Statistical Physics & Condensed Matter Theory I: Exercise

Mean-field theory for the Anderson impurity model

A given metal sample, no matter how pure, will inevitably contain some form of randomly-distributed impurities which can sometimes greatly affect physical properties (like conductivity). In this problem, we study a simplified situation in which a *single* impurity is embedded in the crystal.

Our starting point is the Hamiltonian for the conduction electrons, which we write as

$$H_c = \sum_{\mathbf{k}} \sum_{\sigma} (\varepsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

where $c^{\dagger}_{\mathbf{k}\sigma}$ and $c_{\mathbf{k}\sigma}$ are respectively creation and annihilation operators for the conduction electrons, obeying the canonical anticommutation relations $\{c_{\mathbf{k}\sigma}, c^{\dagger}_{\mathbf{k}'\sigma'}\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma\sigma'}$. The precise form of the dispersion relation $\varepsilon_{\mathbf{k}}$ is not important, although the existence of a well-defined Fermi surface will be assumed later on. Note that we have explicitly written the chemical potential μ for the conduction electrons directly inside their Hamiltonian.

Somewhere within the metal sits an impurity (different type of atom). For simplicity, we represent this atom as a single orbital level (typically the outermost orbital of the impurity, *e.g.* the d-shell for a Fe atom), and we write creation and annihilation operators for electrons on this orbital as $d^{\dagger}_{\sigma}, d_{\sigma}$ respectively. For the impurity level, we take a Hubbard-like Hamiltonian:

$$H_{imp} = H_d + H_U = \sum_{\sigma} (\varepsilon_d - \mu_{d,\sigma}) d^{\dagger}_{\sigma} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow}.$$

Here, ε_d is a given one-body energy, $\mu_{d,\sigma}$ are impurity chemical potentials defined for later convenience, U is a Hubbard interaction parameter and $n_{d\sigma} \equiv d^{\dagger}_{\sigma} d_{\sigma}$ are occupation number operators for the impurity level.

Physically, electrons propagating in the metal will have a wavefunction which overlaps with that of the impurity level. The electrons will thus be able to hop on or off the impurity due to the hybridization between these states. This is taken into account in second quantization by including a hopping term in the Hamiltonian of the form

$$H_{hop} = \sum_{\mathbf{k}} \sum_{\sigma} (t_{\mathbf{k}} d^{\dagger}_{\sigma} c_{\mathbf{k}\sigma} + t^{*}_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma})$$

in which $t_{\mathbf{k}}$ are given complex amplitudes (they depend on the microscopic details). The full Hamiltonian for the Anderson impurity model is thus

$$H_{And} = H_c + H_{imp} + H_{hop}.$$

We would like to know what happens: does the impurity capture an electron? Two? Does the impurity spontaneously magnetize (that is, does it tend to capture one spin projection more than the other)? This problem addresses this question.

a)

The U term is difficult to handle, since it contains a product of four fermionic operators. We will thus simplify the problem by making a mean-field approximation. Argue that we can take

$$H_U \to H_U^{MF} = U\left(\langle n_{d\uparrow}\rangle n_{d\downarrow} + \langle n_{d\downarrow}\rangle n_{d\uparrow} - \langle n_{d\uparrow}\rangle\langle n_{d\downarrow}\rangle\right).$$

b)

Write down the coherent state functional integral for the partition function for this mean-field theory, in the Matsubara representation (use the notation $\bar{\psi}, \psi$ and $\bar{\phi}, \phi$ for the Grassmann variables for the conduction electrons and impurity electrons, respectively).

c)

Show that the partition function can also be written as (*hint: consider a shift* $\psi, \bar{\psi} \to \psi', \bar{\psi}'$)

$$\mathcal{Z} = e^{\beta U\langle n_{d\uparrow}\rangle\langle n_{d\downarrow}\rangle} \int \mathcal{D}(\bar{\psi}', \psi') e^{-S[\bar{\psi}', \psi']} \int \mathcal{D}(\bar{\phi}, \phi) e^{-S[\bar{\phi}, \phi]},$$

in which the fields are decoupled and have free actions

$$S[\bar{\psi}', \psi'] = \sum_{\mathbf{k}} \sum_{\sigma} \sum_{n} \bar{\psi}'_{\mathbf{k}\sigma n}[-i\omega_n + \varepsilon_{\mathbf{k}} - \mu]\psi'_{\mathbf{k}\sigma n},$$
$$S[\bar{\phi}, \phi] = \sum_{\sigma} \sum_{n} \bar{\phi}_{\sigma n}[-i\omega_n + \varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle + \Sigma(i\omega_n, \mu)]\phi_{\sigma n}$$

in which we have defined the 'self-energy' of the impurity electrons as

$$\Sigma(i\omega_n, \mu) \equiv \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}}|^2}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu}$$

which we will explicitly calculate later.

d)

Calculate the partition function explicitly by performing the necessary Grassmann integrations, and show that the free energy $\mathcal{F} = -T \ln \mathcal{Z}$ can be written

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

e)

Let us now look at the self-consistency of the mean-field approach. Argue on the one hand from the definition of the partition function that the expectation value of the impurity electron occupation number must be given by

$$\langle n_{d,\sigma}\rangle = -\frac{\partial \mathcal{F}}{\partial \mu_{d,\sigma}},$$

and, on the other hand, that this derivative equals

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

f)

We are now at the stage where we would like to evaluate $\langle n_{d,\sigma}\rangle$ using the equation above, but before we can proceed we must calculate the self-energy, which we do by first making a number of approximations. First of all, we assume that the only important states of the conduction electrons are those with an energy within a restricted band $-D < \varepsilon_{\mathbf{k}} < D$. We can thus write

$$\Sigma(i\omega_n,\mu) = \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}}|^2}{i\omega_n - \varepsilon_{\mathbf{k}} + \mu} \to \int_{-D}^{D} d\varepsilon \rho_{DOS}(\varepsilon) \frac{|t|^2}{i\omega_n - \varepsilon + \mu}$$

in which $\rho_{DOS}(\varepsilon)$ is the density of states. We then assume that for states within the restricted band, we have $\rho_{DOS}|t|^2 \simeq \Gamma/2\pi$ in which Γ is a positive constant. Show that under these assumptions, the self-energy takes the form[1]

$$\Sigma(i\omega_n,\mu) \to -\frac{\Gamma}{2\pi} \ln \frac{i\omega_n + \mu - D}{i\omega_n + \mu + D}.$$

g) *

Performing the Matsubara sum in question above is a nontrivial task[2] (**I give you the answer here**). Assuming that $\Sigma(\omega + i\delta,\mu) \to \Sigma^r(\mu) + \frac{i}{2}\Gamma \mathrm{sgn}(\delta)$ for $\omega \in [-\mu - D, -\mu + D[$, in which $\Sigma^r(\mu)$ is a real-valued function, the result for the self-consistency equations becomes

$$\langle n_{d,\sigma}\rangle = \int_{-\mu-D}^{-\mu+D} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega}+1} \frac{\Gamma}{(\omega - \varepsilon_d + \mu_{d,\sigma} - U\langle n_{d,-\sigma}\rangle - \Sigma^r)^2 + (\Gamma/2)^2} + \frac{1}{e^{\beta z_0}+1}$$

in which $z_0 = \varepsilon_d - \mu_{d,\sigma} + U\langle n_{d,-\sigma}\rangle + O(\Gamma)$. Taking the $T \to 0$ limit of this equation and assuming infinite bandwidth $D \to \infty$, show that the self-consistency equations become (assuming $z_0 > 0$)[3]

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

h) *

Taking the impurity chemical potentials equal to the bulk one ($\mu_{d,\sigma} = \mu$), and defining $a \equiv \frac{\mu - \varepsilon_d - \Sigma^r}{U}$ and $b \equiv \frac{2U}{\Gamma}$, can you convince yourself that solutions with $\langle n_{d\uparrow}\rangle \neq \langle n_{d\downarrow}\rangle$ exist for certain values of a, b?[4]

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[1] *Hint: remember that* $\int_a^b \frac{dx}{x} = \ln b - \ln a$

[2] If you want to know, this is because the self-energy has two branch cuts.

[3] *Hint: use partial fractions and the identity* $\mathrm{atan}\, x = \frac{1}{2i} \ln \frac{1+ix}{1-ix}$

[4] *Hint:* $\mathrm{atan}\, x = x - x^3/3 + ...$ Also, you can for example assume that $\langle n_{d\sigma}\rangle = \frac{1}{2} + \sigma\delta n$ in which $\delta n << 1$, and that $a \simeq \frac{1}{2}$.