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Finite-temperature properties of the two-orbital Anderson model

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Abstract. The metallic phase of the two-orbital Anderson lattice is studied in the limit of infinite spatial dimensions, where a second-order perturbation treatment is used to solve the single-site problem. Using this approximation, in the Kondo regime, we find that the finite-temperature properties of the conduction electrons exhibit the same behaviour as is observed in the metallic phase of the two-channel Kondo lattice. Possible connections between these two models are discussed.

The normal metallic state of a number of three-dimensional heavy-fermion compounds can be quite well described by the Landau Fermi-liquid theory. At zero temperature (T) the heavy-fermion quasi-particles have an infinite lifetime and a large effective mass. As a consequence of this *coherent* regime the heavy-fermion compounds present at low T a very large electronic specific heat coefficient $\gamma(T) = C(T)/T$ [1]. The physical properties of these materials are related to strongly correlated electrons in 4f/5f orbitals, and the appropriate model Hamiltonian for the description of these properties is the Anderson Hamiltonian [1].

The Fermi-liquid regime in the single-impurity Anderson model can be identified by the behaviour of the f-electron self-energy $\Sigma^f(\omega)$ at low temperatures near of the Fermi level (ε_F). The f-electron self-energy in the single-impurity Anderson model is $\boldsymbol{k}$-independent and respects the Fermi-liquid requirements [2]. Performing a perturbation expansion in the f-electron Coulomb interaction (U) at low T and near ε_F, Yamada showed that Re $\Sigma^f(\omega) \approx -\omega$ and Im $\Sigma^f(\omega) \approx -(\omega^2 + (\pi T)^2)$ [3]. For the lattice case and in the infinite-dimensional limit, where $\Sigma^f(\omega)$ is also $\boldsymbol{k}$-independent [4, 5], it was shown by Georges *et al* [6] that the metallic phase of the periodic (one-orbital) Anderson model can be a Fermi liquid. The behaviours of the real and imaginary parts of $\Sigma^f(\omega)$ for $d = \infty$ were studied by Schweitzer and Czycholl [7] by means of a self-consistent second-order perturbation in U. In this case the imaginary part of $\Sigma^f(\omega)$ vanishes near ε_F in accordance with the Luttinger theorem, and the real part has a negative slope in the same region.

The investigations presented above were carried out only for one-channel versions of the Anderson Hamiltonian. The multichannel one-impurity Anderson model, where a localized f electron hybridizes with several conduction bands (orbitals), was studied in the large-U limit [8, 9]. In this limit the model shows non-Fermi-liquid behaviour. A non-Fermi-liquid behaviour is also present in the multichannel Kondo-impurity problem. This problem was introduced by Nozières and Blandin [10], and the exact solution was obtained by Andrei and Destri [11] and Tsvelick and Wiegmann [12] in terms of the Bethe *ansatz*. The non-Fermi-liquid behaviour in the multichannel Kondo-impurity model comes from the overcompensation

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of the Kondo spins by the conduction electrons [13]. The overcompensation mechanism was also used to explain the non-Fermi-liquid behaviour in the two-channel Kondo (tCK) lattice [14, 15] and the two-channel Anderson (tCA) lattice [16] in the Kondo limit.

A conclusion regarding the non-Fermi-liquid regime in the tCK lattice was reached by Jarrell *et al* [14] looking at the one-particle properties of the conduction electrons. In this case, the real part of the self-energy of the conduction electrons $\Sigma^c(\omega)$ presents a positive slope near the Fermi energy. The imaginary part of $\Sigma^c(\omega)$, instead of going to zero in a quadratic way as in Fermi-liquid systems, goes away from zero as $\omega, T \to 0$. Despite these properties, the system is metallic and the single-particle density of states (DOS) of the conduction electrons has a finite value at the Fermi level. This metallic regime (*incoherent metal*) was used to explain the physical properties of a number of heavy-fermion compounds where the Fermi-liquid paradigm cannot be applied [14, 18]. For example, the incoherent-metal regime has been used to explain the unusual resistivity of UBe_{13} [16].

In addition, in reference [14] the tCK model was studied by means of quantum Monte Carlo (QMC) simulation in the limit of high dimensions. It is well known that the QMC method provides very accurate results at intermediate and high temperatures. However, it does not provide any information about the explicit form of the self-energy of the problem. For example, in the work of Jarrell *et al* [14] the single-particle self-energy was obtained by inverting the relation $G^c(\omega) = D(\omega - \Sigma^c(\omega))$ [17] for different temperatures. It must be noted that the non-analytic form of $\Sigma^c(\omega)$ was postulated from these numerical results. Thus, in order to understand the origin of the incoherent-metal regime in the tCK lattice, it is important to find a model which describes these novel properties and allows us to obtain an explicit form for $\Sigma^c(\omega)$. Here, we address precisely this problem: the study of a multi-orbital model which correctly takes into account the incoherent behaviour of the tCK lattice and provides an explicit form for the self-energy of the conduction electrons of each orbital.

In this article we study a multi-orbital Anderson-lattice (mOA) model in the high-dimension ($d = \infty$) limit. We discuss the formal exact solution of this multi-orbital Hamiltonian as well as the finite-temperature properties of the two-orbital version of this problem. In this case a second-order perturbation treatment is applied to solve the impurity problem in the presence of U. As we have mentioned before, we find that the conduction electrons show the same behaviour as those obtained by Jarrell *et al* [14] for the tCK lattice.

The mOA model consists of the usual f-electron Hamiltonian of the periodic Anderson-lattice model, m identical orbitals of non-interacting conduction electrons and local hybridization between f and conduction electrons. The complete Hamiltonian can be written as

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle ij\rangle\sigma\alpha} c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} + E \sum_{i\sigma} n^f_{i\sigma} + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow} + \sum_{i\sigma\alpha} V_{\alpha\sigma}(c^\dagger_{i\alpha\sigma} f_{i\sigma} + f^\dagger_{i\sigma} c_{i\alpha\sigma}) \qquad (1)$$

where $c^\dagger_{i\alpha\sigma}$ ($c_{i\alpha\sigma}$) creates (destroys) a conduction electron on site i and orbital $\alpha = 1, 2, \ldots, m$ of spin σ, and $f^\dagger_{i\sigma}$ ($f_{i\sigma}$) creates (destroys) a localized f electron on site i of spin σ. The sites i form an infinite-dimensional hypercubic lattice and the hopping is limited to the nearest neighbours. The scaled hopping integral $t^* = 1$ determines the energy unit. The hybridization term $V_{\alpha\sigma}$ is site independent, but it can have different values for different orbitals or spin directions.

To obtain the formal exact solution of the mOA model it is convenient to define a new set of conduction electron operators: $\{a^\dagger_{i1\sigma}, a^\dagger_{i2\sigma}, \ldots, a^\dagger_{im\sigma}\}$. In this case,

$$a^\dagger_{i1\sigma} \equiv (1/\bar{V}_\sigma) \sum_\alpha V_{\alpha\sigma} c^\dagger_{i\alpha\sigma}$$

and the remaining $a^\dagger_{i\alpha\sigma}$-operators are written in such a way as to preserve the definition of $a^\dagger_{i1\sigma}$

and the fermion commutation relations. The normalization factor is

$$\bar{V}_\sigma = \sqrt{\sum_\alpha V_{\alpha\sigma}^2}.$$

In the new representation the mOA Hamiltonian (equation (1)) is written as

$$H = -\frac{t^*}{2\sqrt{d}} \sum_{\langle ij\rangle\sigma\alpha} a_{i\alpha\sigma}^\dagger a_{j\alpha\sigma} + E\sum_{i\sigma} n_{i\sigma}^f + U\sum_i n_{i\uparrow}^f n_{i\downarrow}^f + \sum_{i\sigma} \bar{V}_\sigma (a_{i1\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger a_{i1\sigma}). \tag{2}$$

It is clear from equation (2) that the multi-orbital problem for the f electrons is reduced to a one-orbital problem with a renormalized hybridization $\bar{V}_\sigma$. As the local approximation for the Anderson (one-orbital) lattice is exact in the limit of infinite dimensions [5, 19], the formal exact solution for the f-electron one-particle Green's function for $d \to \infty$ is given by [5]

$$G_{\boldsymbol{k}\sigma}^f(\mathrm{i}\omega_n)^{-1} = \mathrm{i}\omega_n - \Sigma_\sigma^f(\mathrm{i}\omega_n) - \frac{\bar{V}_\sigma^2}{\mathrm{i}\omega_n - \epsilon_{\boldsymbol{k}}}. \tag{3}$$

As we intend in this work to clarify the physical origin of the incoherent properties of the tCK model, the conduction electron Green's function of each particular orbital must be known. In the context of the mapped Hamiltonian (equation (2)), the α-orbital Green's function $G_{ij\sigma}^{\alpha c}(\tau) \equiv -\langle \hat{T} c_{i\alpha\sigma}(\tau) c_{j\alpha\sigma}^\dagger(0)\rangle$ is obtained when the $c_{i\alpha\sigma}$-operators are written in terms of the $a_{i\alpha\sigma}$-operators, and it is straightforward to show that

$$G_{ii\sigma}^{\alpha c}(\mathrm{i}\omega_n) = \left(1 - \frac{V_{\alpha\sigma}^2}{\bar{V}_\sigma^2}\right) D(\mathrm{i}\omega_n) + \frac{V_{\alpha\sigma}^2}{\bar{V}_\sigma^2} D(\mathrm{i}\omega_n - \bar{V}_\sigma^2 \mathcal{G}_\sigma) \tag{4}$$

where $\mathcal{G}_\sigma(\mathrm{i}\omega_n)^{-1} \equiv \mathrm{i}\omega_n - \Sigma_\sigma^f(\mathrm{i}\omega_n)$ and $D(z)$ is the Hilbert transform of the uncorrelated density of states of the conduction band $\rho_0(\epsilon)$ [17]. For a hypercubic lattice for $d = \infty$, $\rho_0(\epsilon) = (1/\sqrt{\pi})\exp(-\epsilon^2)$.

The two terms of equation (4) can be easily understood from the transformation discussed above. The first term of the right-hand side of this equation describes the contributions of the $m - 1$ free orbitals and the second term is related to the one-orbital Anderson problem of equation (2). It is important to notice that the formal exact solution of the mOA model (equations (3) and (4)) is completely general as regards the number of orbitals as well as the values of the hybridization on different orbitals.

In principle, it is possible to assume that the *scattering processes* in each orbital can be described by means of a self-energy [14, 19]. By definition, the α-orbital Green's function can be written in terms of the self-energy of the conduction electrons $\Sigma_{\boldsymbol{k}\sigma}^{\alpha c}(\mathrm{i}\omega_n)$ as

$$G_{\boldsymbol{k}\sigma}^{\alpha c}(\mathrm{i}\omega_n)^{-1} \equiv \mathrm{i}\omega_n - \epsilon_{\boldsymbol{k}} - \Sigma_{\boldsymbol{k}\sigma}^{\alpha c}(\mathrm{i}\omega_n). \tag{5}$$

In order to recover equation (4) by summing equation (5) over the momentum, the self-energy of the α-orbital conduction electrons must be given by

$$\Sigma_{\boldsymbol{k}\sigma}^{\alpha c}(\mathrm{i}\omega_n) = V_{\alpha\sigma}^2 \mathcal{G}_\sigma(\mathrm{i}\omega_n)\left\{1 + \frac{(\bar{V}_\sigma^2 - V_{\alpha\sigma}^2)\mathcal{G}_\sigma(\mathrm{i}\omega_n)}{\mathrm{i}\omega_n - (\bar{V}_\sigma^2 - V_{\alpha\sigma}^2)\mathcal{G}_\sigma(\mathrm{i}\omega_n) - \epsilon_{\boldsymbol{k}}}\right\}. \tag{6}$$

The requirement that in the $d \to \infty$ limit the local interactions give rise to a $\boldsymbol{k}$-independent self-energy for the f electrons is satisfied for the mOA lattice (see equation (3)). However, a $\boldsymbol{k}$-dependent self-energy for the α-orbital conduction electrons is obtained.

The first term of $\Sigma_{\boldsymbol{k}\sigma}^{\alpha c}(\mathrm{i}\omega_n)$, $V_{\alpha\sigma}^2 \mathcal{G}_\sigma(\mathrm{i}\omega_n)$, is the self-energy of the one-orbital Anderson lattice. This term is completely local and describes the scattering processes in the α-orbital. The second term is relevant only for multi-orbital systems, where $\bar{V}_\sigma^2 \neq V_{\alpha\sigma}^2$. As $\bar{V}_\sigma^2 - V_{\alpha\sigma}^2$ is related to all other orbitals different from α, the $\boldsymbol{k}$-dependent term can be considered as

an *effective correction* to the one-orbital self-energy. This effective correction describes the scattering process that occurs in the remaining orbitals.

Different methods can be used to solve the single-site problem in the $d = \infty$ limit [5, 20]. One of these methods is that of the iterative perturbation theory (IPT) [21]. The IPT proves to be a good approximation for describing the Fermi-liquid properties of the Hubbard model [22]. For the particular case of the periodic Anderson model, the IPT results are in good agreement with exact-diagonalization [5] and QMC findings [23]. The IPT method is normally applied for values of $U/t^* < 3$; however, it has the property of correctly taking into account the limit $V \to 0$ [5]. This allows us to study the one-particle properties of the mOA lattice near the Kondo limit.

Let us now turn our attention to the spectral properties of the conduction electrons of the two-orbital Anderson (tOA) model. The one-particle properties of f electrons will not be considered here because they are well known from studies of the periodic Anderson model [5, 7, 23]. In our study we have chosen $U = 2.0$ and $V = 0.3535$. Note that $V = 0.3535$ for $m = 2$ means that $\bar{V} = 0.5$.

In figure 1(a) we display the single-particle density of states (DOS) for the conduction electrons in the tOA model. The DOS has a finite value at the Fermi level for all temperatures. Such metallic behaviour is related to charge fluctuations and to the contribution of the non-hybridized electrons. The $\boldsymbol{k}$-independent real and imaginary parts of the conduction electron self-energy $\Sigma^c(\omega) \equiv V^2\mathcal{G}(\omega)$ (see equation (6)) are plotted in figures 1(b) and 1(c), respectively. As one can see in figure 1(b), the real part of the self-energy exhibits a positive slope near the Fermi level and this slope decreases with increasing temperature. It is well known that for a Fermi-liquid system the slope of Re $\Sigma^c(\omega)$ must be negative. Therefore, as was pointed out in reference [14], the positive slope observed in figure 1(b) describes the

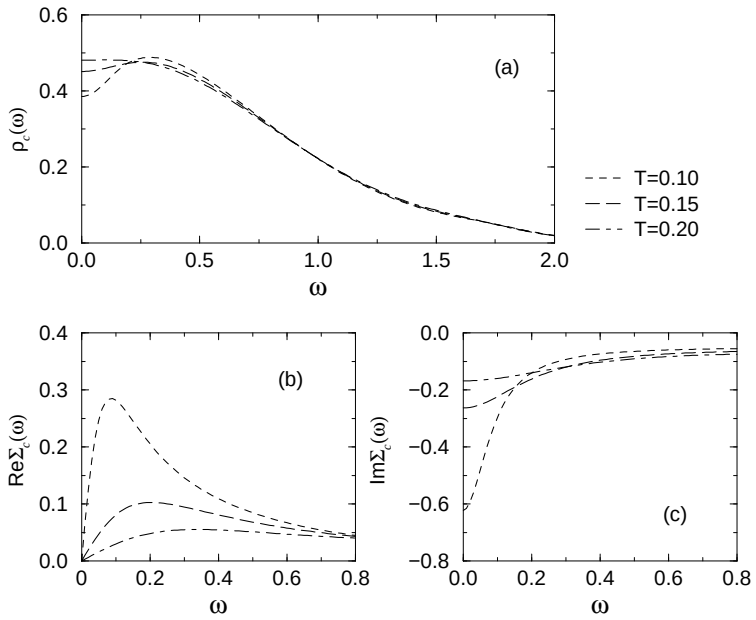

Figure 1. One-particle properties of the conduction electrons for $m = 2$, $V = 0.3535$, $U = 2.0$ and three different temperatures: (a) the density of states; and the (b) real and (c) imaginary parts of the self-energy.

breakdown of the quasiparticle concept. Non-Fermi-liquid properties can be also observed in the imaginary part of the self-energy (see figure 1(c)). From this figure it is clear that Im $\Sigma^c(\omega)$ does not approach the Fermi-liquid form Im $\Sigma(\omega) \approx -(T^2 + \omega^2)$ as $\omega, T \to 0$. Note that a behaviour similar to that presented in figure 1 has been observed in the one-particle properties of the conduction electrons of the tCK lattice [14].

It is worth noticing that the incoherent properties shown in figures 1(b) and 1(c) are closely related to the definition of $\Sigma^c(\omega)$. Concerning this point, we follow the idea of Jarrell *et al* [14] where the self-energy is defined in such a way as to account for the Hilbert transform of the Green's function of the conduction electrons in each channel. It is well known that $\Sigma^f(\omega)$ (see equation (3)) shows Fermi-liquid behaviour at low temperatures near to the Fermi level [7]. From equation (6) one can easily conclude that the Fermi-liquid properties of the f electrons imply incoherent properties for the conduction electrons of the periodic Anderson model as well as the mOA model. Hence, to decide whether a model of two or more different particles is in a coherent regime or not, it is important to consider the behaviour of all particles.

In figure 2 we compare the DOS for the conduction electrons of the tOA model with those of the periodic Anderson model. In this figure we consider two different values of the hybridization: $V = 0.3535$ ($m = 2$) and $V = 0.5$ ($m = 1$), such that the correlation effects are taken into account at the same level for both systems. This allows us to study the effect of the non-hybridized particles in the two-orbital system. For $T = 0.20$ the contribution of these particles completely suppresses the hybridization gap, and a flat region in the DOS for $m = 2$ is observed near the Fermi level. Despite the differences in the Hamiltonian parameters and the methods used to solve the impurity problem, similar flat behaviours have been reported in reference [14] for the tCK model.

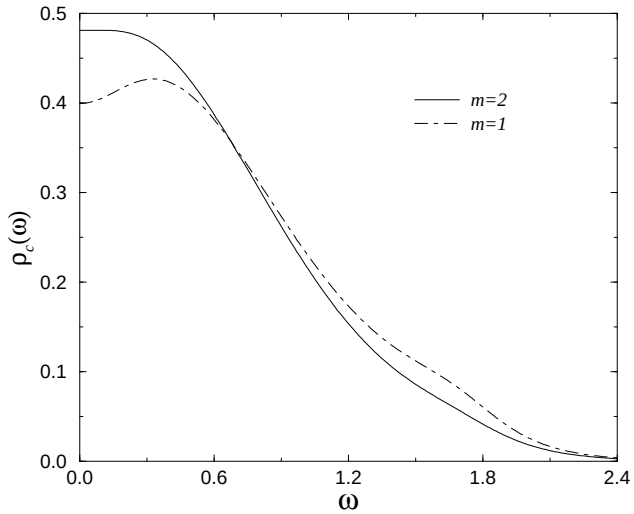

Figure 2. The DOS of the conduction electrons at $T = 0.20$ for $m = 2$ (solid line) and $m = 1$ (dot–dashed line).

Let us now proceed to explain the similarities between our results and those from the tCK model [14]. In the Kondo limit, the mOA model (equation (1)) is mapped onto a multi-orbital Kondo (mOK) model. In order to prove this result, one can apply the resolvent perturbation theory [24] in the subspace defined by the $a_{i1\sigma}$- and f-operators; see equation (2). If the

hybridization is the same for both spin directions, the mOK Hamiltonian is written as

$$H_{\rm Kondo} = -\frac{t^*}{2\sqrt{d}} \sum_{\langle ij\rangle\sigma\alpha} c^{\dagger}_{i\alpha\sigma} c_{j\alpha\sigma} + k \sum_{i\alpha} V^2_{\alpha} \boldsymbol{S}_i \cdot \boldsymbol{s}_{i\alpha} + k \sum_{i\alpha\neq\alpha'} V_{\alpha} V_{\alpha'} [S^z_i (c^{\dagger}_{i\alpha\uparrow} c_{i\alpha'\uparrow} - c^{\dagger}_{i\alpha\downarrow} c_{i\alpha'\downarrow}) + S^+_i c^{\dagger}_{i\alpha\downarrow} c_{i\alpha'\uparrow} + S^-_i c^{\dagger}_{i\alpha\uparrow} c_{i\alpha'\downarrow}] \qquad (7)$$

where $k \equiv U/(|E|(|E| + U))$ [1] and $\boldsymbol{S}_i$, $\boldsymbol{s}_{i\alpha}$ are the Kondo and the α-orbital conduction electron spin operators, respectively. Note that equation (7) is precisely the Schrieffer–Wolf transformation [25] of equation (1).

The first two terms on the right-hand side of equation (7) can be considered as the simplest generalization of the *one-* and *two-channel* Kondo models into a multichannel one. The remaining terms are related to non-diagonal processes of exchange between the impurity and the conduction electrons in the different orbitals. The relevant contributions of these non-diagonal processes will appear only in fourth order in the hybridization term; see equation (6). It is clear that the fourth-order contributions act only as small corrections in the Kondo limit, $(kV_{\alpha}V_{\alpha'})^2 \ll 1$. This explains the agreement between our results and those from the tCK model.

Summarizing, the simplest extension of the periodic Anderson model into a multi-orbital Anderson (mOA) model is introduced for the first time in this article. The model is studied in the limit of high dimensions, where a second-order perturbation treatment (IPT) is used to solve the impurity problem. Using this approximation at finite temperatures, we find that the single-particle properties of the conduction electrons in the Kondo regime for the two-orbital Anderson model are the same as those for the two-channel Kondo lattice. We have explained this agreement in terms of the irrelevance of the non-diagonal exchange processes in the Kondo limit. Finally, we wish to point out the importance of our results, since they open up a new possibility for studying the mCK problem in the limit of high dimensions.

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