Statistical Physics & Condensed Matter Theory I: Exercise

Itinerant electrons with interactions: mean-field theory

We have seen that starting from Hubbard-like models (with on-site Coulomb interaction $U > 0$), a Heisenberg model can be obtained by going to the strongly-interacting limit $U \to \infty$ when the system is half-filled (one electron per site on average).

What happens if U is not that large, and we're working at generic fillings? Consider a d-dimensional crystal with electrons interacting with a purely on-site Coulomb interaction $U > 0$. In Fourier space, we can write the Hamiltonian as

$$H = H_0 + H_{int} = \sum_{\mathbf{k}} \sum_{\sigma} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \frac{U}{2L^d} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{\sigma\sigma'} a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma}$$

in which $\varepsilon_{\mathbf{k}}$ is the kinetic energy part.

The interaction term is impossible to handle exactly. We could simply do perturbation theory in U, but we don't always want to assume that U is small. The purpose of this exercise is to show you another way of handling this interaction.

The key is to find a reasonable way of rewriting the interaction term (containing 4 operators) into terms with 2 operators only (which can then be handled exactly). We thus make the assumption ('mean-field') that we can replace the operator product according to

$$\begin{aligned} a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma} \simeq\; & a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \langle a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}'\sigma'} \rangle_{MF} + a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}'\sigma'} \langle a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \rangle_{MF} \\ & - a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}'\sigma'} \langle a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}\sigma} \rangle_{MF} - a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}\sigma} \langle a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}'\sigma'} \rangle_{MF} \\ & - \langle a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}\sigma} \rangle_{MF} \langle a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}'\sigma'} \rangle_{MF} + \langle a^\dagger_{\mathbf{k}+\mathbf{q}\sigma} a_{\mathbf{k}'\sigma'} \rangle_{MF} \langle a^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} a_{\mathbf{k}\sigma} \rangle_{MF} \end{aligned}$$

in which we take the 'mean-field' expectation values to be given by the (not yet determined) parameters $n_{\mathbf{k}\sigma}$ according to

$$\langle a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}'\sigma} \rangle_{MF} \equiv \delta_{\mathbf{k}\mathbf{k}'} \bar{n}_{\mathbf{k}\sigma}$$

(all other expectation values vanishing).

a)

Show that under this mean-field assumption, the interaction part of the Hamiltonian is replaced by

$$H_{int} \simeq H^{MF}_{int} = U \sum_{\mathbf{k}} \sum_{\sigma\sigma'} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \left[\bar{n}_{\sigma'} - \delta_{\sigma\sigma'} \bar{n}_\sigma\right] - \frac{UL^d}{2} \sum_{\sigma\sigma'} (1 - \delta_{\sigma\sigma'}) \bar{n}_\sigma \bar{n}_{\sigma'}$$

in which

$$\bar{n}_\sigma \equiv \frac{1}{L^d} \sum_{\mathbf{k}} \langle a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \rangle_{MF}$$

are again fixed (though unspecified as of yet) numbers.

b)

The complete mean-field Hamiltonian is thus

$$H^{MF} = H^0 + H^{MF}_{int} \equiv \sum_{\mathbf{k}} \sum_{\sigma} \varepsilon^{MF}_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + C(\{\bar{n}_\sigma\})$$

with

$$\varepsilon^{MF}_{\mathbf{k}\sigma} \equiv \varepsilon_{\mathbf{k}} + U(\bar{n}_\uparrow + \bar{n}_\downarrow - \bar{n}_\sigma) = \varepsilon_{\mathbf{k}} + U\bar{n}_{-\sigma}, \qquad C(\{\bar{n}_\sigma\}) \equiv -\frac{UL^d}{2} \sum_{\sigma\sigma'} (1 - \delta_{\sigma\sigma'})\bar{n}_\sigma \bar{n}_{\sigma'}$$

Since this Hamiltonian is now bilinear in the $a^\dagger$, a operators, everything can be computed exactly. Write down the coherent state path integral representation for the partition function Z^{MF} of the mean-field theory, introducing separate chemical potentials μ_σ for up and down spins, and show that the mean-field free energy can be written

$$\mathcal{F}^{MF} = -T \ln \mathcal{Z}^{MF} = -T \sum_{\mathbf{k}} \sum_{n} \sum_{\sigma} \ln \left[\beta(-i\omega_n + \xi^{MF}_{\mathbf{k}\sigma})\right] + C(\{\bar{n}_\sigma\})$$

in which $\xi^{MF}_{\mathbf{k}\sigma} = \varepsilon^{MF}_{\mathbf{k}\sigma} - \mu_\sigma$.

c)

So far, we have assumed that the mean-field parameters $\bar{n}_\sigma$ were fixed, but we didn't specify to which value. This is done by requiring *self-consistency* of the mean-field treatment. Using the relations $\bar{n}_\sigma = -\frac{1}{L^d}\frac{\partial}{\partial \mu_\sigma}\mathcal{F}^{MF}$, show that (by performing the Matsubara summation using one of the 'Useful formulas') we need to require

$$\bar{n}_\sigma = \frac{1}{L^d} \sum_{\mathbf{k}} n_F(\varepsilon^{MF}_{\mathbf{k}\sigma})$$

d)

Specialize now to the three-dimensional case at zero temperature, assume that $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$, go to the infinite-size limit (so that $\frac{1}{L^3}\sum_{\mathbf{k}}(...) \to \int \frac{d^3k}{(2\pi)^3}(...)$), and take the two chemical potentials to be equal $\mu_\sigma \equiv \mu$. Show that

$$\bar{n}_\sigma = \frac{1}{6\pi^2} k^3_{F\sigma}$$

where the (spin-dependent) Fermi momenta are given by $\frac{\hbar^2}{2m} k^2_{F\sigma} + U\bar{n}_{-\sigma} = \mu$.

e)

Defining the parameters

$$\bar{n} \equiv \bar{n}_\uparrow + \bar{n}_\downarrow, \qquad \zeta = \frac{\bar{n}_\uparrow - \bar{n}_\downarrow}{\bar{n}_\uparrow + \bar{n}_\downarrow}, \qquad \gamma = \frac{2mU\bar{n}^{1/3}}{(3\pi^2)^{2/3}\hbar^2}$$

(note that we must have $0 \leq \zeta \leq 1$), show that the self-consistency conditions can be rewritten (most easily by subtracting the two chemical potentials from each other)

$$\gamma = \frac{1}{\zeta}\left[(1+\zeta)^{2/3} - (1-\zeta)^{2/3}\right].$$

Discuss what happens as a function of the effective interaction parameter γ (hint: look at the left-hand side function of ζ, and find the limits when $\zeta \to 0$ and $\zeta \to 1$). What kind of magnetic state exists for $\gamma < 4/3$, $4/3 < \gamma < 2^{2/3}$ and $\gamma > 2^{2/3}$? Can you explain this physically?