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Effective action for the Kondo lattice model. New approach for $S = 1/2$

F. Bouis[a,*], M.N. Kiselev[a,b]

[a]*Laboratoire Léon Brillouin, CE-Saclay 91191, Gif-sur-Yvette, France*
[b]*Russian Research Center "Kurchatov Institute", 123 182 Moscow, Russia*

Abstract

In the partition function of the Kondo lattice (KL), spin matrices are exactly replaced by bilinear combinations of Fermi operators with the purely imaginary chemical potential $\lambda = -i\pi T/2$ (Popov representation). This new representation of spin operators allows one to introduce new Green's Functions (GF) with Matsubara frequencies $\omega_n = 2\pi T(n+\frac{1}{4})$ for $S=\frac{1}{2}$. A simple temperature diagram technique is constructed with the path integral method. This technique is standard and does not contain the complicated combinatoric rules characteristic of most of the known variants of the diagram techniques for spin systems. The effective action for the almost antiferromagnetic KL problem is derived.

Keywords: Heavy fermions; Kondo lattice; Antiferromagnetism

Many systems in statistical physics are described by Hamiltonians containing spin matrices. Unfortunately, the diagrammatic perturbation theory for spin systems is complicated. Many variants are based on different representations of the spin matrices by Bose or Fermi operators. However, unphysical states always arise leading to constraints and complication of the Feynman codex. In this paper, we construct a simple diagrammatic technique (DT) for spin-$\frac{1}{2}$ that differs from the known techniques in the form of the GF, but which is standard in other respects, does not contain the complicated combinatoric rules characteristic of spin systems and permits one to take into account the constraints rigorously.

It is indeed possible to replace exactly spin-$\frac{1}{2}$ matrices by bilinear combinations of Fermi operators:

$$\sigma^z_{fi} \to S^z_{fi} = \tfrac{1}{2}(a^+_{i\uparrow}a_{i\uparrow} - a^+_{i\downarrow}a_{i\downarrow}),\ \ \sigma^+_{fi} \to S^+_{fi} = a^+_{i\uparrow}a_{i\downarrow},$$

$$\sigma^-_{fi} \to S^-_{fi} = a^+_{i\downarrow}a_{i\uparrow}, \tag{1}$$

by the basic formula shown in Ref. [1]

$$Z = \mathrm{Sp}\ e^{-\beta H} = i^N \mathrm{Sp}\ e^{-\beta(H_f + (i\pi/2\beta)N)}, \tag{2}$$

where H_f is obtained from H by replacement (1), and $N = \sum_{i\sigma} a^+_{i\sigma}a_{i\sigma}$. There is no constraint but the purely imaginary chemical potential of pseudofermions $\lambda = -i\pi T/2$ leads to the mutual cancellation of the unphysical states.

We analyze here the KL model which is a periodic lattice of magnetic atoms modeled by f-orbitals in a metallic background

$$\mathscr{H}_{KL} = -\sum_{ij,\sigma}(t_{ij}+\mu)\Psi^+_{i\sigma}\Psi_{j\sigma} + J_{sf}\sum_i \Psi^+_{i\sigma}\sigma\Psi_{i\sigma'}\boldsymbol{S}_{fi} + g\sum_i (H + h e^{i\boldsymbol{R}_i\boldsymbol{Q}})S^z_{fi}. \tag{3}$$

We add a uniform (H) and a staggered (h) magnetic field ($g = \mu_B g_L$, where μ_B is the Bohr magneton and g_L is the Landé factor). We consider a simple cubic lattice with the notation $\boldsymbol{Q} = \boldsymbol{Q}_{AF} = (\pi,\pi,\pi)$. Using Popov representation of spins, the ratio of the partition function of the interacting system to the partition function of the corresponding free system can be represented in the form of functional

* Corresponding author. Tel.: 331-69-08-96-85; fax: 331-69-08-82-61; e-mail: bouis@llb.saclay.cea.fr.

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integrals as follows:

$$Z/Z_0 = \frac{\int Dv \exp[S - \frac{i\pi}{2\beta}\int_0^\beta d\tau \sum_i \bar{a}_{i,\alpha}(\tau) a_{i,\alpha}(\tau)]}{\int Dv \exp[S_0 - \frac{i\pi}{2\beta}\int_0^\beta d\tau \sum_i \bar{a}_{i,\alpha}(\tau) a_{i,\alpha}(\tau)]}, \tag{4}$$

where the Euclidean action for the KL model is

$$S = \int_0^\beta d\tau \left\{ \sum_i [\bar{\Psi}_{i,\sigma}\partial_\tau \Psi_{i,\sigma} + \bar{a}_{i,\alpha}\partial_\tau a_{i,\alpha}] - \mathscr{H}_{KL}(\tau) \right\}. \tag{5}$$

We note by Dv the integration over the anticommuting Grassmann variables Ψ_σ, a_α. By making the replacement $a_{i,\alpha}(\tau) \to a_i^\alpha(\tau)\exp((i\pi/2\beta)\tau)$, etc., which cancels the last term in both exponents in numerator and denominator of Eq. (4), we come to the following boundary conditions for Grassmann fields: $\Psi_\sigma(\beta) = -\Psi_\sigma(0), \bar{\Psi}_\sigma(\beta) = -\bar{\Psi}_\sigma(0)$, $\bar{a}^\alpha(\beta) = -i\bar{a}^\alpha(0), a^\alpha(\beta) = ia^\alpha(0)$. Going over to the momentum representation for all Grassmann variables and assuming $\boldsymbol{s}_{sk} = \sum_p \bar{\Psi}_{p+k}\sigma\Psi_p$ we obtain

$$S = \sum_k \bar{\Psi}_{k,\sigma} G_0^{-1} \Psi_{k,\sigma} + \sum_p \bar{a}_p^\alpha \mathscr{G}_0^{-1} a_p^\alpha + J_{\mathrm{sf}} \sum_k \boldsymbol{s}_{sk}\boldsymbol{S}_{f-k} + \tfrac{1}{2} hg \sum_k \bar{a}_k^\alpha \sigma^z a_{k+Q}^{\alpha'}, \tag{6}$$

where the inverse GF of Ψ-fields is $G_0^{-1} = i2\pi T(n+1/2) - \varepsilon_k + \mu$ with dispersion $\varepsilon_k = -\sum_\delta t_{i,i+\delta} e^{i\delta k}$ and the inverse GF of a^α Grassmann fields is $\mathscr{G}_{0\alpha}^{-1} = i2\pi T(m + \frac{1}{4}) - \frac{1}{2} gH\sigma_{\alpha\alpha}^z$ with unusual Matsubara frequencies. Note that Popov representation can be used for spins $S = 1$ also. In this case the frequencies are shifted to $\omega_m = 2\pi T(m + 1/3)$. Moreover the method has been extended to arbitrary spin in Ref. [8].

We now confine ourselves to the limiting case $T_N \sim T_K \sim T_0$ [2] assuming the same energy scale for antiferromagnetic (AF) and Kondo correlations. It allows us to integrate over the fast Ψ fields with energies $\varepsilon \sim \mu \gg T_0$ using the bare electrons GF. We can also integrate over the fast fields a^α ($\omega \gg T_0$) taking into account one-site Kondo renormalization of vertices ($J_{\mathrm{sf}} \to \mathscr{J}_{\mathrm{sf}}$) and self-energy parts ($G_0 \to G$) [3]. As a result, a simple DT is constructed. Contrary to other DT (see, e.g. Refs. [4,5]) the constraint on the spin subsystem is taken into account exactly. The new action which is written in terms of slow Ψ and a^α variables contains an additional AF Heisenberg interaction between spins due to the indirect RKKY exchange [3,4]:

$$S_{\mathrm{eff}} = \sum_k \bar{\Psi}_{k,\sigma}^{\mathrm{slow}} G^{-1} \Psi_{k,\sigma}^{\mathrm{slow}} + \sum_k \mathscr{J}_{\mathrm{sf}} \boldsymbol{s}_{sk}^{\mathrm{slow}} \boldsymbol{S}_{f-k} + S_{\mathrm{H}}. \tag{7}$$

The last term in (7) can be analyzed separately and represented by auxiliary three-component Bose fields $\phi^\gamma(k)$ [1]

$$S_{\mathrm{H}} = \sum_{k_1 k_2 \sigma} \bar{a}_{k_1}^\alpha [\mathscr{G}_0^{-1}\delta_{k_1,k_2} + \sigma^z h \delta_{k_1+Q,k_2}] a_{k_2}^\alpha - \sum_k [\tfrac{1}{2}\phi_k^3 S_{-k}^z + \eta_k^* S_k^- + \eta_k S_k^+] + S_0[\phi] \tag{8}$$

with the following notation: $S_0 = -\frac{1}{4}\sum_k (\Gamma_k^{\mathrm{RKKY}})^{-1}\phi_k^\gamma \phi_{-k}^\gamma$, $\eta_k^* = (\eta_k)^*$ and $\eta_k = (\phi_k^1 - i\phi_k^2)/2$. In the case $T_K \ll T_N$ only magnetic terms in the effective action are important. We note by W the matrix of the quadratic form in a^α variables. Integrating over all a^α fields one can find the nonpolynomial action of the AF Heisenberg model in terms of Bose fields [6]:

$$S_{\mathrm{H}} = S_0[\phi^3, \eta] + \log\det W[\phi^3, \eta]. \tag{9}$$

In the case considered, namely $T_N \sim T_K \sim T_0$ the procedure of derivation of the effective action is a little bit complicated. Taking into account the second term in Eq. (7) one has to replace $\phi^\gamma \to \phi^\gamma - 2\mathscr{J}_{\mathrm{sf}} s_{s,k}^{\gamma\mathrm{slow}}$ in Eq. (9). As a result, the effective action can be rewritten as follows:

$$S_{\mathrm{eff}} = \sum_k \bar{\Psi}_{k,\sigma}^{\mathrm{slow}} G^{-1} \Psi_{k,\sigma}^{\mathrm{slow}} + S_0[\phi^3, \eta] + \log\det W[\phi_k^\gamma - 2\mathscr{J}_{\mathrm{sf}} \boldsymbol{s}_{sk}^{\gamma\mathrm{slow}}]. \tag{10}$$

Eqs. (7)–(10) are the key result of the present work. This effective action describes the low-energy properties of the KL model. The last term in Eq. (9) takes into account the mutual influence of conduction electrons and spins. Magnetic instabilities of both kind of electrons could then be easily analyzed.

Let us concentrate on the former problem (8). The spin subsystem undergoes a phase transition with $T_c = T_0$ corresponding to the appearance of a nonzero staggered magnetization ρ as $h \to 0$. This problem is related to the Bose-condensation of the field $\phi_k^3 = \tilde{\phi}_k^3 + \rho(\beta N)^{1/2}\delta_{k,Q}\delta_\omega$ and in one-loop approximation results in the usual mean-field equation for AF order parameter [6] in the presence of Kondo-scattering processes [3]. Note that a magnetic transition in the localized system may induce a magnetic transition in the itinerant system.

Taking into account the compensation equation [3,6] and calculating the $\log\det W[\phi^3, \eta]$ approximately by the method of stationary phase the following expression for the spin subsystem effective action can be obtained:

$$S_{\mathrm{H}}^{\mathrm{eff}} = \sum_k \eta_k^* \chi_t^{-1} \eta_k + \sum_k \phi_k^{3*} \chi_\ell^{-1} \phi_{-k}^3 - 1/4 \sum_k (\Gamma_k^{\mathrm{RKKY}})^{-1} \phi_k^\gamma \phi_{-k}^\gamma, \tag{11}$$

where χ_t and χ_ℓ are transverse and longitudinal susceptibilities, respectively. As usual, the transverse susceptibility describes the AF magnons excitations. At the temperature range $T > T_0$ when the condensate solution is absent the effective action has the same form except that the transverse and longitudinal susceptibilities describe the paramagnon excitations which can result in some untrivial effects in heavy-fermion compounds [7]. These excitations introduce a new energy scale corresponding to the critical behavior.

Summarizing, we constructed a simple diagrammatic technique which allows one to analyze the effective action of the KL model when the energy scales for AF and Kondo correlations are the same. This effective action describes the slow electron subsystem interacting with the spin fluctuations of either magnon or paramagnon type.

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