

## Problem Set 5:

Handout: Fri, Jun 19, 2020; Solutions: Fri, Jul 03, 2020

### Problem 1 (counts as 3 problems) Kondo model

Consider the Kondo Hamiltonian,

$$\hat{\mathcal{H}}_K = \int d^3\mathbf{k} \sum_{\sigma} \epsilon(k) \hat{c}_{\mathbf{k},\sigma}^{\dagger} \hat{c}_{\mathbf{k},\sigma} + J \hat{\mathbf{S}} \cdot \hat{\mathbf{S}}_e(\mathbf{0}), \quad (1)$$

with the band electron spin at the location  $\mathbf{r} = \mathbf{0}$  of the Kondo spin  $\hat{\mathbf{S}}$ :

$$\hat{\mathbf{S}}_e(\mathbf{0}) = (2\pi)^{-3} \int d^3\mathbf{k} d^3\mathbf{k}' \sum_{\alpha,\beta} \hat{c}_{\mathbf{k},\alpha}^{\dagger} \frac{1}{2} \boldsymbol{\sigma}_{\alpha,\beta} \hat{c}_{\mathbf{k}',\beta} \quad (2)$$

(1.a) By an expansion into plane waves, show that the Kondo problem reduces to a 1D Hamiltonian  $\hat{\mathcal{H}}_K^{1D}$  which decouples from the rest of the system:

$$\hat{\mathcal{H}}_K = \hat{\mathcal{H}}_K^{1D} + \hat{\mathcal{H}}'_K. \quad (3)$$

Derive an expression for  $\hat{\mathcal{H}}'_K$  and show that

$$\hat{\mathcal{H}}_K^{1D} = \int_0^{\Lambda_{UV}} dk \sum_{\sigma} \epsilon(k) \hat{s}_{k,\sigma}^{\dagger} \hat{s}_{k,\sigma} + J \hat{\mathbf{S}} \cdot \hat{\mathbf{S}}_e(\mathbf{0}), \quad (4)$$

where:

$$\hat{\mathbf{S}}_e(\mathbf{0}) = \sum_{\alpha,\beta} \hat{s}_{\alpha}^{\dagger}(0) \frac{1}{2} \boldsymbol{\sigma}_{\alpha,\beta} \hat{s}_{\beta}(0), \quad \hat{s}_{\sigma}(0) = \frac{1}{\sqrt{2\pi}} \int_0^{\Lambda_{UV}} dk \hat{s}_{k,\sigma}. \quad (5)$$

(1.b) Linearizing the band Hamiltonian Eq. (4) around the Fermi energy,  $\epsilon(k) \simeq \hbar k v_F$ , yields:

$$\hat{\mathcal{H}}_K^{1D} \simeq \int_{-\infty}^{\infty} dk \sum_{\sigma} \hbar v_F k \hat{s}_{k,\sigma}^{\dagger} \hat{s}_{k,\sigma} + J \hat{\mathbf{S}} \cdot \hat{\mathbf{S}}_e(\mathbf{0}). \quad (6)$$

This Hamiltonian can be *bosonized* by defining spin- and charge- density operators,

$$\hat{\rho}(k) = \sum_{\sigma=\pm} \int_{-\infty}^{\infty} dp \hat{s}_{p+k,\sigma}^{\dagger} \hat{s}_{p,\sigma}, \quad \hat{\rho}(-k) = \hat{\rho}^{\dagger}(k) \quad (7)$$

$$\hat{\sigma}(k) = \sum_{\sigma=\pm} \int_{-\infty}^{\infty} dp \sigma \hat{s}_{p+k,\sigma}^{\dagger} \hat{s}_{p,\sigma}, \quad \hat{\sigma}(-k) = \hat{\sigma}^{\dagger}(k). \quad (8)$$

Calculate the *commutation relations* of  $\hat{\rho}$  and  $\hat{\sigma}$ , assuming a band with all states at  $p < 0$  occupied. Show that they define *bosonic operators*,  $\hat{\rho} \propto \hat{b}_{-k}$  and  $\hat{\sigma}(k) \propto \hat{a}_{-k}$ . For the new bosonic operators we will show in the tutorial that:

$$\hat{\mathcal{H}}_K^{1D} = \hbar v_F \int_0^{\infty} dk k \left( \hat{a}_k^{\dagger} \hat{a}_k + \hat{b}_k^{\dagger} \hat{b}_k \right) + J \hat{\mathbf{S}} \cdot \hat{\mathbf{S}}_e(\mathbf{0}). \quad (9)$$

(1.c) The Kondo interaction can be written as:

$$J\hat{\mathbf{S}} \cdot \hat{\mathbf{S}}_e(0) = \frac{J_z}{2} \hat{S}^z \sum_{\sigma=\pm} \sigma \hat{s}_\sigma^\dagger(0) \hat{s}_\sigma(0) + J_\perp \left[ \hat{S}^+ \hat{s}_-^\dagger(0) \hat{s}_+(0) + \text{h.c.} \right], \quad (10)$$

with  $J_z = J_\perp = J$ . Express the  $J_z$ -term by the new bosonic operators  $\hat{a}_k$  and  $\hat{b}_k$ . As usual,  $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ .

(1.d) Show that the operators

$$\hat{\psi}_\sigma(x) = (2\pi a)^{-1/2} \exp \left[ \hat{j}_\sigma(x) \right], \quad \text{with} \quad (11)$$

$$\hat{j}_\sigma(x) = \int_0^\infty dk e^{-ak/2} C_k \left( \hat{b}_k + \sigma \hat{a}_k \right) e^{i\sigma kx} - \text{h.c.} \quad (12)$$

and an appropriately defined normalization constant  $C_k = \alpha/\sqrt{k}$  (to be determined), obey *fermionic anti-commutation relations* for given spin  $\sigma$ :

$$\{\hat{\psi}_\sigma(x), \hat{\psi}_\sigma^\dagger(x')\} = \delta(x - x'). \quad (13)$$

In the above expression,  $a$  defines a short-distance cut-off which may be sent to  $a \rightarrow 0$  in the end.

*Hint:* Show first that  $[\hat{j}_\sigma(x), \hat{j}_{\sigma'}(y)] = -i\pi\sigma \text{sgn}(x - y) \delta_{\sigma,\sigma'}$ .

*Note:* To obtain full fermionic anti-commutations, also between different spins  $\sigma \neq \sigma'$ , one needs to include additional zero-modes in the representation (11). For simplicity we discard them now.

(1.e) You may now identify the fermionic operators  $\hat{s}_\sigma(0) \equiv \hat{\psi}_\sigma(0)$ . Using this relation, express the  $J_\perp$ -part of the Kondo interaction in Eq. (10) by the bosonic fields  $\hat{a}_k$  and  $\hat{b}_k$ . Show that the interaction decouples from the  $\hat{b}_k$  operators – i.e. only the spin channel described by  $\hat{a}_k$  couples to the Kondo impurity.

*Hint:* The result is:

$$J_\perp \hat{S}^+ \hat{s}_-^\dagger(0) \hat{s}_+(0) = \frac{J_\perp}{2\pi a} \hat{S}^+ e^{\hat{\xi}}, \quad \hat{\xi} = \int_0^\infty dk e^{-ak/2} 2C_k \left( \hat{a}_k - \hat{a}_k^\dagger \right). \quad (14)$$

(1.f) Show that the resulting Kondo Hamiltonian  $\hat{\mathcal{H}}_K^a$  for the interacting modes  $\hat{a}_k$  is equivalent to a spin-boson model, by applying the unitary transformation:  $\hat{U} = \exp[\hat{S}^z \hat{\xi}]$ , i.e. show that:

$$\hat{U}^\dagger \hat{\mathcal{H}}_K^a \hat{U} = \text{spin-boson model.} \quad (15)$$

Derive the resulting spin-boson Hamiltonian explicitly.

**Problem 2** Effective polaron mass:

Consider the 3D Fröhlich Hamiltonian:

$$\hat{\mathcal{H}}_F = \frac{\hat{\mathbf{p}}^2}{2M} + \int d^3\mathbf{k} \omega_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \int d^3\mathbf{k} V_{\mathbf{k}} e^{i\mathbf{k}\cdot\hat{\mathbf{x}}} \left( \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \right), \quad (16)$$

with  $V_{\mathbf{k}} \propto \alpha^{1/2}$ .

(2.a) Use Rayleigh-Schrödinger perturbation theory to first order in  $\alpha$  and start from the unperturbed eigenstates  $|\mathbf{q}\rangle|n_{\mathbf{k}} = 0\rangle$  to derive their renormalized energy:

$$E_0(\mathbf{q}) = \frac{\mathbf{q}^2}{2M} - \int d^3\mathbf{k} \frac{V_{\mathbf{k}}^2}{\omega_{\mathbf{k}} + \frac{\mathbf{k}^2}{2M} - \frac{\mathbf{k}\cdot\mathbf{q}}{M}}. \quad (17)$$

(2.b) Use Eq. (17) to derive a formal expression for the effective polaron mass  $M^*$ , to first order in  $\alpha$ . Assume that  $V_{\mathbf{k}} = V_k$  and  $\omega_{\mathbf{k}} = \omega_k$  are rotationally invariant and simplify the resulting integrals as far as possible.