Statistical Physics & Condensed Matter Theory I: Exercise

Mean-field theory for the Anderson impurity model: solution

a)

We can write $n_{d\sigma} - \langle n_{d\sigma}\rangle = \delta n_{d\sigma}$ and expect this to be very small (*i.e.* under the mean-field approximation, we expect that fluctuations are very small as compared to the average value, $\delta n_{d\sigma} \ll \langle n_{d\sigma}\rangle$). Then,

$$(n_{d\uparrow} - \langle n_{d\uparrow}\rangle)(n_{d\downarrow} - \langle n_{d\downarrow}\rangle) = \delta n_{d\uparrow}\delta n_{d\downarrow} \sim 0 \Rightarrow n_{d\uparrow}n_{d\downarrow} \sim \langle n_{d\uparrow}\rangle n_{d\downarrow} + \langle n_{d\downarrow}\rangle n_{d\uparrow} - \langle n_{d\uparrow}\rangle\langle n_{d\downarrow}\rangle.$$

b)

The functional integral can be written as usual by evaluating the creation/annihilation operators onto the coherent states, and moving to the Matsubara representation:

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi)\int \mathcal{D}(\bar{\phi},\phi)e^{-S[\bar{\psi},\psi,\bar{\phi},\phi]}$$

with $\mathcal{D}(\bar{\psi},\psi) = \prod_{\mathbf{k}\sigma n}\beta d\bar{\psi}_{\mathbf{k}\sigma n}d\psi_{\mathbf{k}\sigma n}$, $\mathcal{D}(\bar{\phi},\phi) = \prod_{\sigma n}\beta d\bar{\phi}_{\sigma n}\phi_{\sigma n}$ and

$$S = \sum_{\mathbf{k}}\sum_{\sigma}\sum_{n}\bar{\psi}_{\mathbf{k}\sigma n}[-i\omega_n + \varepsilon_{\mathbf{k}} - \mu]\psi_{\mathbf{k}\sigma n} + \sum_{\sigma}\sum_{n}\bar{\phi}_{\sigma n}[-i\omega_n + \varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle]\phi_{\sigma n} + \sum_{\mathbf{k}}\sum_{\sigma}\sum_{n}\left(t_{\mathbf{k}}\bar{\phi}_{\sigma n}\psi_{\mathbf{k}\sigma n} + t^*_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\sigma n}\phi_{\sigma n}\right)$$

c)

To absorb the coupling term, we can defined shifted fermionic fields according to

$$\psi'_{\mathbf{k}\sigma n} = \psi_{\mathbf{k}\sigma n} + \frac{t^*_{\mathbf{k}}}{-i\omega_n + \varepsilon_{\mathbf{k}} - \mu}\phi_{\sigma n}, \qquad \bar{\psi}'_{\mathbf{k}\sigma n} = \bar{\psi}_{\mathbf{k}\sigma n} + \frac{t_{\mathbf{k}}}{-i\omega_n + \varepsilon_{\mathbf{k}} - \mu}\bar{\phi}_{\sigma n}.$$

We can then write

$$\bar{\psi}_{\mathbf{k}\sigma n}[-i\omega_n + \varepsilon_{\mathbf{k}} - \mu]\psi_{\mathbf{k}\sigma n} + t_{\mathbf{k}}\bar{\phi}_{\sigma n}\psi_{\mathbf{k}\sigma n} + t^*_{\mathbf{k}}\bar{\psi}_{\mathbf{k}\sigma n}\phi_{\sigma n} = \bar{\psi}'_{\mathbf{k}\sigma n}[-i\omega_n + \varepsilon_{\mathbf{k}} - \mu]\psi'_{\mathbf{k}\sigma n} - \frac{|t_{\mathbf{k}}|^2}{-i\omega_n + \varepsilon_{\mathbf{k}} - \mu}\bar{\phi}_{\sigma n}\phi_{\sigma n}$$

which then gives the action in the question after identification of the self-energy function.

d)

For the partition function, we simply need to use the identity (for a general ε)

$$\int d(\bar{\psi}_{\mathbf{k}\sigma n},\psi_{\mathbf{k}\sigma n})e^{-\bar{\psi}_{\mathbf{k}\sigma n}\varepsilon\psi_{\mathbf{k}\sigma n}} = \beta\int d\bar{\psi}_{\mathbf{k}\sigma n}d\psi_{\mathbf{k}\sigma n}(1 - \bar{\psi}_{\mathbf{k}\sigma n}\varepsilon\psi_{\mathbf{k}\sigma n}) = \beta\varepsilon.$$

Since all the $\psi_{\mathbf{k}\sigma n}$ and $\phi_{\sigma n}$ are decoupled, the whole partition function is simply the product of all single-mode integrals, namely

$$\mathcal{Z} = \prod_{\mathbf{k}\sigma n} \beta[-i\omega_n + \varepsilon_{\mathbf{k}} - \mu] \times \prod_{\sigma n} \beta[-i\omega_n + \varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle + \Sigma(i\omega_n, \mu)].$$

Taking the logarithm gives the free energy $\mathcal{F} = -T \ln \mathcal{Z}$ as in the question.

e)

We have

$$\partial_{\mu_{d,\sigma}} \mathcal{Z} = \partial_{\mu_{d,\sigma}} \text{ Tr } e^{-\beta H} = -\beta \text{ Tr } (e^{-\beta H} \partial_{\mu_{d,\sigma}} H) = +\beta \text{ Tr } (e^{-\beta H} d_\sigma^\dagger d_\sigma) = \beta \mathcal{Z} \langle n_{d,\sigma}\rangle$$

where we have used $\langle ...\rangle \equiv \frac{1}{\mathcal{Z}} \text{ Tr } (e^{-\beta H} ...)$. We thus get

$$\langle n_{d,\sigma}\rangle = \beta^{-1} \frac{1}{\mathcal{Z}} \partial_{\mu_{d,\sigma}} \mathcal{Z} = T \partial_{\mu_{d,\sigma}} \ln \mathcal{Z} = -\partial_{\mu_{d,\sigma}} \mathcal{F}.$$

On the other hand, from the previous result for the partition function, we immediately get

$$-\frac{\partial \mathcal{F}}{\partial \mu_{d,\sigma}} = T \sum_n \frac{1}{i\omega_n - \varepsilon_d + \mu_{d,\sigma} - U\langle n_{d,-\sigma}\rangle - \Sigma(i\omega_n, \mu)}.$$

f)

Under the assumptions given, we have the simple elementary integral

$$\int_{-D}^{D} d\varepsilon \rho_{DOS}(\varepsilon) \frac{|t|^2}{i\omega_n - \varepsilon + \mu} = \frac{\Gamma}{2\pi} \int_{-D}^{D} d\varepsilon \frac{1}{i\omega_n - \varepsilon + \mu}$$
$$= -\frac{\Gamma}{2\pi} \ln[i\omega_n - \varepsilon + \mu]|_{-D}^{D} = -\frac{\Gamma}{2\pi} \ln \frac{i\omega_n + \mu - D}{i\omega_n + \mu + D}.$$

g) *

FOR YOUR INFORMATION: The Matsubara summation is performed by noticing the that self-energy has branch cuts along the lines $i\omega_n \in \,]-\infty, -\mu - D]$ as well as $i\omega_n \in \,]-\infty, -\mu + D]$. Cancelling cuts for $i\omega_n \in [-\infty, -\mu - D]$ mean that once we deform the original Matsubara contour, we remain with an isolated pole at some $z_0 = \varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle + O(\Gamma)$, together with the integral just above and below the branch cut $i\omega_n \in [-\mu - D, -\mu + D]$. This gives the result in the question after noticing that along the branch cut, $\Sigma(\omega + i\delta, \mu) \to \Sigma^r(\mu) + \frac{i}{2}\Gamma \text{sgn}(\delta)$ for $\omega \in [-\mu - D, -\mu + D[$, in which $\Sigma^r(\mu)$ is a real-valued function.

At $T \to 0$, we can drop the isolated pole contribution (assuming $z_0 > 0$), and perform the integral over ω simply by writing

$$\frac{\Gamma}{(\omega - \varepsilon_d + \mu_{d,\sigma} - U\langle n_{d,-\sigma}\rangle - \Sigma^r)^2 + (\Gamma/2)^2} = \frac{1}{i}\left(\frac{1}{\omega - \varepsilon_d + \mu_{d,\sigma} - U\langle n_{d,-\sigma}\rangle - \Sigma^r - i\Gamma/2} - \text{ h.c.}\right)$$

so (writing $\varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle + \Sigma^r \equiv c$)

$$\langle n_{d,\sigma}\rangle = \int_{-\infty}^{0} \frac{d\omega}{2\pi} \frac{1}{i} \frac{1}{\omega - c - i\Gamma/2} + \text{ h.c. } = \frac{1}{2\pi i} \ln \frac{-c - i\Gamma/2}{-c + i\Gamma/2} = \frac{1}{2\pi i}\left(i\pi - \ln \frac{1 + ic/(\Gamma/2)}{1 - ic/(\Gamma/2)}\right)$$

which as required yields

$$\langle n_{d,\sigma}\rangle = \frac{1}{2} - \frac{1}{\pi} \text{ atan}\left(\frac{\varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle + \Sigma^r}{\Gamma/2}\right).$$

h) *

Here, the self-consistency relations are rewritten as

$$\langle n_{d,\sigma}\rangle = \frac{1}{2} - \frac{1}{\pi}\ \text{atan}\ [(\langle n_{d,-\sigma} - a)b].$$

This self-consistency could be solved on a computer; let us here more simply just try to show that nontrivial (magnetized) solutions exist. Let us suppose for simplicity that the magnetization is really small, that is

$$\langle n_{d,\sigma}\rangle = \frac{1}{2} + \sigma\delta, \qquad \delta \ll 1.$$

This requires that $(\langle n_{d,\sigma}\rangle - a)b$ also be very small, which means that $a \simeq 1/2$. Let us thus set $a = 1/2$, so $(\langle n_{d,\sigma}\rangle - a)b = \sigma\delta b$. Expanding the *atan*, we get

$$\frac{1}{2} + \sigma\delta = \frac{1}{2} - \frac{1}{\pi}(-\delta b + (\delta b)^3/3 + ...).$$

Subtracting the case $\sigma = -$ from the $\sigma = +$ one gives

$$2\delta = \frac{2}{\pi}(\delta b - (\delta b)^3/3 + ...) \rightarrow \delta(b - \pi) = \delta^3 b^3/3 \rightarrow \delta^2 = \frac{3}{b^3}(b - \pi).$$

This equation has a solution for real $\delta > 0$ when $b > \pi$, that is when the interaction is strong enough. The magnetization then increases as a square root from the critical interaction strength $b = \pi$. If a deviates slightly from 1/2 linearly with δ, then b just gets rescaled, so there are also solutions in that case. Therefore, mean-field theory predicts that the Anderson model's impurity spontaneously magnetizes in the presence of interactions, although these interactions are fully spin-symmetric.