Finite-temperature slave-boson description of the ferromagnetic instabilities of the Anderson lattice

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Abstract. Using the Kotliar and Ruckenstein slave-boson formalism we consider the finite-U Anderson lattice. We study the appearance of ferromagnetic instabilities and their stabilities. We study both the groundstate and the finite temperature regimes as a function of the Coulomb repulsion, density and f-level location. In the insulating regime there is a ferromagnetic instability that competes with the paramagnetic phase. In the metallic regime there are two ferromagnetic phases as the coupling grows. We calculate the critical temperatures as a function of coupling.

In this work we consider ferromagnetic regimes of the Anderson lattice in the metallic phase and at finite temperatures. The magnetic instabilities [1] were obtained successfully using a slave-boson formalism [2, 3]. Most heavy fermion systems are nonmagnetic but there are exceptions such as antiferromagnetic like TmSe, UNiSm, UAγCu₄, UCu₇, U₂Zn₁₇ (typically with small moments due to the Kondo effect) and some ferromagnetic such as Fe₃Si₁₋ₓGeₓ. The antiferromagnetic phase typically prevails close to half-filling or quarter filling but if the system is not near commensurability a ferromagnetic instability may appear.

The model we study is the Anderson lattice, with Na sites, where two sets of electron operators are described by the Hamiltonian

\[
H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} (\epsilon_f - \sigma B) f_{k,\sigma}^\dagger f_{k,\sigma} + U \sum_i d_i^\dagger d_i + V \sum_{i,\sigma} \left( e_i^\dagger e_i + p_i^\dagger p_i + f_{i,\sigma}^\dagger f_{i,\sigma} - 1 \right) + \sum_{i,\sigma} \lambda_i \left( e_{i,\sigma}^\dagger e_{i,\sigma} + p_{i,\sigma}^\dagger p_{i,\sigma} - d_i^\dagger d_i \right)
\]

Here V is the hybridization between the c-electrons, described by the band \( \epsilon_k \), and the f-electrons, described by the energy \( \epsilon_f \), and U is the coupling between the f-electrons if located at the same site. We associate four bosons to the various states f-electrons can occupy [2]. The bosons \( e, d \) are associated with empty and doubly-occupied sites, respectively and the bosons \( p, f \) with a singly-occupied site with spin component \( \sigma \). There is an enlargement of the Hilbert space and restrictions must be implemented at each site \( e_{i,\sigma}^\dagger e_{i,\sigma} + p_{i,\sigma}^\dagger p_{i,\sigma} + f_{i,\sigma}^\dagger f_{i,\sigma} = 1 \) and \( f_{i,\sigma}^\dagger f_{i,\sigma} = p_{i,\sigma}^\dagger p_{i,\sigma} + d_i^\dagger d_i \) through Lagrange multipliers \( \lambda_i \) and \( \lambda_{i,\sigma} \), respectively. In the physical subspace the operators \( f_{i,\sigma} \) are replaced by \( f_{i,\sigma} Z_{i,\sigma} \) where

\[
Z_{i,\sigma} = (1 - d_i^\dagger d_i - p_{i,\sigma}^\dagger p_{i,\sigma})^{-1/2} (e_{i,\sigma}^\dagger p_{i,\sigma} + p_{i,-\sigma}^\dagger d_i)(1 - e_{i,\sigma}^\dagger p_{i,-\sigma} - p_{i,\sigma}^\dagger p_{i,-\sigma})^{-1/2}.
\]

The usual procedure consists in taking a mean-field approach where we assume the slave bosons to be condensed. In the cases of paramagnetic or ferromagnetic
solutions we take $Z_{i,\sigma} = Z_{i,\sigma} = Z_{\sigma}, \epsilon_{i}^{\uparrow} = \epsilon_{i} = \epsilon, d_{i}^{\downarrow} = d_{i} = d, p_{i,\sigma}^{\downarrow} = p_{i,\sigma} = p_{\sigma}$. The paramagnetic solution is described by $p_{1} = p_{\downarrow}$. As a consequence $\lambda_{\uparrow} = \lambda_{\downarrow}$. In the mean-field approximation the Hamiltonian can be simplified to

$$H = \sum_{k,\sigma} (\epsilon_{k} - \mu) c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{k,\sigma} (\epsilon_{f} - \mu - \sigma B + \lambda_{\sigma}) f_{k,\sigma}^{\dagger} f_{k,\sigma} + V \sum_{k,\sigma} Z_{\sigma} \left( c_{k,\sigma}^{\dagger} f_{k,\sigma} + f_{k,\sigma}^{\dagger} c_{k,\sigma} \right) + U N_{s} d^{2} + N_{s} \lambda \left( e^{2} + d^{2} + p_{\uparrow}^{2} + p_{\downarrow}^{2} - 1 \right) - N_{s} \sum_{\sigma} \lambda_{\sigma} (p_{\sigma}^{2} + d^{2}) \quad (2)$$

The procedure now consists of determining the mean-field values of the condensed bosons using the Helmann-Feynmann theorem by taking derivatives of the Hamiltonian with respect to these parameters.

These derivatives lead to the mean-field equations that have to be solved self-consistently. This leads to

$$V \sum_{k,\sigma} \frac{\partial Z_{\sigma 1}}{\partial p_{\sigma}} \left( \langle c_{k,\sigma 1}^{\dagger} f_{k,\sigma 1} \rangle + \langle f_{k,\sigma 1}^{\dagger} c_{k,\sigma 1} \rangle \right) + 2 N_{s} (\lambda - \lambda_{\sigma}) p_{\sigma} = 0$$

$$V \sum_{k,\sigma 1} \frac{\partial Z_{\sigma 1}}{\partial d_{\sigma}} \left( \langle c_{k,\sigma 1}^{\dagger} f_{k,\sigma 1} \rangle + \langle f_{k,\sigma 1}^{\dagger} c_{k,\sigma 1} \rangle \right) + 2 U N_{s} d + 2 N_{s} d (\lambda - \lambda_{\uparrow} - \lambda_{\downarrow}) = 0$$

$$V \sum_{k,\sigma 1} \frac{\partial Z_{\sigma 1}}{\partial e_{\sigma}} \left( \langle c_{k,\sigma 1}^{\dagger} f_{k,\sigma 1} \rangle + \langle f_{k,\sigma 1}^{\dagger} c_{k,\sigma 1} \rangle \right) + 2 N_{s} e \lambda = 0 \quad (3)$$

together with the restrictions $N_{s} (e^{2} + d^{2} + p_{\uparrow}^{2} + p_{\downarrow}^{2} - 1) = 0$ and $\sum_{k} \langle f_{k,\sigma}^{\dagger} f_{k,\sigma} \rangle - N_{s} (p_{\sigma}^{2} + d^{2}) = 0$.

The solution of these equations requires the evaluation of the various fermion operator averages. This can be done in various ways such as using Green function methods or directly diagonalizing the Hamiltonian operator by performing a rotation of the fermionic operators as indicated in [4]. We will now discuss the results.

The insulator case was considered before in [3] and the paramagnetic (PM) solution for the metallic case was considered in [5] together with the effects of orbital degeneracy. We take $V = 1$ and $t = 2.5\sqrt{V}$. In Figs. 1-2 we show the dependence of $p_{\uparrow}, p_{\downarrow}$ as a function of $U/V$ for $\mu = 0, -0.2$ (the magnetization is given by $M = p_{\uparrow}^{2} - p_{\downarrow}^{2}$ and is shown in Fig. 3 for these values of $\mu$ and $\mu = -0.6$). In the case $\mu = 0 (n = 2)$ the system is half-filled and an insulator with a finite gap in the spectrum. In this case for small values of $U/V$ the system is in a PM phase ($p_{\uparrow} = p_{\downarrow}$) as previously found (note that here we consider a tight-binding band instead of a flat c-electron density of states). Increasing the coupling there is a discontinuous phase transition to a ferromagnetic phase [3] as also seen experimentally [6]. Decreasing the chemical potential leads to a metallic regime. In this case one finds two ferromagnetic phases
as found in the very large $U$ limit in [7] as the $f$-level position is varied. At high values of $U/V$ we find a strong ferromagnetic phase (SFM) as in the insulator regime. Decreasing the coupling the system jumps discontinuously to another (weak) ferromagnetic phase (WFM), with a smaller magnetization. Decreasing further the Coulomb interaction the system changes again discontinuously (at $T = 0$) to the PM regime (note that there are metastable phases; the stable phases are selected comparing the energies of the various mean-field solutions found. The metastable phases are represented by dashed lines in Figs. 1, 2). Note that in the WFM phase the magnetization decreases as the coupling increases until the phase is replaced by the more stable SFM phase. Also the double occupancy decreases discontinuously at the transition. The difference between the two ferromagnetic phases is explained in Figs. 4-6 where the bands are shown for three different values of $U/V$ corresponding to the three phases (keeping $\mu = -0.2$) choosing a direction such that $k = k_x = k_y$. In the PM regime there are two bands as expected (with double degeneracy). As the coupling increases a first ferromagnetic phase appears. In this regime the bands split slightly such that for low momenta both bands are still above the chemical potential (the energies are measured with respect to the chemical potential). Therefore both bands are empty. For high momentum one band is filled and the other one is empty leading to a non-zero, but weak, magnetization. Increasing further $U/V$ in both low and high momenta one band is filled and the other one is empty leading to an increased magnetization. The discontinuity in the magnetization occurs since the level crossing through the chemical potential is discontinuous. A similar description using a spin-rotation invariant slave-boson method was considered in [8].

The influence of the $f$-level position is easily understood. The magnetization is maximum.
when the $f$-level position is such that there is one band filled and one band empty, that is when the bands are centered around the chemical potential. As expected when $\epsilon_f$ is negative and $U$ not large the level has a high double occupancy. On the other hand when the $f$-level position is above the chemical potential the $f$-level is mostly empty.

Finally we present results at finite temperatures. In Fig. 7 we show the effect of temperature on $p_\uparrow, p_\downarrow$ for a temperature such that the WFM phase is still present and in Fig. 8 a temperature for which the weak phase has merged with the PM phase. In the first case the magnetization is small, as shown in the following figures. At this temperature the strong phase is basically unaffected. In Fig. 9 we show the magnetization of the two phases as a function of temperature. The results show that the transition between the WFM phase and the PM phase is of second order in $T$. Note that the quantum phase transition at zero temperature is of first order in $U/V$.

On the other hand the transition to the SFM phase either from the weak phase or from the PM regime at a temperature above the critical temperature for the WFM phase is of first order, consistently with the quantum phase transition at zero temperature. The critical temperature of the strong phase is much higher. As the temperature grows, the splitting of $p_\uparrow$ and $p_\downarrow$ for the WFM phase goes to zero at the low $U$ boundary and the PM phase is extended up to the value of $U$ where the SFM phase is the most stable. The splitting between $p_\uparrow$ and $p_\downarrow$ remains large.

In Fig. 10 we plot the critical temperature as a function of coupling $U$ for the two phases.

In summary, in the insulator case at zero temperature there is a first order phase transition to a SFM phase. At finite temperature the same type of order prevails. In the metallic regime there are two phases at zero temperature with quantum phase transitions that are of first order both to the WFM phase and to the SFM phase. These phases are obtained in succession as the coupling grows. At finite temperature the transition from the WFM phase to the PM phase is now second order while the transition to the SFM phase remains first order.

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