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ARTICLE

Competing antiferromagnetic phases of the under-screened Anderson lattice model (INVITED)

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We investigate the magnetic phases of the Under-screened Anderson Lattice Model (UALM) for nearly half-filled 5f bands and find a competition between two distinct magnetic phases. The version of the UALM that we consider consists of two correlated 5f bands that, in the paramagnetic state, hybridize with a single conduction band. At the Néel temperature, the paramagnetic state undergoes a second-order transition to antiferromagnetically ordered states, in which the Néel order parameter induces a mixing between the states with different 5f characters. As pressure is applied, there is a line of first-order transitions that separates two Néel phases. Furthermore, as the pressure is increased, the Néel temperature decreases as if the system is being driven towards a quantum critical point. However, the nature of the paramagnetic instability changes from second-order to first-order before the Neel temperature reaches absolute zero.

Keywords: unders-creened Anderson lattice model; spin density waves; competing phases: phase diagram; uranium compounds;

1. Introduction

The Under-screened Anderson Lattice Model (UALM) has been used to describe the anomalous properties of several uranium compounds. The UALM is the natural generalization of the Under-screened Kondo Impurity Model (UKIM) for crystalline compounds. The UKIM describes localized moments S which interact with conduction electrons via an on-site antiferromagnetic interaction which, through the Kondo effect, induces a compensating antiparallel spin polarization of the conduction electrons that only partially quenches the moment on the impurity site [1]. This leads to a residual moment and hence, an entropy associated with the impurity at T=0. The uranium monochalcogenides exhibit resistivities that follow logarithmic temperature dependencies at high temperatures, which indicates that Kondo scattering is at work. The logarithmic temperature dependence of the resistivities is interrupted at temperatures of the order of 100 K, where the materials order magnetically [2,3]. For the ferromagnetic uranium monochalcogenides, the saturated ordered magnetic moments are consistent with partial Kondo compensation of the free uranium moments inferred from the high-temperature Curie-Weiss form of the susceptibilities. While some cerium compounds do exhibit signatures of the Kondo effect at high temperatures and undergo magnetic ordering at low-temperatures, the transition temperatures and the saturated ordered moments of the uranium compounds are orders of magnitude smaller than those of the corresponding cerium compounds [4]. Therefore, one may expect that the UALM may be appropriate to describe the uranium monochalcogenides [5,6]. Furthermore, one may expect that the UALM may also describe the antiferromagnetic ordering observed in the uranium-pnictides [7,8] and $UIrSi_3$ [9]. It has been proposed that the UALM may describe the enigmatic "Hidden Ordered" phase of the itinerant 5f material URu_2Si_2 [10,11].

In this paper, we survey the antiferromagnetically ordered phases of the UALM for nearly half-filled 5f bands, as found by mean-field theory. We incorporate a direct 5f to 5f hopping matrix element in the UALM that introduces a delocalization of the residual 5f local moments. We investigate the pressure-temperature phase diagram by assuming that the main effect of applying pressure is to reduce the inter-atomic spacings and, thereby, increase the band-width which reduces the tendency for magnetic ordering.

2. The Under-screened Anderson lattice model

The under-screened Anderson Lattice Model, used in the present work, is described by the Hamiltonian

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$$H = H_f + H_d + H_{fd} \tag{1}$$

Where

$$H_f = \sum_{\underline{k},\sigma,\chi} E_f^{\chi}(\underline{k}) f_{\underline{k},\sigma}^{\dagger} f_{\underline{k},\sigma}$$
$$+\left(\frac{U-J}{2N}\right)\sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi\neq\chi'} f_{\underline{k}+\underline{q},\sigma}^{\dagger,\chi} f_{\underline{k},\sigma}^{\chi} f_{\underline{k}'-\underline{q},\sigma}^{\dagger,\chi'} f_{\underline{k}',\sigma}^{\chi'}$$
$$+\left(\frac{U}{2N}\right)\sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi,\chi'} f_{\underline{k}+\underline{q},\sigma}^{\dagger,\chi} f_{\underline{k},\sigma}^{\chi} f_{\underline{k}'-\underline{q},-\sigma}^{\dagger,\chi'} f_{\underline{k}',-\sigma}^{\chi'}$$
$$+\left(\frac{J}{2N}\right)\sum_{\underline{k},\underline{k}',\underline{q},\sigma,\chi\neq\chi'} f_{\underline{k}+\underline{q},\sigma}^{\dagger,\chi} f_{\underline{k},\sigma}^{\chi'} f_{\underline{k}'-\underline{q},-\sigma}^{\dagger,\chi'} f_{\underline{k}',-\sigma}^{\chi},$$

$$H_d = \sum_{\underline{k},\sigma} \varepsilon(\underline{k}) d_{\underline{k},\sigma}^{\dagger} d_{\underline{k},\sigma}.$$

The dispersion relation of the conduction electrons is given by:

$$\varepsilon(k) = -2t[\cos(ak_x) + \cos(ak_y) + \cos(ak_z)]$$

where a is the lattice parameter, W=6t and 2W is the total band-width. The hybridization tem is:

$$H_{fd} = \sum_{\underline{k},\sigma,\chi}\left(V_{\chi}(\underline{k}) f_{\underline{k},\sigma}^{\dagger,\chi} d_{\underline{k},\sigma} + V_{\chi}(\underline{k}) d_{\underline{k},\sigma}^{\dagger} f_{\underline{k},\sigma}^{\chi}\right).$$

The first term in the Hamiltonian describes two 5f bands (labeled by $\chi=(\alpha,\beta)$), while the other terms represent the screened Coulomb interaction, U, and the Hund's rule interaction, J. The term H_d describes the conduction band in which $\varepsilon(k)$ is the nearest-neighbor tight binding hopping energy and the H_{fd} term represents the hybridization. We shall assume that $V_{\beta}(k)=0$, which does not affect the results. The first term H_f is treated in the mean-field approximation, in which the fluctuations $\Delta\hat{n}_{f\underline{q}\sigma}^{\chi} = \left(\hat{n}_{f\underline{q},\sigma}^{\chi} - \left\langle\hat{n}_{f\underline{q},\sigma}^{\chi}\right\rangle\right)$ are considered as being small when compared with the average value of $\hat{n}_{f\underline{q}\sigma}^{\chi}$. The expectation value of $\hat{n}_{f\underline{q}\sigma}^{\chi}$ is re-written in terms of the Néel order parameters via

$$\left\langle\hat{n}_{f\underline{q},\sigma}^{\chi}\right\rangle = \frac{n_f^{\chi}}{2}\delta_{\underline{q}0} + \eta(\sigma) m_f^{\chi} \delta_{\underline{q},\pm\underline{Q}} \tag{2}$$

where $\underline{Q}=(\pi,\pi,\pi)$ and $\eta(\sigma)=\pm1$ for $\sigma=\uparrow,\downarrow$ respectively. The quantity m_f^{χ} is identified with the spin density wave (SDW) order parameter and satisfies a pair of coupled equations

$$m_f^{\alpha} = \left(U m_f^{\alpha} + J m_f^{\beta}\right)\chi_f^{\alpha,\alpha}(\Delta_{\alpha})$$

$$m_f^{\beta} = \left(U m_f^{\beta} + J m_f^{\alpha}\right)\chi_f^{\beta,\beta}(\Delta_{\beta}) \tag{3}$$

which involves the energy gaps $\Delta_{\alpha(\beta)}$

$$\Delta_{\alpha(\beta)} = U m_f^{\alpha(\beta)} + J m_f^{\beta(\alpha)} \tag{4}.$$

The α susceptibility that appears in the above equations is given by

$$\chi_f^{\alpha,\alpha}(\Delta_{\alpha}) = \frac{1}{4\pi i N}\sum_{\underline{k}}\oint f(\omega) F^{\alpha\alpha}(\underline{k}+\underline{Q}) d\omega \tag{5}$$

where $f(\omega)$ is the Fermi-function and the contour encircles the real axis. The function $F^{\alpha\alpha}(\underline{k}+\underline{Q})$ is related to the 5f Green's function $G^{\alpha\alpha}(\underline{k}+\underline{Q})$. The β susceptibility is given by

$$\chi_f^{\beta,\beta}(\Delta_{\beta}) = \frac{1}{2N}\sum_{\underline{k}}\left[\frac{f(E_{\beta}^{+}(\underline{k})) - f(E_{\beta}^{-}(\underline{k}))}{\sqrt{(t\varepsilon(\underline{k}))^2 + (\Delta_{\beta})^2}}\right]$$

in which

$$E_{\beta}^{\pm}(\underline{k}) = \varepsilon_f \pm \sqrt{t^2\varepsilon^2(\underline{k}) + |\Delta_{\beta}|^2}\,. \tag{6}$$

The Helmholtz Free-Energy F_N can be expressed in terms of the Néel order parameters as

$$F_N = -k_B T\sum_{\gamma,\underline{k}}\ln\left(1+\exp\left[-\frac{(E^{\gamma}(\underline{k})-\mu)}{k_B T}\right]\right) + \mu N_t \tag{7}$$
$$+\frac{N}{U^2+J^2}\left[U(\Delta_{\alpha}^2+\Delta_{\beta}^2) - 2J\Delta_{\alpha}\Delta_{\beta}\right]$$

3. Numerical results

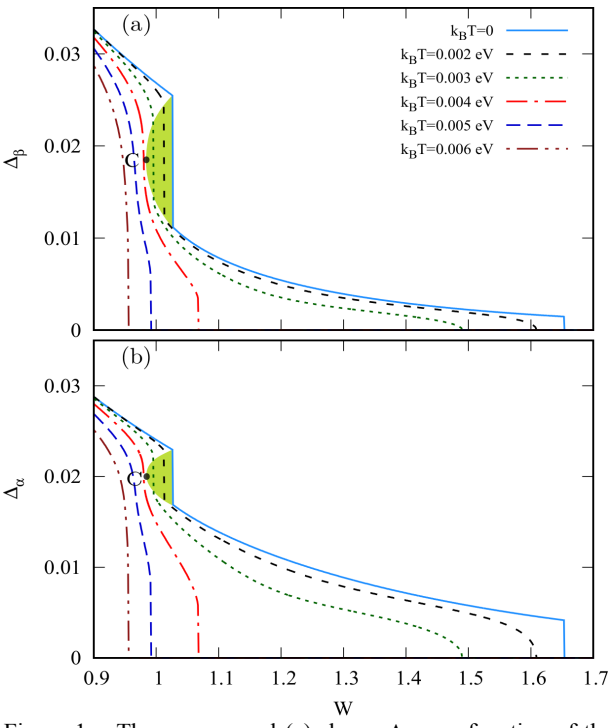

Figure 1. The upper panel (a) shows Δ_β as a function of the band-width W, for various temperatures. The lower panel (b) shows Δ_α for the same range of temperatures and band-widths.

The results presented in this section were calculated with the parameter values U=5,J=0.165, V_α=1/10 and the value of the effective 5f level energy was taken to be E_f=0.3 eV. The occupation number of the 5f bands was chosen as being close to 2.

The gaps Δ_α and Δ_β as a function of the conduction band-width (half-width) W, are shown in **Figure 1** for different temperatures. Note that the increase of W acts in the sense of suppressing the Néel state. Besides that, at low temperatures, for instance $k_B T = 0$, Δ_β exhibits a discontinuity at $W \approx 1.03$. Indeed, near $W = 1.03$, the system of equations has several solutions. The area highlighted by the green color shows the region where there are multiple solutions for Δ_α and Δ_β. The point C indicates the smallest value of W and the highest temperature, for which Δ_α and Δ_β show discontinuous behavior. In the regions where the equations possess multiple solutions (shown in green), the Helmholtz Free-Energy has been used to determine which of the solutions for Δ_α and Δ_β are more stable. The behavior of the gap Δ_α is similar to that of Δ_β, as can be seen in Figure 1(b).

The discontinuity exhibited by Δ_α and Δ_β indicates that a first-order transition occurs between two competing SDW's, here called SDW1 and SDW2. The temperature at the point C is $k_B T \approx 0.004$ eV. For $k_B T >$ 0.004 eV, the gaps Δ_β and Δ_α vary continuously and go to zero at T_N. However, another interesting result is found at very low temperatures and large values of the band-width W. For $k_B T > 0.001$ eV, the phase transition between the SDW2 and the paramagnetic phase is a second-order type of phase transition. However, at $k_B T$ = 0, both Δ_α and Δ_β exhibit a discontinuous behavior indicating another first-order phase transition between the SDW2 and the paramagnetic phase. The replacement of a second-order transition between the SDW2 and the paramagnetic phase at higher temperature by a first-order transition at lower temperatures suggests the presence of a tri-critical point. This tri-critical point has been located at $k_B T \approx 0.001$ eV.

The nature of the phase transition is illustrated by a complementary analysis of the behavior of Δ_α and Δ_β as a function of temperature T. **Figure 2** shows the gaps as a function of T, for several values of the band-widths W. For W=0.90 eV and W=0.95 eV, both Δ_β and Δ_α decreases with the temperature and fall continuously to zero at T_N, which is a feature of a second-order phase transition. It should be noted that these values of W are smaller than the value of the band-width at the point C of figure 1. However, for W=1.00 eV, i.e., for W located in the region where multiple solutions exist (as shown in Figure 1), although the gaps go to zero continuously at T_N, they exhibit a discontinuity at $k_B T \approx 0.0028$ eV. For W=1.025 eV, a similar behavior is observed, however, in this case, the discontinuity occurs at $k_B T \approx 0.0007$ eV. This behavior is a manifestation of a first-order transition between the two competing SDW1 and SDW2. This finding is in accord with the results presented in Figure 1. For W = 1.10 and 1.20 eV, the gaps vanish continuously, as is also the case for W= 0.90 eV and W= 0.95 eV. For W = 1.650 eV the gaps decrease with the temperature and fall discontinuously to zero at T_N. The inset of Figure 2(a) shows, in detail, the discontinuity of Δ_β at $k_B T \approx 0.0008$ eV. A similar discontinuity of Δ_α can be seen in Figure 2(b).

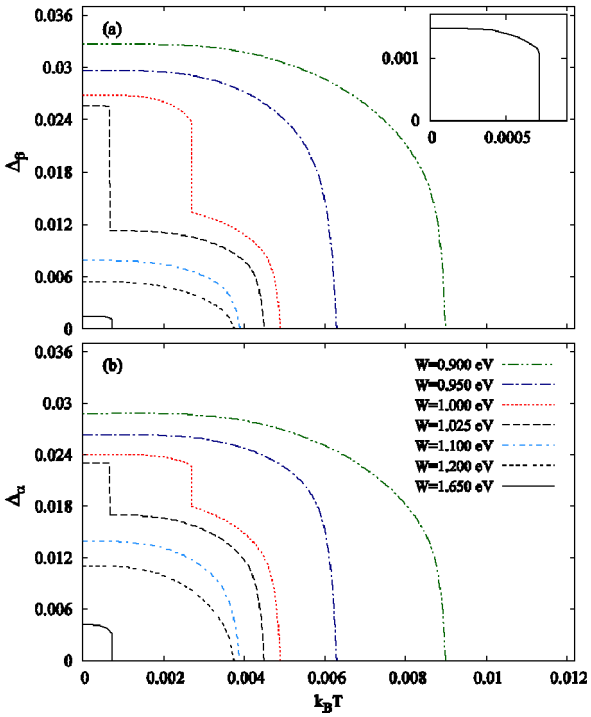

Figure 2. The upper panel (a) shows Δ_β as a function of temperature T, for various band-widths W. The lower panel (b) shows that Δ_α exhibits similar behavior.

4. Conclusions

We have investigated the magnetic phase diagram of the UALM where the 5f bands are almost half-filled as a function of the 5f band-widths. The UALM supports Néel phases in which the ordering in one 5f band induces ordering in the second 5f band. As the 5f band-width increases, we find that the two gaps Δ_α, Δ_β and the induced sub-lattice magnetizations vary continuously but exhibit a distinct jump indicating a first-order transition between the two competing Néel phases. As the band-width increases, the tendency for magnetic order decreases, as is evidenced by a decrease in the Néel temperature, T_N. Initially, the paramagnetic state becomes unstable to the Néel state via a second-order instability at T_N. The decrease in T_N with band-width suggests that the material will have a quantum critical point. However, before the system reaches the quantum critical point, the phase transition changes from second-order to first-order. The change of order of the transition is understood in terms of a slight mismatch between the position of the Fermi-energy and

the energy at which the nesting would be optimal. The change in the order occurs when the energy lowering produced by the reconstruction of the Fermi-surface exceeds the entropy term in the Helmholtz Free-Energy. Since the mean-field approximation is not expected to be applicable in the critical region, defined by the Ginzburg criterion, the effects of commensurate and incommensurate fluctuations requires further investigation.

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