Condensed Matter Theory II: Many-Body Theory (TKM II)   SoSe 2023

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Homework assignment 8
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1. Electron-phonon self-energy in Matsubara formalism (10 + 5 = 15 points)

The electronic self-energy from electron-phonon interaction reads:

$$\Sigma(\mathbf{p},\omega_n) = -2\int \frac{\mathrm{d}^d q}{(2\pi)^d}\,\frac{1}{\beta}\sum_{\nu_n} \mathscr{G}_{M,0}(\mathbf{p}-\mathbf{q},\omega_n-\nu_n)\mathscr{D}_{M,0}(\mathbf{q},\nu_n).$$

(a) Transform the summation over bosonic frequency ν_n into a contour integral in the complex energy plane and express the result as an integral over the momentum $\mathbf{q}$ involving Fermi and Bose distribution functions.

Solution: Using the expressions for the free Green's functions (from Sec. 4.7 of the lecture notes):

$$\Sigma(\mathbf{p},\omega_n) = \frac{2}{\beta}\sum_{\nu_n}\int \frac{\mathrm{d}^d q}{(2\pi)^d}\frac{1}{\mathrm{i}(\omega_n+\nu_n)-\varepsilon_{\mathbf{p}-\mathbf{q}}}\frac{\omega_{\mathbf{q}}^2}{\nu_n^2+\omega_{\mathbf{q}}^2} \tag{1}$$

$$= \frac{1}{\beta}\sum_{\nu_n}\int \frac{\mathrm{d}^d q}{(2\pi)^d}\frac{\omega_{\mathbf{q}}}{\mathrm{i}(\omega_n+\nu_n)-\varepsilon_{\mathbf{p}-\mathbf{q}}}\left(\frac{1}{\omega_{\mathbf{q}}-\mathrm{i}\nu_n}+\frac{1}{\omega_{\mathbf{q}}+\mathrm{i}\nu_n}\right) \tag{2}$$

$$\tag{3}$$

where we used

$$\frac{1}{\nu_n^2+\omega_{\mathbf{q}}^2} = \frac{1}{(\omega_{\mathbf{q}}-\mathrm{i}\nu_n)(\omega_{\mathbf{q}}+\mathrm{i}\nu_n)} \tag{4}$$

$$= \frac{1}{2\omega_{\mathbf{q}}(\omega_{\mathbf{q}}-\mathrm{i}\nu_n)}+\frac{1}{2\omega_{\mathbf{q}}(\omega_{\mathbf{q}}+\mathrm{i}\nu_n)}. \tag{5}$$

To rewrite the sum over bosonic frequencies ν_n as an integral, we consider

$$\oint_{\mathcal{C}}\frac{\mathrm{d}z}{2\pi\mathrm{i}}\mathcal{F}(z)n_{\mathrm{B}}(z) = \frac{1}{\beta}\sum_{\nu_n}\mathcal{F}(\nu_n) + \sum_{z\in\mathrm{Res}(\mathcal{F}(z))}\mathcal{F}(z)n_{\mathrm{B}}(z) \tag{6}$$

where the contour integral vanishes for our integrand. We end up with

$$\Sigma(\mathbf{p},\omega_n) = -\int\frac{\mathrm{d}^d q}{(2\pi)^d}\sum_{z\in\mathrm{Res}(\mathcal{F}(z))}\frac{\omega_{\mathbf{q}}}{\mathrm{i}\omega_n+z-\varepsilon_{\mathbf{p}-\mathbf{q}}}\left(\frac{1}{\omega_{\mathbf{q}}-z}+\frac{1}{\omega_{\mathbf{q}}+z}\right)n_{\mathrm{B}}(z) \tag{7}$$

where

$$\mathcal{F}(z) = \frac{\omega_{\mathbf{q}}}{\mathrm{i}\omega_n+z-\varepsilon_{\mathbf{p}-\mathbf{q}}}\left(\frac{1}{\omega_{\mathbf{q}}-z}-\frac{1}{\omega_{\mathbf{q}}+z}\right). \tag{8}$$

Calculating the residues at $z_1 = \omega_{\mathbf{q}}$, $z_2 = -\omega_{\mathbf{q}}$ and $z_3 = \varepsilon_{\mathbf{p}-\mathbf{q}} - \mathrm{i}\omega_n$, we find

$$\Sigma(\mathbf{p}, \omega_n) = -\int \frac{\mathrm{d}^d q}{(2\pi)^d} \left[-\frac{n_{\mathrm{B}}(\omega_{\mathbf{q}})\omega_{\mathbf{q}}}{\mathrm{i}\omega_n + \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}}} + \frac{n_{\mathrm{B}}(-\omega_{\mathbf{q}})\omega_{\mathbf{q}}}{\mathrm{i}\omega_n - \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}}} \right. \tag{9}$$

$$\left. + n_{\mathrm{B}}(\varepsilon_{\mathbf{p}-\mathbf{q}} - \mathrm{i}\omega_n)\omega_{\mathbf{q}} \left(\frac{1}{\omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}} + \mathrm{i}\omega_n} + \frac{1}{\omega_{\mathbf{q}} + \varepsilon_{\mathbf{p}-\mathbf{q}} - \mathrm{i}\omega_n} \right) \right] \tag{10}$$

using

$$n_{\mathrm{B}}(\varepsilon - \mathrm{i}\omega_n) = \frac{1}{\exp(\beta[\varepsilon - \mathrm{i}(2n+1)\pi/\beta]) - 1} \tag{11}$$

$$= -\frac{1}{\exp(\beta\varepsilon) + 1} \tag{12}$$

$$= -n_{\mathrm{F}}(\varepsilon) \tag{13}$$

(note that ω_n is a fermionic Matsubara frequency); and $n_{\mathrm{B}}(-\omega) = -(1 + n_{\mathrm{B}}(\omega))$we find

$$\Sigma(\mathbf{p}, \omega_n) = \int \frac{\mathrm{d}^d q}{(2\pi)^d} \omega_{\mathbf{q}} \left[\frac{n_{\mathrm{B}}(\omega_{\mathbf{q}}) + n_{\mathrm{F}}(\varepsilon_{\mathbf{p}-\mathbf{q}})}{\mathrm{i}\omega_n + \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}}} + \frac{1 - n_{\mathrm{F}}(\varepsilon_{\mathbf{p}-\mathbf{q}}) + n_{\mathrm{B}}(\omega_{\mathbf{q}})}{\mathrm{i}\omega_n - \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}}} \right] \tag{14}$$

(b) For a one-dimensional system with $\varepsilon_p = p^2/2m - \mu$, calculate $\operatorname{Im}\Sigma^R(\mathbf{p}, \omega)$: Analytically continue $\Sigma(\mathbf{p}, \omega_n)$ from discrete Matsubara frequencies $\omega_n > 0$ to a frequency just above the real axis: $\mathrm{i}\omega_n \to \omega + \mathrm{i}0$, take the imaginary part and perform the q-integration.

Solution: Analytic continuation:

$$\Sigma^{\mathrm{R}}(\mathbf{p}, \omega) = \int \frac{\mathrm{d}^d q}{(2\pi)^d} \omega_{\mathbf{q}} \left[\frac{n_{\mathrm{B}}(\omega_{\mathbf{q}}) + n_{\mathrm{F}}(\varepsilon_{\mathbf{p}-\mathbf{q}})}{\omega + \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}} + \mathrm{i}0} + \frac{1 - n_{\mathrm{F}}(\varepsilon_{\mathbf{p}-\mathbf{q}}) + n_{\mathrm{B}}(\omega_{\mathbf{q}})}{\omega - \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}} + \mathrm{i}0} \right] \tag{15}$$

Taking the imaginary part, going to $d = 1$:

$$\operatorname{Im}\left[\Sigma^{\mathrm{R}}(\mathbf{p}, \omega)\right] = -\pi \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{(2\pi)} \omega_{\mathbf{q}} \left[(n_{\mathrm{B}}(\omega_{\mathbf{q}}) + n_{\mathrm{F}}(\varepsilon_{\mathbf{p}-\mathbf{q}}))\delta(\omega + \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}}) \right. \tag{16}$$

$$\left. + (1 - n_{\mathrm{F}}(\varepsilon_{\mathbf{p}-\mathbf{q}}) + n_{\mathrm{B}}(\omega_{\mathbf{q}}))\delta(\omega - \omega_{\mathbf{q}} - \varepsilon_{\mathbf{p}-\mathbf{q}}) \right] \tag{17}$$

since $\mu \gg |\omega|$, both δ-functions have two roots; say q_1 and q_2, and q_3 and q_4.

$$\operatorname{Im}\left[\Sigma^{\mathrm{R}}(\mathbf{p}, \omega)\right] = -\frac{1}{2} \sum_{i=1}^{2} \left(\left[\frac{n_{\mathrm{B}}(\omega_q) + n_{\mathrm{F}}(\varepsilon_{p-q})}{\left| \frac{\partial}{\partial q}(\varepsilon_{p-q} - \omega_q) \right|} \right]_{q=q_i} + \sum_{i=3}^{4} \left[\frac{n_{\mathrm{B}}(\omega_q) + 1 - n_{\mathrm{F}}(\varepsilon_{p-q})}{\left| \frac{\partial}{\partial q}(\varepsilon_{p-q} + \omega_q) \right|} \right]_{q=q_i} \right) \tag{18}$$

2. RKKY interaction in finite temperature (5 + 10 + 10 + 5 + 5 = 35 points)

Let us consider two impurity spins embedded in a metal. If the spins are close enough, they will interact with each other via the spin-polarization of the conduction electrons. This effect is known as the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction.

An impurity spin in a free 3D Fermi gas interacts with the local electronic spin density by means of the Hamiltonian

$$H_{\mathrm{imp}} = J\Sigma_i \hat{S}_i(\mathbf{x}=0), \tag{19}$$

where the local spin density operator is given by

$$\hat{S}_i(\mathbf{x}) = \frac{\hbar}{2}\psi^\dagger_\alpha(\mathbf{x})\sigma^i_{\alpha\beta}\psi_\beta(\mathbf{x}) \tag{20}$$

and Σ_i is a component of the impurity spin-vector, which is treated as an external field localized at $\mathbf{x}=0$.

Let us assume that $J \ll 0$, and determine the coupling between the two impurity spins.

(a) Determine the Matsubara Green's function for a non-interacting 3D Fermi gas as a function of position $\mathbf{r}$ and Matsubara frequency ω_n at large distances ($k_{\mathrm{F}}r \gg 1$) and for $\omega_n \ll E_{\mathrm{F}}$.

Solution: $G_{\mathrm{M}}(\mathbf{r},\omega_n)$ in the limit $k_{\mathrm{F}}r \gg 1$:

$$G_{\mathrm{M}}(\mathbf{r},\omega_n) = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{\exp(\mathrm{i}\mathbf{pr})}{\mathrm{i}\omega_n - \varepsilon_{\mathbf{p}}} \tag{21}$$

$$= \frac{1}{(2\pi)^2}\frac{2}{r}\int_0^\infty \mathrm{d}p\, \frac{p\sin(pr)}{\mathrm{i}\omega_n - \frac{p^2}{2m} + \frac{p_{\mathrm{F}}^2}{2m}} \tag{22}$$

$$= -\frac{1}{(2\pi)^2}\frac{2m\pi}{r}\exp\left(-rp_{\mathrm{F}}\sqrt{-1-2\mathrm{i}m\omega_n/p_{\mathrm{F}}^2}\right) \tag{23}$$

We expand the square root:

$$\sqrt{-1-2\mathrm{i}m\omega_n/p_{\mathrm{F}}^2} \overset{m\omega_n/p_{\mathrm{F}}^2 \ll 1}{\approx} \mathrm{sign}(\omega_n)[-\mathrm{i} + m\omega_n/p_{\mathrm{F}}^2] \tag{24}$$

$$= -\mathrm{i}\cdot\mathrm{sign}(\omega_n)[1 + \mathrm{i}m\omega_n/p_{\mathrm{F}}^2] \tag{25}$$

We find

$$G_{\mathrm{M}}(\mathbf{r},\omega_n) \approx -\frac{m}{2\pi r}\exp(\mathrm{i}r\mathrm{sign}(\omega_n)\,[p_{\mathrm{F}} + \mathrm{i}\omega_n/v_{\mathrm{F}}]) \tag{26}$$

(b) Calculate the spin susceptibility

$$\left[\mathcal{D}^M_{SS}\right]_{i,j}(\mathbf{r},\tau) := -\left\langle \mathcal{T}_\tau \hat{S}_i(\mathbf{r},\tau)\hat{S}_j(0,0)\right\rangle_0 \tag{27}$$

where the (thermal) trace is defined in lecture Eq. (4.106). (The calculation is similar to that for $T=0$ in exercise 3 (a) from sheet 6.)

Solution: We know from the lecture that Wick's theorem works analogously to $T=0$ at $T>0$, with the zero-temperature Green's functions replaced by Matsubara Green's functions. Taking into account signs, we get

$$\left[\mathcal{D}^M_{SS}\right]_{i,j}(\mathbf{r},\tau) = \frac{1}{2}\delta_{i,j}G_{\mathrm{M}}(\mathbf{r},\tau)G_{\mathrm{M}}(-\mathbf{r},-\tau). \tag{28}$$

(c) At finite temperature, find the static ($\omega = 0$) spin polarization $s_i(\mathbf{x}) = \langle \hat{S}_i(\mathbf{x}) \rangle$ in the electronic system at large distances away from a single impurity spin. Consider the spin susceptibility in the limit $T \to 0$. Show that the polarization oscillates as a function of r and find the oscillation period.

Solution: The static spin polarization is given in terms of the retarded susceptibility as

$$s_i(\mathbf{x}, \omega = 0) = J \left[\mathcal{D}^{\mathrm{R}}_{SS}\right]_{i,j} (\mathbf{x}, \omega = 0)\Sigma_j \tag{29}$$

We calculate the (discrete) Fourier-transform of the Matsubara spin susceptibility:

$$\left[\mathcal{D}^{M}_{SS}\right]_{i,j} (\mathbf{r}, \omega_n) = \frac{1}{2}\delta_{i,j} \int_0^\beta \mathrm{d}\tau \exp(\mathrm{i}\omega_n \tau) G_{\mathrm{M}}(\mathbf{r}, \tau) G_{\mathrm{M}}(-\mathbf{r}, -\tau) \tag{30}$$

$$= \frac{T}{2}\delta_{i,j} \sum_{\varepsilon_m} G_{\mathrm{M}}(\mathbf{r}, \varepsilon_m) G_{\mathrm{M}}(-\mathbf{r}, \varepsilon_m + \omega_n) \tag{31}$$

Since $\left[\mathcal{D}^{M}_{SS}\right]_{i,j} (\mathbf{r}, \tau) = \left[\mathcal{D}^{M}_{SS}\right]_{i,j} (\mathbf{r}, \tau + \beta)$ (as can be seen from the periodicity of the Green's functions), ω_n is a bosonic Matsubara frequency.
In order to evaluate Eq. (31) in the limit $rk_{\mathrm{F}} \gg 1$, we use the corresponding expression for the Matsubara Green's function (26). We find

$$\left[\mathcal{D}^{M}_{SS}\right]_{i,j} (\mathbf{r}, \omega_n) = \frac{\delta_{i,j}}{2} \left(\frac{m}{2\pi r}\right)^2 T \sum_{\varepsilon_m} \mathrm{e}^{\mathrm{i}r\mathrm{sign}(\varepsilon_m)[p_{\mathrm{F}} + \mathrm{i}\varepsilon_m/v_{\mathrm{F}}]} \mathrm{e}^{\mathrm{i}r\mathrm{sign}(\omega_n + \varepsilon_m)[p_{\mathrm{F}} + \mathrm{i}(\omega_n + \varepsilon_m)/v_{\mathrm{F}}]} \tag{32}$$

Here, it is OK to use the small ε expression for the Green's function, since high ε_m terms vanish exponentially in the sum. For obtaining the analytic continuation (to find the retarded response function) we need the susceptibility at $\omega_n > 0$. In this case, the sum can be solved:

$$\left[\mathcal{D}^{M}_{SS}\right]_{i,j} (\mathbf{r}, \omega_n) = \frac{\delta_{i,j}}{2} \left(\frac{m}{2\pi r}\right)^2 \exp(-r\omega_n/v_{\mathrm{F}}) \left[\frac{T\cos(2p_{\mathrm{F}} r)}{\sinh(2\pi r T/v_{\mathrm{F}})} + \frac{\omega_n}{\pi}\right] \tag{33}$$

Next, we need to perform the analytic continuation to find the retarded response function. To this end, we consider the function

$$\mathcal{F}_{i,j}(z) := \frac{\delta_{i,j}}{2} \left(\frac{m}{2\pi r}\right)^2 \exp(\mathrm{i}rz/v_{\mathrm{F}}) \left[\frac{T\cos(2p_{\mathrm{F}} r)}{\sinh(2\pi r T/v_{\mathrm{F}})} - \frac{\mathrm{i}z}{\pi}\right] \tag{34}$$

which is analytic for $z \in \mathbb{C}_+$. Furthermore, it holds $\mathcal{F}_{i,j}(\mathrm{i}\omega_n) = \left[\mathcal{D}^{M}_{SS}\right]_{i,j} (\mathbf{r}, \omega_n)$. Therefore, the retarded spin susceptibility is given by

$$\left[\mathcal{D}^{\mathrm{R}}_{SS}\right]_{i,j} (\mathbf{r}, \omega) := \frac{\delta_{i,j}}{2} \left(\frac{m}{2\pi r}\right)^2 \exp(\mathrm{i}r\omega/v_{\mathrm{F}}) \left[\frac{T\cos(2p_{\mathrm{F}} r)}{\sinh(2\pi r T/v_{\mathrm{F}})} - \frac{\mathrm{i}\omega}{\pi}\right]. \tag{35}$$

For $T \to 0$ and in the static limit $\omega \to 0$ we get

$$\left[\mathcal{D}^{\mathrm{R}}_{SS}\right]_{i,j} (\mathbf{r}, \omega = 0) := \frac{\delta_{i,j}}{2} \left(\frac{m}{2\pi r}\right)^2 \frac{\cos(2p_{\mathrm{F}} r)}{2\pi r/v_{\mathrm{F}}} \tag{36}$$

$$= \frac{\delta_{i,j}}{2} \frac{m p_{\mathrm{F}}}{(2\pi r)^3} \cos(2p_{\mathrm{F}} r). \tag{37}$$

Thus, the spin polarization at $T \to 0$ is

$$s_i(\mathbf{x}, \omega = 0) = J\frac{\Sigma_i}{2}\frac{mp_\mathrm{F}}{(2\pi r)^3}\cos(2p_\mathrm{F} r). \tag{38}$$

From the cosine we get an oscillation with period π/p_F.

(d) Study the temperature dependence of the spin polarization. What changes qualitatively as compared to the zero temperature case?

Solution: At finite temperature, we have

$$s_i(\mathbf{x}, \omega = 0) = \frac{J\Sigma_i}{2}\left(\frac{m}{2\pi r}\right)^2 \frac{T\cos(2p_\mathrm{F} r)}{\sinh(2\pi r T/v_\mathrm{F})}. \tag{39}$$

This means that the oscillations are dampened exponentially with increasing temperature.

(e) Assume that there are two localized spins $\mathbf{\Sigma_1}$ and $\mathbf{\Sigma}_2$ at distance r from each other ($rk_\mathrm{F} \gg 1$). The energy of the system will depend on the relative orientation of the two spins and can be written as

$$E = K\mathbf{\Sigma}_1 \cdot \mathbf{\Sigma}_2$$

Calculate the coupling constant K between the two spins by evaluating $\langle H_\mathrm{imp}\rangle$.

Solution: We have

$$\langle H_\mathrm{imp}\rangle = J\Sigma_i\langle S_i(\mathbf{x} = 0)\rangle \tag{40}$$

$$= J^2\mathbf{\Sigma}_1 \cdot \mathbf{\Sigma}_2\frac{1}{2}\left(\frac{m}{2\pi r}\right)^2 \frac{T\cos(2p_\mathrm{F} r)}{\sinh(2\pi r T/v_\mathrm{F})} \tag{41}$$

We thus find

$$K = J^2\frac{1}{2}\left(\frac{m}{2\pi r}\right)^2 \frac{T\cos(2p_\mathrm{F} r)}{\sinh(2\pi r T/v_\mathrm{F})} \tag{42}$$