Statistical Physics & Condensed Matter Theory I: Exercise

1 Hubbard model: solution

a) After a simple Fourier transform, we get

$$H = -t \sum_{\sigma} \sum_{k} 2 \cos k a^{\dagger}_{k\sigma} a_{k\sigma} + \frac{U}{N} \sum_{kk'q} a^{\dagger}_{k+q\uparrow} a^{\dagger}_{k'-q\downarrow} a_{k'\downarrow} a_{k\uparrow}.$$

b) The Grassmann integration for the partition function is

$$\mathcal{Z}^{(0)} = \int \mathcal{D}(\bar{\psi}, \psi) e^{-S_0[\bar{\psi},\psi]} = \prod_{kn\sigma} \int d(\bar{\psi}_{kn\sigma}, \psi_{kn\sigma}) e^{-\bar{\psi}_{kn\sigma}[-i\omega_n + \xi_k]\psi_{kn\sigma}}$$
$$= \prod_{kn\sigma} \beta \int d\bar{\psi}_{kn\sigma} d\psi_{kn\sigma} (1 - \bar{\psi}_{kn\sigma}[-i\omega_n + \xi_k]\psi_{kn\sigma}) = \prod_{kn\sigma} (\beta[-i\omega_n + \xi_k]),$$

so the free energy is

$$\mathcal{F}^{(0)} = -T \ln \mathcal{Z}^{(0)} = -T \sum_{kn\sigma} \ln(\beta[-i\omega_n + \xi_k]) = -T \sum_{k\sigma} \left(\sum_{n} \ln[\beta(-i\omega_n + \xi_k)] \right).$$

The Matsubara sum is done using the formula given. We thus get what is given in the question.

c) In the zero temperature limit, $\beta \to +\infty$, so the logarithm is nonvanishing only if $\xi_k < 0$, in which case it is equal to ξ_k. The factor of 2 comes from spin degeneracy. If we take μ in the interval $[-2t, 2t]$, we can define a Fermi momentum using the condition $\xi_{k_F} = 0$, so $k_F = \text{ acos } (\frac{-\mu}{2t})$. In the thermodynamic limit, the free energy density becomes

$$\begin{aligned} f^{(0)} &= -T \frac{1}{N} 2 \sum_{|k|<k_F} \xi_k = -2T \int_{-k_F}^{k_F} \frac{dk}{2\pi} (-2t \cos k - \mu) \\ &= -\frac{T}{\pi} (-2t 2 \sin k_F - \mu 2 k_F) = \frac{4Tt}{\pi} \sin k_F + \frac{2T\mu}{\pi} k_F. \end{aligned}$$

This can be written as an explicit function of μ through the definition of k_F. For $\mu > 2t$, we stay at $k_F = \pi$. For $\mu < -2t$, we stay at $k_F = 0$.

d) For the free Green's function, the Grassmann integration is

$$\mathcal{G}^{(0)}_{k,n} \equiv \frac{1}{\mathcal{Z}^{(0)}} \int \mathcal{D}(\bar{\psi}, \psi) \bar{\psi}_{kn\sigma} \psi_{kn\sigma} e^{-S_o[\bar{\psi},\psi]} = \frac{\int d(\bar{\psi}_{kn\sigma}, \psi_{kn\sigma}) \bar{\psi}_{kn\sigma} \psi_{kn\sigma} e^{-\bar{\psi}_{kn\sigma}[-i\omega_n + \xi_k]\psi_{kn\sigma}}}{\int d(\bar{\psi}_{kn\sigma}, \psi_{kn\sigma}) e^{-\bar{\psi}_{kn\sigma}[-i\omega_n + \xi_k]\psi_{kn\sigma}}}$$
$$= \frac{\int d(\bar{\psi}_{kn\sigma}, \psi_{kn\sigma}) \bar{\psi}_{kn\sigma} \psi_{kn\sigma}}{\int d(\bar{\psi}_{kn\sigma}, \psi_{kn\sigma})(1 - \bar{\psi}_{kn\sigma}[-i\omega_n + \xi_k]\psi_{kn\sigma})} = \frac{-\beta}{\beta[-i\omega_n + \xi_k]} = \frac{1}{i\omega_n - \xi_k}.$$

In the first step, we dropped all integrals for fields with indices other than $kn\sigma$, for which the numerator and denominator cancel. The actual integrals are done as in Useful formulas.

e) The first order correction to the free energy is given from the first order correction to the partition function, which is

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi)e^{-S_0-S_{int}} = \int \mathcal{D}(\bar{\psi},\psi)e^{-S_0}(1-S_{int}+\mathcal{O}(2)) = \mathcal{Z}^{(0)}+\mathcal{Z}^{(1)}+\mathcal{O}(2)$$

where $\mathcal{Z}^{(1)} \equiv -\mathcal{Z}^{(0)}\langle S_{int}\rangle_0$, so

$$\mathcal{F} = -T\ln(\mathcal{Z}^{(0)}+\mathcal{Z}^{(1)}+\mathcal{O}(2)) = -T\ln\mathcal{Z}^{(0)} - T\ln(1+\frac{\mathcal{Z}^{(1)}}{\mathcal{Z}^{(0)}}+\mathcal{O}(2)) = \mathcal{F}^{(0)}+T\langle S_{int}\rangle_0+\mathcal{O}(2).$$

Here, the interaction part of the action is as in a), with $a^\dagger \to \bar{\psi}$ and $a \to \psi$.

f) Performing the average using Wick's theorem, the only term that survives is the Hartree-like term, since for the Fock one, the spin indices don't match. Note that here, the Hartree term is nonzero, since the interaction is purely local in site index j, meaning that it has uniform Fourier components for all frequencies including zero. We thus get

$$\begin{aligned}
\mathcal{F}^{(1)} &= \frac{UT^2}{N}\sum_{kk'q}\sum_{nn'm}\langle\bar{\psi}_{k+q,n+m,\uparrow}\bar{\psi}_{k'-q,n'-m,\downarrow}\psi_{k',n',\downarrow}\psi_{k,n,\uparrow}\rangle_0 \\
&= \frac{UT^2}{N}\sum_{kk'q}\sum_{nn'm}\langle\bar{\psi}_{k+q,n+m,\uparrow}\psi_{k,n,\uparrow}\rangle_0\langle\bar{\psi}_{k'-q,n'-m,\downarrow}\psi_{k',n',\downarrow}\rangle_0 \\
&= \frac{UT^2}{N}\sum_{kk'}\sum_{nn'}\mathcal{G}^{(0)}_{kn}\mathcal{G}^{(0)}_{k'n'} = \frac{UT^2}{N}\left(\sum_{kn}\mathcal{G}^{(0)}_{kn}\right)^2.
\end{aligned}$$

Doing the Mastubara sum with the Useful formulas, we have (going to zero temperature and the thermodynamic limit)

$$f^{(1)} = \frac{\mathcal{F}^{(1)}}{N} = \frac{U}{N^2}\left(\sum_k n_F(\varepsilon_k)\right)^2 \to U\left(\frac{1}{N}\sum_k\theta(-\xi_k)\right)^2 = U\left(\int_{-k_F}^{k_F}\frac{dk}{2\pi}1\right) = U\frac{k_F^2}{\pi^2}.$$