3] Hint: $1 + U = \frac{1}{1-U} + \mathcal{O}(U^2)$.