Supplemental Material for "Lifshitz phase transitions in the ferromagnetic regime of the Kondo lattice model"

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STATIC MEAN-FIELD THEORY

The $S = 1/2$ case

We perform a mean-field decomposition in the KLM written in the form:

$$\mathcal{H} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + J \sum_i \mathbf{s}_i \cdot \mathbf{S}_i + \mu_B H \sum_i (g_c s_{z,i} + g_f S_{z,i}), \tag{1}$$

where H is the external magnetic field oriented along the z axis, μ_B the Bohr magneton, while g_c and g_f are the Landé factors. For simplicity, we consider flat non-interacting conduction-band density of states (DOS):

$$\rho^0_c = 1/2D, \tag{2}$$

where D is the half-bandwidth.

The interaction term for localized spins with $S = 1/2$ is decomposed in terms of the hybridization operators [1, 2]

$$\chi^\mu = \frac{1}{\sqrt{2}} \sum_{\alpha,\beta} f^\dagger_\alpha \sigma^\mu_{\alpha\beta} c_\beta, \tag{3}$$

where c, f are annihilation operators for itinerant and localized electrons, respectively, and the spin indexes α and β range over spin up and down. The index μ ranges over $0, 1, 2, 3$; the operator σ^0 is the identity, while other σ^i are the Pauli matrices. These operators are complete in the spin sector $1/2 \otimes 1/2 = 1 \oplus 0$, and therefore the interaction part can be split into:

$$\mathbf{s} \cdot \mathbf{S} = \left(\frac{1}{2} c^\dagger \boldsymbol{\sigma} c\right) \cdot \left(\frac{1}{2} f^\dagger \boldsymbol{\sigma} f\right) = -3/4 \chi^{0\dagger} \chi^0 + 1/4 \boldsymbol{\chi}^\dagger \cdot \boldsymbol{\chi}. \tag{4}$$

This expression is exact.

We perform the standard mean-field procedure: $AB \approx \langle A \rangle B + A \langle B \rangle - \langle A \rangle \langle B \rangle$. We assume that only the singlet part $\langle \chi^0 \rangle$ is nonzero and we use the $U(1)$ gauge freedom to make $\langle \chi_0 \rangle$ real.

The second mean-field decomposition is done in the magnetic channel (assuming the magnetization is along the z axis):

$$\mathbf{s} \cdot \mathbf{S} = s_z \tilde{m}_f + \tilde{m}_c S_z - \tilde{m}_c \tilde{m}_f, \tag{5}$$

where

$$\tilde{m}_c = \langle s^z \rangle \quad \text{and} \quad \tilde{m}_f = \langle S^z \rangle \tag{6}$$

are the expectation values of the z component of conduction-band and localized-electron spin. These are proportional to the magnetization of $c(f)$ electrons:

$$m_{f(c)} = -\mu_B g_{f(c)} \tilde{m}_{f(c)}. \tag{7}$$

In order to fix the average number of electrons we introduce the chemical potential μ. We also introduce Lagrangian multipliers λ_i to enforce the local constraint $\langle n_{f,i} \rangle = 1$ on the f electrons:

$$\sum_i \lambda_i \sum_\sigma \left(f^\dagger_{i,\sigma} f_{i,\sigma} - 1 \right). \tag{8}$$

This constraint is fulfilled only as an average over all f electrons, $\lambda_i \equiv \lambda$. We may then perform a FT:

$$\lambda \sum_k \sum_\sigma \left(f^\dagger_{k\sigma} f_{k\sigma} - 1 \right). \tag{9}$$

Thus λ plays the role of the effective f level energy: the f level occupancy is controlled by the difference between λ and μ.

At constant μ, the thermodynamic potential that we need to minimize is

$$K(\mu, \ldots) = H(N_{\text{total}}, \ldots) - \mu N_{\text{total}} = H - \mu(N_c + N_f) = H - \mu \sum_{k,\sigma} \left(c^\dagger_{k\sigma} c_{k\sigma} + f^\dagger_{k\sigma} f_{k\sigma} \right). \tag{10}$$

The mean-field thermodynamic potential takes the following wave-vector representation:

$$\mathcal{K}_{MF} = \sum_{k\sigma} \left(c^\dagger_{k,\sigma} \, f^\dagger_{k,\sigma} \right) \tilde{M}_k \begin{pmatrix} c_{k,\sigma} \\ f_{k,\sigma} \end{pmatrix} + \sum_k E_0, \tag{11}$$

where the matrix M_k is

$$\tilde{M}_k = \begin{pmatrix} \epsilon_{k,\sigma} - \mu & -c\chi_0 \\ -c\chi_0 & \lambda_\sigma - \mu \end{pmatrix}. \tag{12}$$

with

$$\epsilon_{k,\sigma} = \epsilon_k + \epsilon_\sigma = \epsilon_k + J\tilde{m}_f \frac{\sigma}{2} + \mu_B g_c H \frac{\sigma}{2} = \epsilon_k + \mu_B g_c \tilde{H}_c \frac{\sigma}{2}, \tag{13}$$

$$\lambda_\sigma = \lambda + J\tilde{m}_c \frac{\sigma}{2} + \mu_B g_f H \frac{\sigma}{2} = \lambda + \mu_B g_f \tilde{H}_f \frac{\sigma}{2}, \tag{14}$$

$$c = \frac{3}{4}\frac{1}{\sqrt{2}} J = \frac{3J}{4\sqrt{2}}, \tag{15}$$

$$E_0 = +\frac{3}{4} J \chi_0^2 - J\tilde{m}_c \tilde{m}_f - \lambda. \tag{16}$$

The effective field felt by the $c(f)$ electrons is given by

$$\tilde{H}_{c(f)} = H + \frac{J\tilde{m}_{f(c)}}{\mu_B g_{c(f)}}. \tag{17}$$

In general, the equation of motion (EOM) can be written as

$$z\langle\langle A, B\rangle\rangle = -\langle\langle [\mathcal{K}_{MF}, A], B\rangle\rangle + \langle\langle [A, B]\rangle\rangle, \tag{18}$$

where A, B are arbitrary fermionic operators. We find

$$\begin{aligned} zG_{cc,k\sigma} &= 1 + (\epsilon_{k\sigma} - \mu)\, G_{cc,k\sigma} - c\chi_0 G_{fc,k\sigma}, \\ zG_{ff,k\sigma} &= 1 + (\lambda_\sigma - \mu)\, G_{ff,k\sigma} - c\chi_0 G_{cf,k\sigma}, \\ zG_{cf,k\sigma} &= (\epsilon_{k\sigma} - \mu) G_{cf,k\sigma} - c\chi_0 G_{ff,k\sigma}, \\ zG_{fc,k\sigma} &= (\lambda_\sigma - \mu) G_{fc,k\sigma} - c\chi_0 G_{cc,k\sigma}. \end{aligned} \tag{19}$$

Note also that $G_{cf}(z) = G_{fc}(z)$, since the matrix $\tilde{M}_k$ is symmetric. It follows

$$\begin{aligned} (z - \epsilon_{k\sigma} + \mu) G_{cc,k\sigma} &= 1 - c\chi_0 G_{fc,k\sigma}, \\ (z - \lambda_\sigma + \mu) G_{ff,k\sigma} &= 1 - c\chi_0 G_{cf,k\sigma}, \\ (z - \epsilon_{k\sigma} + \mu) G_{cf,k\sigma} &= -c\chi_0 G_{ff,k\sigma}, \\ (z - \lambda_\sigma + \mu) G_{fc,k\sigma} &= -c\chi_0 G_{cc,k\sigma}, \end{aligned} \tag{20}$$

and consequently

$$(z - \lambda_\sigma + \mu)^2 G_{ff,k\sigma} = (c\chi_0)^2 G_{cc,k\sigma}. \tag{21}$$

In this approach, writing $z = \omega + i\delta$, the Fermi level corresponds to $\omega = 0$. We use a different convention. We absorb μ into z: $\tilde{z} = z + \mu$. Also the Green's functions take $\tilde{z}$ as their argument. With this choice, spectral functions are obtained with replacement $\tilde{z} = \omega + i\delta$ and there are no explicit μ in the expressions for Green's functions. μ only appears as an integration limit (or in the Fermi-Dirac distribution). We drop writing the tilde in $\tilde{z}$ in the following.

The quasiparticle band edges are

$$\begin{aligned}
\omega_{1,\sigma} &= \frac{1}{2}\left(\epsilon_\sigma + \lambda_\sigma - D - \sqrt{(\epsilon_\sigma - \lambda_\sigma - D)^2 + 4c^2\chi_0^2}\right), \\
\omega_{2,\sigma} &= \frac{1}{2}\left(\epsilon_\sigma + \lambda_\sigma + D - \sqrt{(\epsilon_\sigma - \lambda_\sigma + D)^2 + 4c^2\chi_0^2}\right), \\
\omega_{3,\sigma} &= \frac{1}{2}\left(\epsilon_\sigma + \lambda_\sigma - D + \sqrt{(\epsilon_\sigma - \lambda_\sigma - D)^2 + 4c^2\chi_0^2}\right), \\
\omega_{4,\sigma} &= \frac{1}{2}\left(\epsilon_\sigma + \lambda_\sigma + D + \sqrt{(\epsilon_\sigma - \lambda_\sigma + D)^2 + 4c^2\chi_0^2}\right).
\end{aligned} \tag{22}$$

In the multiindex (i, σ), σ is spin, while i enumerates the band edges from the lowest to the highest. Furthermore

$$\epsilon_\sigma = J\tilde{m}_f\frac{\sigma}{2} + \mu_B g_c H\frac{\sigma}{2} = \mu_B g_c \tilde{H}_c\frac{\sigma}{2}. \tag{23}$$

The final closed-form expressions for the spectral functions are

$$\rho_{c,\sigma}(\omega) = \rho_c^0 \sum_{i=1}^{4}(-1)^{i-1}\theta(\omega - \omega_{i,\sigma}), \tag{24}$$

$$\rho_{f,\sigma}(\omega) = \frac{(c\chi_0)^2}{(\omega - \lambda_\sigma)^2}\rho_{c,\sigma}(\omega). \tag{25}$$

We also have

$$\rho_{cf,\sigma}(\omega) = -\frac{c\chi_0}{\omega - \lambda_\sigma}\rho_{c,\sigma}(\omega). \tag{26}$$

The energy eigenvalues are

$$E_{k,\sigma} = \frac{1}{2}\left(\epsilon_{k,\sigma} + \lambda_\sigma \pm \sqrt{(\epsilon_{k,\sigma} - \lambda_\sigma)^2 + 4c^2\chi_0^2}\right). \tag{27}$$

Mean-field equations

We can derive the system of mean-field equation using the fluctuation-dissipation theorem at $T = 0$:

$$\begin{aligned}
\langle AB\rangle &= -\int_\mu^\infty \frac{d\omega}{\pi} G''_{AB}(\omega) \\
&= \int_{-\infty}^{\mu} d\omega \rho_{BA}(\omega).
\end{aligned} \tag{28}$$

We obtain

$$n_c = \sum_\sigma \langle c_\sigma^\dagger c_\sigma\rangle = \sum_\sigma \int d\omega \rho_{c,\sigma}(\omega), \tag{29}$$

$$1 = n_f = \sum_\sigma \langle f_\sigma^\dagger f_\sigma\rangle = \sum_\sigma \int d\omega \rho_{f,\sigma}(\omega), \tag{30}$$

$$\tilde{m}_c = 1/2\sum_\sigma \sigma\langle c_\sigma^\dagger c_\sigma\rangle = 1/2\sum_\sigma \int \sigma d\omega \rho_{c,\sigma}(\omega), \tag{31}$$

$$\tilde{m}_f = 1/2\sum_\sigma \sigma\langle f_\sigma^\dagger f_\sigma\rangle = 1/2\sum_\sigma \int \sigma d\omega \rho_{f,\sigma}(\omega). \tag{32}$$

In all integrals, the lower integration limit is $-\infty$, while the upper is the chemical potential μ.

For the gap equation we take the symmetrized spectral function

$$A_{cf,\sigma} = -\frac{1}{2\pi}[\mathrm{Im}G_{cf}(\omega + i\delta) + \mathrm{Im}G_{fc}(\omega + i\delta)] = \rho_{cf,\sigma}.$$

This gives:

$$\frac{1}{2}\langle f_\uparrow^\dagger c_\uparrow + c_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger c_\downarrow + c_\downarrow^\dagger f_\downarrow\rangle = \frac{1}{2}2\sqrt{2}\langle\chi_0\rangle = \tag{33}$$

$$\sum_\sigma \int d\omega A_{fc,\sigma}(\omega) = -c\chi_0 \sum \int d\omega \frac{1}{\omega - \lambda_\sigma}\rho_{c,\sigma}(\omega) \tag{34}$$

We now assume $\chi_0 \neq 0$. Using $c = 3J/(4\sqrt{2})$, we finally find the gap equation

$$\boxed{\sum_\sigma \int_{-\infty}^{\mu} d\omega \frac{\rho_{c,\sigma}(\omega)}{\omega - \lambda_\sigma} = -8/3J.} \tag{35}$$

This set of non-linear equations had been previously derived in Refs. [1, 2], while in Ref. [3] a somewhat different mean-field decoupling was used.

Evaluation of energy

The total energy can be evaluated as

$$\begin{aligned} E_{\mathrm{GS}} &= \langle H_{\mathrm{MF}}\rangle \\ &= \sum_k \left\langle \sum_{ij} c_{ki}^\dagger c_{kj} M_{k,ij} + E_0 \right\rangle \\ &= \sum_k \left(\sum_{ij} \int_{-\infty}^{\mu} A_{\epsilon_k,ij}(\omega) M_{\epsilon_k,ij} \mathrm{d}\omega + E_0 \right). \end{aligned} \tag{36}$$

We used a symmetrized spectral function

$$A_{ij}(\omega) = \frac{1}{2}\left[-\frac{1}{\pi}\mathrm{Im}G_{ij}(\omega + i\delta) - \frac{1}{\pi}\mathrm{Im}G_{ji}(\omega + i\delta)\right], \tag{37}$$

since

$$\int_{-\infty}^{\mu} A_{ij}(\omega)\mathrm{d}\omega = \frac{1}{2}\langle c_i^\dagger c_j + c_j^\dagger c_i\rangle. \tag{38}$$

Then

$$\frac{E_{\mathrm{GS}}}{N} = E_0 + \int_{-D}^{D} \rho(\epsilon) d\epsilon \int_{-\infty}^{\mu} \mathrm{Tr}[\mathbf{A}_\epsilon(\omega)\mathbf{M}_\epsilon]\mathrm{d}\omega. \tag{39}$$

Note that both $\mathbf{A}$ and $\mathbf{M}$ have out-of-diagonal matrix elements. Now we use

$$\mathrm{Tr}[\mathbf{A}(\omega)\mathbf{M}] = -\frac{1}{\pi}\mathrm{ImTr}[\mathbf{G}(\omega + i\delta)\mathbf{M}] = -\frac{1}{\pi}\mathrm{ImTr}[(\omega + i\delta - \mathbf{M})^{-1}\mathbf{M}] = -\frac{1}{\pi}\mathrm{ImTr}[(\omega + i\delta - \mathbf{M})^{-1}\omega] = \mathrm{Tr}[\mathbf{A}(\omega)]\omega, \tag{40}$$

which follows from the fact that $\mathrm{Im}[1/(z - x)]$ is a delta distribution, and we have used a transformation to the eigenbasis and back to replace $\mathbf{M}$ by ω in the third step. Thus, after the integration over ϵ,

$$\frac{E_{\mathrm{GS}}}{N} = E_0 + \sum_\sigma \int_{-\infty}^{\mu} \omega d\omega \left[\rho_{c,\sigma}(\omega) + \rho_{f,\sigma}(\omega)\right]. \tag{41}$$

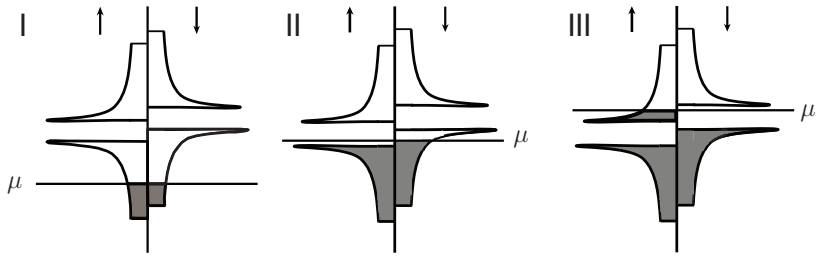

Figure 1. Sketch of the possible placements of the bands with respect to the chemical potential. The phase I correspond to the phase B', phase II to the phase A and phase III to the phase B in the DMFT calculations.

We also have

$$\begin{aligned}\frac{N_c+N_f}{N} &= \int_{-D}^{D}\rho(\epsilon)d\epsilon\int_{-\infty}^{\mu}\mathrm{Tr}[A_\epsilon(\omega)]d\omega \\ &= \sum_\sigma\int_{-\infty}^{\mu}\left[\rho_{c,\sigma}(\omega)+\rho_{f,\sigma}(\omega)\right]d\omega,\end{aligned} \tag{42}$$

thus finally,

$$\frac{K_{\mathrm{GS}}}{N} = E_0+\sum_\sigma\int_{-\infty}^{\mu}d\omega(\omega-\mu)\left[\rho_{c,\sigma}(\omega)+\rho_{f,\sigma}(\omega)\right]. \tag{43}$$

We would like to evaluate Eq. (43) for two different cases represented on Fig. 1, namely cases I and II:

$$\begin{aligned}\frac{K_{GS}}{N} &= E_0+\sum_\sigma\int_{-\infty}^{\mu}d\omega(\omega-\mu)\left(1+\frac{(c\chi_0)^2}{(\omega-\lambda_\sigma)^2}\right)\rho_{c\sigma}(\omega) \\ &= E_0+E_c+(c\chi_0)^2\sum_\sigma\int_{-\infty}^{\mu}d\omega\frac{\omega-\lambda_\sigma+\lambda_\sigma-\mu}{(\omega-\lambda_\sigma)^2}\rho_{c\sigma}(\omega) \\ &= E_0+E_c+(c\chi_0)^2\sum_\sigma\int_{-\infty}^{\mu}d\omega\frac{\rho_{c,\sigma}(\omega)}{\omega-\lambda_\sigma}+\sum_\sigma(\lambda_\sigma-\mu)n_{f,\sigma} \\ &= E_0+E_c+(c\chi_0)^2(-8/3J)+\sum_\sigma(\lambda_\sigma-\mu)n_{f,\sigma},\end{aligned} \tag{44}$$

where $E_c=\int_{-\infty}^{\mu}d\omega(\omega-\mu)\rho_{c,\sigma}(\omega)$ and in the last line we have use the gap equation, see Eq. (35). We need to evaluate

$$\begin{aligned}2\sum_\sigma(\lambda_\sigma-\mu)n_{f,\sigma} &= \sum_\sigma\left(\lambda-\mu+\mu_B g_f\tilde{H}_f\frac{\sigma}{2}\right)n_{f\sigma} \\ &= (\lambda-\mu)n_f+2\mu_B g_f\tilde{H}_f\tilde{m}_f.\end{aligned} \tag{45}$$

For $H=0$, this is equal to

$$(\lambda-\mu)n_f+J\tilde{m}_c\tilde{m}_f. \tag{46}$$

Case I is when $\omega_{1,\sigma}<\mu<\omega_{2,\sigma}$ for both spin orientations. We can write:

$$E_c = \rho_{c,0}\sum_\sigma[(\mu^2-\omega_{1,\sigma}^2)/2]-\mu n_c \tag{47}$$

and

$$\begin{aligned}\frac{K_{GS}}{N} &= \frac{3}{4}J\chi_0^2-J\tilde{m}_c\tilde{m}_f-\lambda+\rho_{c,0}\sum_\sigma[(\mu^2-\omega_{1,\sigma}^2)/2]-\mu n_c-\frac{3}{4}J\chi_0^2+\sum_\sigma(\lambda_\sigma-\mu)n_{f,\sigma} \\ &= -J\tilde{m}_c m_f-\lambda+\rho_{c,0}\sum_\sigma[(\mu^2-\omega_{1,\sigma}^2)/2]-\mu n_c+(\lambda-\mu)n_f+J\tilde{m}_c\tilde{m}_f \\ &= \rho_{c,0}\sum_\sigma[(\mu^2-\omega_{1,\sigma}^2)/2]-\mu[n_c+n_f]\end{aligned} \tag{48}$$

where in the second line we have used Eq. (46) and in the last line $\langle n_f \rangle = 1$.

Case II is when $\omega_{2,\uparrow} < \mu < \omega_{3,\uparrow}$ and only difference is that $\mu \to \omega_{2,\uparrow}$ in integration limit for $\uparrow$ c electrons. Therefore, the only difference is in the evaluation of E_c:

$$E_c = \rho_c^0 \left(\frac{\mu^2 - \omega_{1,\downarrow}^2}{2} + \frac{\omega_{2,\uparrow}^2 - \omega_{1,\uparrow}^2}{2} \right) - \mu n_c. \tag{49}$$

The $S = 1$ case

We next proceed with an analogous treatment for the $S = 1$ problem. We decompose the interaction term into doublet and quadruplet terms, $1/2 \otimes 1 = 1/2 \oplus 3/2$. We find:

$$\mathbf{s} \cdot \mathbf{S} = -\sum_{i=1}^{2} \chi_{d,i}^\dagger \chi_{d,i} + (1/2) \sum_{i=1}^{4} \chi_{q,i}^\dagger \chi_{q,i}, \tag{50}$$

where $\chi_{d,i}(\chi_{q,j})$ are the doublet ($i = 1, 2$) and the quadruplet ($j = 1, 2, 3, 4$) sets of operators under the spin $SU(2)$ symmetry, namely:

$$\chi_{d,1} = -\sqrt{1/3} c_\downarrow^\dagger f_0 - \sqrt{2/3} c_\uparrow^\dagger f_1, \qquad \chi_{d,2} = \sqrt{2/3} c_\downarrow^\dagger f_{-1} + \sqrt{1/3} c_\uparrow^\dagger f_0, \tag{51}$$

$$\chi_{q,1} = -c_\uparrow^\dagger f_{-1}, \quad \chi_{q,2} = -\sqrt{1/3} c_\downarrow^\dagger f_{-1} + \sqrt{2/3} c_\uparrow^\dagger f_0, \quad \chi_{q,3} = \sqrt{2/3} c_\downarrow^\dagger f_0 - \sqrt{1/3} c_\uparrow^\dagger f_1, \quad \chi_{q,4} = -c_\downarrow^\dagger f_1. \tag{52}$$

These operators again form a complete set in the spin sector. The decomposition in Eq. (50) is exact.

We focus on the doublet part and set all quadruplet fields to zero, $\langle \chi_{q,j} \rangle = 0$. We explicitly break the SU(2) symmetry by setting $\langle \chi_{d,2} \rangle = 0$ and use the $U(1)$ gauge freedom to make $\langle \chi_{d,1} \rangle$ real. In analogy with the $S = 1/2$ case, we make a second mean-field decomposition in the magnetic channel. The mean-field Hamiltonian has a simple wave-vector representation:

$$\mathcal{K}_{MF} = \sum_k \left(c_{k,\downarrow}^\dagger \, c_{k,\uparrow}^\dagger \, f_{k,-1}^\dagger \, f_{k,0}^\dagger \, f_{k,+1}^\dagger \right) \tilde{M}_k \begin{pmatrix} c_{k,\downarrow} \\ c_{k,\uparrow} \\ f_{k,-1} \\ f_{k,0} \\ f_{k,+1} \end{pmatrix} + \sum_k E_0, \tag{53}$$

where the matrix $\tilde{M}_k$ is

$$\begin{pmatrix} \epsilon_{k,\downarrow} - \mu & 0 & 0 & J\chi_{d,1}/\sqrt{3} & 0 \\ 0 & \epsilon_{k,\uparrow} - \mu & 0 & 0 & \sqrt{2/3} J\chi_{d,1} \\ 0 & 0 & \lambda_{-1} - \mu & 0 & 0 \\ J\chi_{d,1}/\sqrt{3} & 0 & 0 & \lambda_0 - \mu & 0 \\ 0 & \sqrt{2/3} J\chi_{d,1} & 0 & 0 & \lambda_1 - \mu \end{pmatrix} \tag{54}$$

and

$$\epsilon_{k,\sigma} = \epsilon_k + J\tilde{m}_f \frac{\sigma}{2} + \mu_B g_c H \frac{\sigma}{2} = \epsilon_k + \mu_B g_c \tilde{H}_c \frac{\sigma}{2}, \tag{55}$$

$$\lambda_i = \lambda + J\tilde{m}_c i + \mu_B g_f H i = \lambda + \mu_B g_f \tilde{H}_f i, \tag{56}$$

$$E_0 = J\chi_{d,1}^2 - J\tilde{m}_c \tilde{m}_f - \lambda, \tag{57}$$

with $\sigma = \pm 1$, $i = -1, 0, 1$. The effective field felt by the $c(f)$ electrons is given by

$$\tilde{H}_{c(f)} = H + \frac{J\tilde{m}_{f(c)}}{\mu_B g_{c(f)}}. \tag{58}$$

The EOMs are

$$\begin{aligned}
(z-\epsilon_{k,\downarrow}+\mu)G_{c_\downarrow,k} &= 1+\sqrt{\frac{1}{3}}J\chi_{d1}G_{f_0,c_\downarrow,k}\\
(z-\epsilon_{k,\uparrow}+\mu)G_{c_\uparrow,k} &= 1+\sqrt{\frac{2}{3}}J\chi_{d1}G_{f_1,c_\uparrow,k}\\
(z-\lambda_{-1}+\mu)G_{f_{-1},k} &= 1\\
(z-\lambda_0+\mu)G_{f_0,c_\downarrow,k} &= \sqrt{\frac{1}{3}}J\chi_{d1}G_{c_\downarrow,c_\downarrow,k}\\
(z-\epsilon_{k,\downarrow}+\mu)G_{c_\downarrow f_0,k} &= \sqrt{\frac{1}{3}}J\chi_{d1}G_{f_0,f_0,k}
\end{aligned} \tag{59}$$

and note also that $G_{ij,k}(z)=G_{ji,k}(z)$, while for the diagonal elements we used $G_{ii,k}(z)=G_{i,k}(z)$. Consequently

$$\begin{aligned}
(z-\lambda_0+\mu)^2G_{f_0,k} &= (z-\lambda_0+\mu)\left(1+\frac{(J\chi_{d1})^2}{3}G_{c_\downarrow,k}\right)\\
(z-\lambda_1+\mu)^2G_{f_1,k} &= (z-\lambda_1+\mu)\left(1+\frac{2(J\chi_{d1})^2}{3}G_{c_\uparrow,k}\right).
\end{aligned} \tag{60}$$

Once more we absorb μ into z: $\tilde{z}=z+\mu$ and drop writing tilde in $\tilde{z}$ in the following. The quasiparticles band edges $\omega_{i,\sigma}$ are:

$$\begin{aligned}
\omega_{1,\sigma} &= \left(3\epsilon_\sigma-3D+3\lambda_\sigma-\sqrt{9(\epsilon_\sigma-D-\lambda_\sigma)^2+12F_\sigma(J\chi_{d,1})^2}\right)/6\\
\omega_{2,\sigma} &= \left(3\epsilon_\sigma+3D+3\lambda_\sigma-\sqrt{9(\epsilon_\sigma+D-\lambda_\sigma)^2+12F_\sigma(J\chi_{d,1})^2}\right)/6\\
\omega_{3,\sigma} &= \left(3\epsilon_\sigma-3D+3\lambda_\sigma+\sqrt{9(\epsilon_\sigma-D-\lambda_\sigma)^2+12F_\sigma(J\chi_{d,1})^2}\right)/6\\
\omega_{4,\sigma} &= \left(3\epsilon_\sigma+3D+3\lambda_\sigma+\sqrt{9(\epsilon_\sigma+D-\lambda_\sigma)^2+12F_\sigma(J\chi_{d,1})^2}\right)/6,
\end{aligned} \tag{61}$$

where ϵ_σ has been defined in the section on the $S=1/2$ model, while

$$F(1)=2, \quad F(-1)=1. \tag{62}$$

and, furthermore,

$$\lambda_\downarrow=\lambda_0, \tag{63}$$

$$\lambda_\uparrow=\lambda_1. \tag{64}$$

The spectral functions are given by:

$$\rho_{c,\sigma}(\omega)=\rho_c^0\sum_{i=1}^{4}(-1)^{i-1}\theta(\omega-\omega_{i,\sigma}), \tag{65}$$

$$\rho_{f,-1}(\omega)=\delta(\omega-\lambda_{-1}), \tag{66}$$

$$\rho_{f,0}(\omega)=F_{-1}\frac{(J\chi_{d,1})^2}{3(z-\lambda_0)^2}\rho_{c,\downarrow}(\omega), \tag{67}$$

$$\rho_{f,1}(\omega)=F_1\frac{(J\chi_{d,1})^2}{3(z-\lambda_1)^2}\rho_{c,\uparrow}(\omega). \tag{68}$$

$$\rho_{f_1 c_\uparrow}(\omega) = \sqrt{\frac{2}{3}} \frac{(J\chi_{d,1})}{(\omega - \lambda_1)} \rho_{c_\uparrow}(\omega). \tag{69}$$

$$\rho_{f_0 c_\downarrow}(\omega) = \sqrt{\frac{1}{3}} \frac{(J\chi_{d,1})}{(\omega - \lambda_0)} \rho_{c_\downarrow}(\omega). \tag{70}$$

The f_{-1} must be unoccupied, otherwise the number of f electrons cannot be exactly 1. Thus $\lambda_{-1} > \mu$. This also implies that f_{-1} must be the highest in energy of the f states, thus $\tilde{m}_c < 0$ and consequently $\tilde{m}_f > 0$.

The mean-field equations

Using the fluctuaction-dissipation theorem at $T = 0$, we find

$$n_c = \sum_\sigma \langle c^\dagger_\sigma c_\sigma \rangle = \sum_\sigma \int d\omega \rho_{c,\sigma}(\omega), \tag{71}$$

$$1 = n_f = \sum_i \langle f^\dagger_i f_i \rangle = \sum_i \int d\omega \rho_{f,i}(\omega), \tag{72}$$

$$\tilde{m}_c = 1/2 \sum_\sigma \sigma \langle c^\dagger_\sigma c_\sigma \rangle = 1/2 \sum_\sigma \int \sigma d\omega \rho_{c,\sigma}(\omega), \tag{73}$$

$$\tilde{m}_f = \sum_i i \langle f^\dagger_i f_i \rangle = \sum_i i \int d\omega \rho_{f,i}(\omega). \tag{74}$$

For the gap equation we take symmetrized spectral function $A_{c\sigma;fi} = -\frac{1}{2\pi}[\mathrm{Im}G_{c\sigma;fi}(\omega + i\delta) + \mathrm{Im}G_{fi;c\sigma}(\omega + i\delta)] = \rho_{c\sigma;f,i}$, where $G_{c\sigma;fi}(z) = \langle\langle c^\dagger_\sigma; f_i \rangle\rangle_z$, etc. For the evaluation of $\langle \chi_1 \rangle$ we will need two off-diagonal spectral functions:

$$\rho_{c\downarrow;f0} = \frac{J\chi_1}{\sqrt{3}(z - \lambda_0)} \rho_{c\downarrow}(\omega) \tag{75}$$

$$\rho_{c\uparrow;f1} = \frac{\sqrt{2/3} J\chi_1}{z - \lambda_1} \rho_{c\uparrow}(\omega). \tag{76}$$

The expectation value is

$$\langle \chi_1 \rangle = \frac{1}{2}[-\sqrt{1/3}(\langle c^\dagger_\downarrow f_0 + f^\dagger_0 c_\downarrow \rangle) - \sqrt{2/3}(c^\dagger_\uparrow f_1 + f^\dagger_1 c_\uparrow)] = -\sqrt{1/3} \int A_{c\downarrow,f0}(\omega) d\omega - \sqrt{2/3} \int A_{c\uparrow,f1}(\omega) d\omega \tag{77}$$

$$= -\sqrt{1/3} \frac{J\chi_1}{\sqrt{3}} \int d\omega \rho_{c\downarrow}/(\omega - \lambda_0) - \sqrt{2/3}\sqrt{2/3} J\chi_1 \int d\omega \rho_{c,\uparrow}(\omega)/(\omega - \lambda_1) \tag{78}$$

$$= -(J\chi_1/3) \left[\int d\omega \rho_{c,\downarrow}(\omega)/(\omega - \lambda_0) \right] - 2J\chi_1/3 \left[\int d\omega \rho_{c\uparrow}(\omega)/(\omega - \lambda_1) \right]. \tag{79}$$

Finally, we obtain the gap equation:

$$\boxed{\int d\omega \rho_{c\downarrow}(\omega)/(\omega - \lambda_0) + 2 \int d\omega \rho_{c\uparrow}(\omega)/(\omega - \lambda_1) = -3/J.} \tag{80}$$

This equation has essentially the same structure as the gap equation for the $S = 1/2$ case.

Evaluation of energy

The total energy can be evaluated in analogy to the $S = 1/2$ case. We find

$$\frac{K_{\mathrm{GS}}}{N} = E_0 + \sum_\sigma \int_{-\infty}^{\mu} d\omega(\omega - \mu)[\rho_{c,\sigma}(\omega) + \rho_{f,i(\sigma)}(\omega)] + (\lambda_{-1} - \mu)\theta(\omega - \lambda_{-1}) \tag{81}$$

We evaluate Eq. 81 for two different cases represented on Fig. 1. For case I, $E_c = \rho_{c,0} \sum_\sigma [(\mu^2 - \omega_{1,\sigma}^2)/2] - \mu n_c$, thus

$$\frac{K_{GS}}{N} = \rho_{c,0} \sum_\sigma [(\mu^2 - \omega_{1,\sigma}^2)/2] + \lambda(n_{f0} + n_{f1}) - \mu(n_f + n_c) \tag{82}$$

In the case II,

$$E_c = \rho_c^0 \left(\frac{\mu^2 - \omega_{1,\downarrow}^2}{2} + \frac{\omega_{2,\uparrow}^2 - \omega_{1,\uparrow}^2}{2} \right) - \mu n_c. \tag{83}$$

PHASE DIAGRAMS FOR $S = 1/2$ AND $S = 1$

We now discuss the different possible mean-field phases for the $S = 1/2$ and $S = 1$ Kondo lattice models.

One possible phase is a pure saturated ferromagnetic phase with magnetization $m_f = -g_f \mu_B S$ and with zero hybridisation, $\chi_{d,1} = 0$. If conducting electrons are completely polarized we call it the polar phase and the magnetization of conducting electrons is then given by

$$m_{c,P-I} = \mu_B g_c n_c/2. \tag{84}$$

For intermediate coupling regime, we distinguish between the ferromagnetic phases I, II, and III, which all have a finite value of the hybridisation parameter $\chi_{d,1}$ (thus a spectral gap). They are schematically represented in in Fig. 1. The phase I with the electron pockets, corresponds to the phase B' in the DMFT calculations. The phase II with the chemical potential in the gap corresponds to the DMFT phase A. The numerical results in the phase II clearly indicate that as we lower J the transition into phase III is expected, but when $\mu > \omega_{3,\uparrow}$ we were not able to find convergent solution in the regime of small J, as marked by the the dashed line in Fig. 2, see also [2]. This phase III would correspond to the phase B in the DMFT calculations, where this is a stable phase.

The phase boundary between the phase I and II or between the phase II and III is given by the condition

$$\tilde{m}_c + \tilde{m}_f = (2S - n)/2, \tag{85}$$

for the expectation values of spin z component, which shows plateau behaviour irrespective of the Landé factors or, equivalently,

$$m_c/g_c + m_f/g_f = -\mu_B(2S - n)/2. \tag{86}$$

This is equivalent to the condition that

$$\mu = \omega_{2(3),\uparrow} \tag{87}$$

for transition between the phases I$\rightarrow$ II (II$\rightarrow$ III).

The pure Kondo singlet (paramagnetic) phase is defined by $m_c = 0, m_f = 0, \chi_{d,1} \neq 0$. We only find it for $S = 1/2$. In the $S = 1$ model the hole pocket never emerges; instead, the chemical potential becomes attached near the top of the bottom band for large J. In fact, similar behavior is also observed in the DMFT solutions. The boundary between phase I and the Kondo phase is determined by the condition

$$m_f = m_c = 0. \tag{88}$$

The boundary between the phases I,II and polar-I is given by the condition

$$\chi_{d,1} = 0. \tag{89}$$

We conclude that the qualitative features of the static MF and DMFT phase diagrams are rather similar, except that in the static mean-field theory the phase III is not stable. The main difference compared to previous works [2–4] is the finding that in the MF treatment the metamagnetic transition is described by the transition I $\rightarrow$ II, while in the DMFT there are two different scenarios for metamagnetic transitions, either the transition I $\rightarrow$ II or the transition II $\rightarrow$ III, where only the former is expected for physically relevant model parameters.

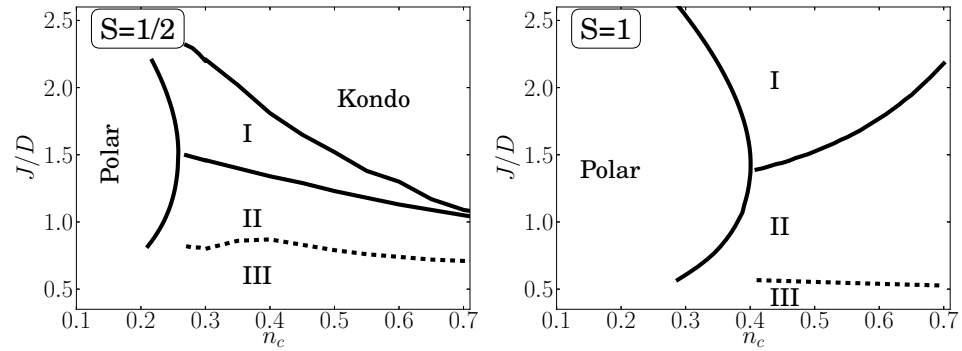

Figure 2. Ground state phase diagram of the KLM: (a) $S = 1/2$, (b) $S = 1$ with Landé factors $g_c = g_f = 1$. For the description of phases I, II, see the discussion in the text and Fig. 1. Phase Polar-I represent polarized phase with zero hybridisation and Kondo phase is paramagnetic phase ($m_c = m_f = 0$.). The dashed line represent the transition into phase where we could not find the convergent solution, but phase III is expected, see discussion in the text.

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