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Griffiths phase of the Kondo insulator fixed point

E. Miranda[a,*], V. Dobrosavljević[b]

[a]*Instituto de Física 'Gleb Wataghin', DFESCM, Unicamp, C.P. 6165, Campinas, SP, 13083-970, Brazil*
[b]*Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306, USA*

Abstract

Heavy-fermion compounds have long been identified as systems which are extremely sensitive to the presence of impurities and other imperfections. In recent years, both experimental and theoretical work has demonstrated that such disorder can lead to unusual, non-Fermi liquid behavior for most physical quantities. In this paper, we show that this anomalous sensitivity to disorder, as well as the resulting Griffiths-phase behavior, directly follow from the proximity of metallic heavy-fermion systems to the Kondo insulator fixed point.

Keywords: Heavy-fermion systems; Non-Fermi liquid; Disordered systems; Anderson localization

Much of the recent interest in strongly correlated electronic systems, such as heavy-fermion compounds, has been sparked by a gamut of unusual properties found in experiments. Most notably, many such materials display unusual, non-Fermi liquid (NFL) behavior which is often consistently observed in both the thermodynamic and transport measurements. While the precise origin of these anomalies remains a highly controversial issue, both the experimental and the theoretical advances have provided convincing evidence[1] that disorder may be at the origin of such behavior, at least for certain classes of materials. The purpose of this paper is to clarify the *physical content* behind one of the proposed mechanisms for such disorder-driven NFL behavior.

Based on an initial success in explaining the anomalous behavior of $UCu_{5-x}Pd_x$ by means of the so-called Kondo disorder model (KDM) [2–8], we have recently extended the analysis to describe Anderson localization effects in a strongly correlated environment [9,10]. It is our intention to show here how the emergence of NFL properties can be described in terms of a quantum Griffiths phase induced by Anderson localization effects. Furthermore, the onset of anomalous behavior occurs already at relatively weak disorder, an effect we ascribe to the *proximity to the Kondo insulator fixed point*. In a clean compound, unitary Kondo scatterers act coherently to create a hybridization gap and the state is the familiar Kondo insulator. A small deviation from unitarity leads to the formation of heavy-fermionic quasi-particles. In a disordered system, however, large spatial fluctuations induce the appearance of random unitary scatterers or 'Kondo insulator droplets' which are responsible for a strong *renormalized effective disorder*. These droplets, in turn, are regions of depleted density of states (DOS) which fail to quench nearby localized moments. The latter ultimately lead to the NFL behavior.

Heavy-fermion non-Fermi liquids are characterized by logarithmic or weak power-law divergence of the magnetic susceptibility $\chi(T)$ and the specific heat coefficient $\gamma(T) = C_V(T)/T$ and a resistivity that behaves as $\rho(T) = \rho_o + AT^{\alpha}$, with $\alpha < 2$. Deviations from normal Fermi-liquid behavior have also been observed in optical conductivity [11,12], magneto-resistance [13], dynamic magnetic susceptibility [14], NMR and μSR [2–5] measurements.

Several mechanisms have recently been proposed to account for such anomalous behavior. One of them is provided by the proximity to an ordering transition at zero temperature, a quantum critical point (QCP) [15–17], where critical modes mediate unscreened long-range interactions between carriers. Indeed, magnetic ordering is fairly common in heavy-fermion physics and in many of the cleaner compounds a strong case can be

* Corresponding author. Fax: + 55-19-289-3137.
E-mail address: emiranda@ifi.unicamp.br (E. Miranda).

[1] For an overview, see Ref. [1].

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made in favor of a QCP interpretation [18–22]. However, our current treatment of QCP's has not produced a unified picture able to account for all the observed behavior of these systems [23].

Another possible route relies on the local dynamical frustration of exotic impurity models, where the local moment cannot decide with which conduction electron channel it will Kondo bind [24,25]. Although a complete understanding of the single impurity case is available, there remains the question of the relevance of inter-site correlations [26,27]. This is important because most of the studied systems are *not* in the dilute limit [28].

More recently, the idea that NFL behavior can occur due to the presence of disorder in a strongly correlated environment has been proposed. The pioneering work relied heavily on the Cu NMR linewidths of $UCu_{5-x}Pd_x$ and its temperature dependence [2–5]. The KDM, a phenomenological model of a system with a broad distribution of Kondo temperatures T_K, was then proposed to account for the data. The presence of a wide range of energy scales led to a picture where different spins were quenched at widely different temperatures. Thus, the singular behavior could be attributed to a few rare spins which remained unquenched (and therefore, highly polarizable) at the lowest temperatures. These ideas were put on a firmer foundation by means of a dynamical mean field theory (DMFT) [29] treatment of strong correlations and disorder, where the KDM found its natural setting [6–8]. The KDM had considerable success in describing a whole series of experiments, including thermodynamic responses [2–8], neutron scattering [6–8,14], optical conductivity [11,12] and magneto-resistance [13]. More recently, we have introduced a microscopic model which incorporates Anderson localization effects [9,10], a feature absent from the KDM. We will discuss some of these recent results below.

Alternatively, it has been proposed that the physics of these compounds is intimately tied to disorder effects in the proximity to magnetic ordering [30–32]. The effect of spatial inhomogeneities together with the tendency of the Kondo effect to destroy magnetic order would then lead to the formation of large clusters of magnetically ordered material close to the phase boundary but still within the disordered phase. Similarly, these large ordered clusters would be responsible for the NFL behavior.

In all proposed disorder-based mechanisms, the low-temperature anomalies result from a broad distribution of local energy scales in the system. In addition, these energy scales are viewed as the appropriate Kondo temperatures describing either individual spins or clusters of spins embedded in a metal. In all the theories, these Kondo temperatures assume a strong, exponential dependence on the parameters describing the fluctuator in question, hence their broad distribution even for moderate disorder. In the simplest KDM, the emergence of low T_K sites is a result of the randomness in the immediate environment of a given spin. In the 'spin cluster' picture, the 'cluster Kondo temperature' is exponentially dependent on the cluster size, a quantity which can be expected to be large close to any magnetic quantum critical point. Finally, in a very recent work, the depression of T_K was proposed to be a result of Anderson localization effects, which lead to a reduction of the local density of conduction electron states required for Kondo screening.

From a general point of view, all three proposed scenarios may be relevant and can be expected to contribute. A more immediate question is the relative practical significance of these processes and their general robustness with respect to different material characteristics. In this respect, recent experiments have provided evidence that the local disorder inherent to the KDM picture may not be sufficient to account for the observed anomalies [33,34]. Similarly, the emergence of large magnetically ordered clusters can be anticipated only in the very close vicinity of magnetic transitions. More importantly, it is difficult to imagine how the cluster picture could even come close to providing enough residual entropy to account for the observed specific heat anomalies in the physical temperature range.

In contrast, we will show that the localization-based scenario provides a very robust and quantitatively relevant mechanism for the NFL behavior. Since the corresponding fluctuations must be present in any moderately disordered system, this route should be of direct relevance to most disordered heavy-fermion compounds, irrespective of the proximity to any magnetic ordering. Our key point is that the corresponding Griffiths phase is a direct consequence of the proximity not to any magnetic, but rather to the Kondo insulator fixed point. The deviation from the Kondo insulator provides an energy scale which is universally small for any heavy-fermion metal, since it is defined by the underlying Kondo energy. This observation also provides a simple explanation for the notorious sensitivity of HF systems to disorder, a feature which we believe is at the origin of all the observed anomalies.

We start from a disordered infinite-U Anderson lattice Hamiltonian

$$H = \sum_{ij\sigma} (-t_{ij} + \varepsilon_i \delta_{ij}) c^\dagger_{i\sigma} c_{j\sigma} + \sum_{j\sigma} E_f f^\dagger_{j\sigma} f_{j\sigma} + \sum_{j\sigma} V_j (c^\dagger_{j\sigma} f_{j\sigma} + \text{h.c.}), \quad (1)$$

where $c_{i\sigma}$ destroys a conduction electron at site i and spin σ from a broad uncorrelated band with hopping t_{ij} and $f_{j\sigma}$ destroys an f-electron at site j with spin σ. Since $U \to \infty$, the constraint $n^f_j = \sum_\sigma f^\dagger_{j\sigma} f_{j\sigma} \leqslant 1$ is assumed.

Typically, alloying introduces substitutions either in the f-shell sub-lattice ('Kondo holes'), e.g. $U_{1-x}Y_xPd_3$, or the non-f-shell subsystem ('Ligand disorder'), e.g. $UCu_{5-x}Pd_x$. It is reasonable to assume that the former

case should be modeled by a distribution of E_{fj}, whereas the latter is expected to introduce randomness both in V_j and ε_j. Most of our results remain unchanged irrespective of the kind of disorder.

We work within the framework of the recently introduced statistical dynamical mean field theory (SDMFT) [35,36]. It is a natural generalization of the DMFT, which retains the latter's treatment of local correlations while going beyond it by incorporating Anderson localization effects. It is most easily implemented on a Bethe lattice of coordination z (we have used $z = 3$ in our simulations). Each lattice site j defines an effective local action for the f-orbital which should be thought of as resulting from integrating out all the other electronic degrees of freedom. It is written as $(U \to \infty)$ [9]

$$S_{\text{eff}}^{(j)} = \int_0^\beta d\tau \sum_\sigma f_{j,\sigma}^\dagger(\tau)(\partial_\tau + E_{fj}) f_{j,\sigma}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma f_{j,\sigma}^\dagger(\tau)\Delta_j(\tau - \tau') f_{j,\sigma}(\tau'), \quad (2)$$

$$\Delta_j(\omega) = \frac{V_j^2}{\omega - \varepsilon_j - \sum_{k=1}^{z-1} t_{jk}^2 G_{ck}^{(j)}(\omega)}. \quad (3)$$

Here, $G_{ck}^{(j)}(\omega)$ is the local c-electron Green's function on the nearest-neighbor site k with site j removed; in other words, a 'cavity' has been created where there once was site j. Note how, as in the DMFT [29], we neglect higher-order Green's functions in the process. $G_{ck}^{(j)}(\omega)$, on the other hand, is determined recursively by relating it to a similar quantity on the next nearest-neighbor site l

$$G_{ck}^{(j)(-1)}(\omega) = \omega - \varepsilon_k - \sum_{l=1}^{z-1} t_{kl}^2 G_{cl}^{(k)}(\omega) - \Phi_k(\omega), \quad (4)$$

$$\Phi_k(\omega) = \frac{V_k^2}{\omega - E_{fk} - \Sigma_{fk}(\omega)}. \quad (5)$$

Finally, the self-consistency loop is closed by requiring that the *local* self-energy $\Sigma_{fk}(\omega)$ be obtained from the solution of the effective action $S_{\text{eff}}^{(k)}$ (see Eq. (2), Refs. [35,36,9]). We note that the self-consistent set of stochastic equations (2)–(5) reduces to the DMFT when the limit $z \to \infty$ is taken (with the appropriate rescaling $t_{ij} \sim t/\sqrt{z}$), in which case the disorder is treated on the CPA level and, therefore, shows no localization effects [37–39]. This was a severe limitation of the previous treatment [6–8] which is here remedied. On the other hand, the non-interacting limit ($U = 0$) reduces to the self-consistent theory of localization of Abou-Chacra et al. [40], which is known to exhibit an Anderson metal–insulator transition (MIT) for $z \geqslant 3$.

We would like to stress that the hybridization function equation (3) 'seen' by each f-orbital has strong spatial fluctuations, reflecting the disorder inside a correlation volume enclosing several lattice sites in its neighborhood. The spectral information is carried by the extended conduction electron wave function, which acts to correlate the different Anderson impurity problems defined by Eq. (2) (see Fig. 1). This leads to a distribution of Kondo temperatures. On the other hand, the effect of this *ensemble* of single-impurity problems is to create a renormalized effective disorder 'seen' by the conduction electrons (cf. Eqs. (4) and (5)). The net effect on the relevant distribution functions of this *highly non-local* self-consistency turns out to be robust and universal.

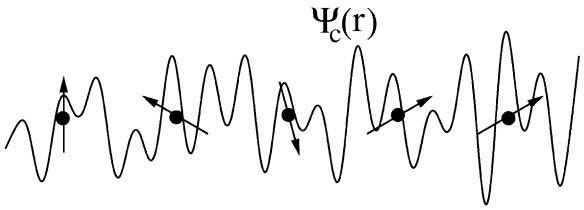

Fig. 1. The conduction electron wave function $\Psi_c(\vec{r})$ has strong amplitude fluctuations due to disorder and correlate several local moments within a correlation length's distance.

The stochastic equations (2)–(5) were solved by standard sampling techniques [40] and provided us with the statistical distributions of the most important physical quantities. The single-impurity problem of Eqs. (2) and (3) was solved in the large-N mean-field approximation at $T = 0$ [41–43], which has the desirable feature of correctly reproducing the exponential form of the Kondo temperature. We have made sure the statistics and numerical procedures were accurate enough to obtain Kondo temperatures spanning many orders of magnitude (~ 15) in order to probe the long tails of the distribution functions.

One of our main results is the identification of a NFL region at relatively weak disorder [10]. This is triggered by the appearance of a fraction of localized moments with very low T_K's, as can be seen in Fig. 2. Indeed, the T_K distribution exhibits *power-law* behavior as $T_K \to 0$

$$P(T_K) \sim T_K^{(\alpha-1)}, \quad (6)$$

where the exponent α varies continuously with the amount of disorder (see the inset of Fig. 2). This can be shown to lead to singular thermodynamic responses

$$\chi(T) \sim \gamma(T) \sim \frac{1}{T^{(1-\alpha)}}, \quad (7)$$

as has been observed in several heavy-fermion alloys [44]. The 'marginal' case $\alpha = 1$ leads to a logarithmic divergence of the same quantities. The occurrence of such NFL behavior in a system with a wide distribution of T_K's had been proposed in the context of the KDM [6–8]. However, in the KDM the presence of these spins could only be obtained through a finely tuned choice of the bare disorder distribution. By contrast, in our current

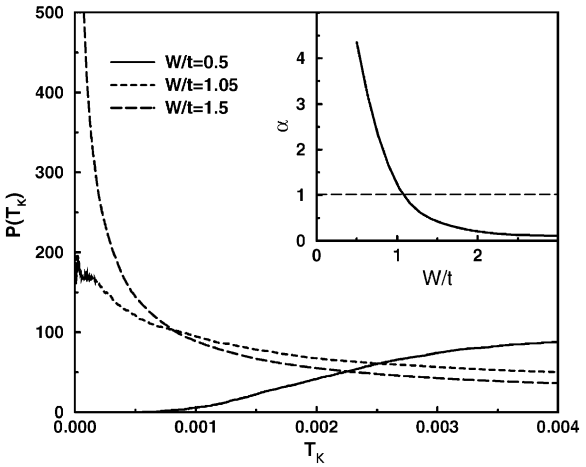

Fig. 2. Distribution of T_K showing the emergence of NFL behavior. Here, ε_i's are distributed uniformly with width W and we have used $z = 3$, $E_f = -1$, $V = 0.5$ and $\mu = -0.1$. Inset: the exponent α of Eq. (6). The dashed line indicates the marginal case $\alpha = 1$.

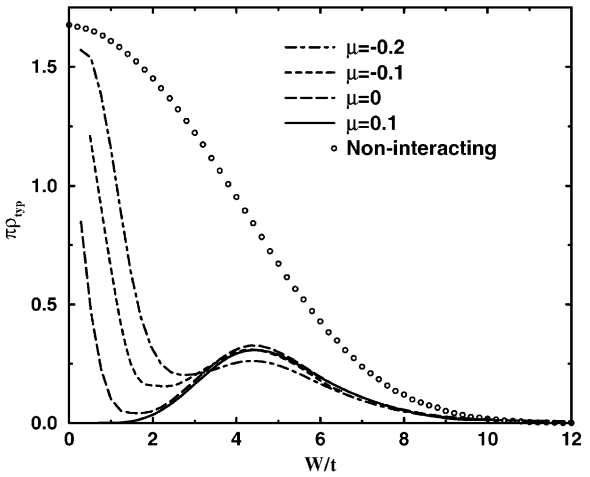

Fig. 3. Localization properties of the conduction electrons as monitored by their typical DOS as a function of disorder, for several values of the chemical potential μ. The other parameters are the same as in Fig. 2. $\mu = 0.1$ corresponds to a Kondo insulator in the clean case. While the non-interacting case is monotonically decreasing, the interaction-induced renormalized disorder leads to a dip for small values of W/t. We attribute this dip to the proximity to the Kondo insulator fixed point.

treatment this behavior is an unavoidable consequence of the spatial fluctuations of the conduction electron wave function amplitude. Due to the extended nature of this wave function and the consequent correlation between T_K values on different sites (Fig. 1) we should expect a high degree of robustness and universality in these distributions. This is indeed what we have found for different types of disorder distributions. We also note that the case depicted in Fig. 2 corresponds to conduction band disorder *only*, for which the KDM would predict *no* T_K fluctuations.

Diverging thermodynamic responses with disorder-dependent exponents due to rare regions with very low T_K's are characteristic of Griffiths phases [45]. Since Anderson localization effects are the driving mechanism here, we associate this Griffiths phase to the proximity to a disorder-driven metal–insulator transition (MIT). This can be checked through an examination of the typical density of states (DOS) of the conduction electrons $\rho_{typ} = \exp\{\langle \ln \rho_j \rangle\}$; $\rho_j = (1/\pi)\,\mathrm{Im}\, G_{cj}(\omega = 0)$, a quantity known to vanish at the MIT. We show our results in Fig. 3. The Griffiths phase is observed for relatively small amounts of disorder ($W/t \approx 1$), whereas the MIT occurs at much higher values ($W/t \approx 12$). Surprisingly, however, the typical DOS is a *non-monotonic* function of the disorder strength (for $-0.2 \lesssim \mu \lesssim 0.3$), in sharp contrast to the non-interacting case (Fig. 3).

In order to gain more insight into this rather non-intuitive behavior, we look at the effective renormalized disorder 'seen' by the conduction electrons. It is clear from Eq. (4) that, in addition to the bare disorder in the ε_k's, scattering from the strongly correlated f-sites adds an *effective* disorder described by the quantity $\Phi_k(\omega)$ of

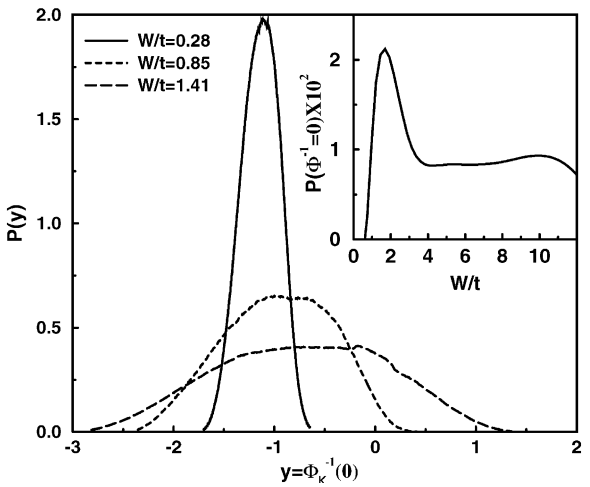

Fig. 4. Distribution of $\Phi_k^{-1}(0)$ as a function of disorder. The inset shows the concentration of unitary scatterers ($\Phi_k^{-1}(0) = 0$). Same parameters as in Fig. 2, but with $\mu = 0$.

Eq. (5). In particular, unitary scattering ($\delta = \pi/2$) corresponds to $\Phi(0) \to \infty$. A diverging $\Phi(0)$ in the clean case leads to the formation of a hybridization gap and Kondo insulating behavior. It is precisely the appearance of the first unitary scatterers (USCs) once disorder is introduced which is responsible for the sharp drop in ρ_{typ} seen in Fig. 3. This can be clearly seen from the distribution of $\Phi_k^{-1}(0)$ as a function of disorder in Fig. 4.

Therefore, the following picture emerges from our results. The clean system has a small energy scale, the

Kondo temperature T_K, which sets the distance from the Kondo resonance to the Fermi energy. When disorder is introduced, the positions of the Kondo resonances start to fluctuate and a distribution of $\Phi_k(0)$ ensues, giving rise to a renormalized effective disorder. The latter initially broadens monotonically and USCs are quickly formed, having a dramatic effect on the conducting properties. The extreme sensitivity of the system to even weak disorder is therefore a result of the existence of the small energy scale T_K, which sets the proximity to the Kondo insulator. Thus, the deeper in the Kondo limit, the more sensitive the system will be to disorder. Note that the value of $\Phi_k(0)$ is *not* set by T_K but is rather a local measure of *particle–hole asymmetry* (see Ref. [6]). As the disorder is further increased, the DOS depletion of the Kondo (pseudo-)gap is washed way and the concentration of USCs saturates. Finally, once the nearby Kondo fixed point is securely destroyed, conventional localization effects set in and the system proceeds to an Anderson-like MIT. That the actual MIT is not very much affected by the renormalized disorder is evidenced by the fact that we observe it to occur at the same point as the non-interacting system. It is the competition between renormalized and bare disorder which, in a three-stage process, leads to the non-monotonic behavior of Fig. 3.

It is worth stressing that the emergence of the Griffiths-phase behavior already at very weak disorder directly follows from the described disorder renormalization as induced by the proximity of an incipient Kondo insulator. Indeed, this mechanism leads to a very large *effective* disorder as seen by conduction electrons, which in turn produces the localization-induced local density of states fluctuations, and the resulting broad distributions of Kondo temperatures. In other correlated systems, such as the disordered Hubbard model [35,36], the Kondo gap is not present, and the relevant Griffiths phase proves to be restricted to the immediate vicinity of the Mott–Anderson transition, in dramatic contrast to what we find here.

In conclusion, we have elucidated the mechanism of the Griffiths phase observed in our studies of disordered Anderson lattices. Within our theory, the NFL behavior proves to be intimately related to the physics of disordered metals close to the Kondo insulator fixed point.

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References

[1] Conference on Non-Fermi Liquid Behavior in Metals, J. Phys.: Condens. Matter 8 (48) 1996.
[2] O.O. Bernal et al., Phys. Rev. Lett. 75 (1995) 2023.
[3] D.E. MacLaughlin et al., J. Phys.: Condens. Matter 8 (1996) 9855.
[4] D.E. MacLaughlin et al., Phys. Rev. B 58 (1998) 11849.
[5] Chia-Ying Liu et al., cond-mat/9909215.
[6] E. Miranda, V. Dobrosavljević, G. Kotliar, J. Phys.: Condens. Matter 8 (1996) 9871.
[7] E. Miranda, V. Dobrosavljević, G. Kotliar, Phys. Rev. Lett. 78 (1997) 290.
[8] E. Miranda, V. Dobrosavljević, G. Kotliar, Physica B 230 (1997) 569.
[9] E. Miranda, V. Dobrosavljević, Physica B 259–261 (1999) 359.
[10] E. Miranda, V. Dobrosavljević, cond-mat/0023209.
[11] L. Degiorgi, H.R. Ott, J. Phys.: Condens. Matter 8 (1996) 9901.
[12] A. Chattopadhyay, M. Jarrell, Phys. Rev. 56 (1997) 2920.
[13] A. Chattopadhyay et al., cond-mat/9805127.
[14] M. C. Aronson et al., Phys. Rev. Lett. 75 (1995) 725.
[15] M.A. Continentino, G. Japiassu, A. Troper, Phys. Rev. B 39 (1989) 9734.
[16] A.J. Millis, Phys. Rev. B 48 (1993) 7183.
[17] A. Rosch et al., Phys. Rev. Lett. 79 (1997) 159.
[18] H.V. Löhneysen et al., Phys. Rev. Lett. 72 (1994) 3262.
[19] F.M. Grosche et al., Physica B 223 + 224 (1996) 50.
[20] N.D. Mathur et al., Nature 394 (1998) 39.
[21] A. Schröder et al., Phys. Rev. Lett. 80 (1998) 5623.
[22] O. Stockert et al., Phys. Rev. Lett. 80 (1998) 5627.
[23] A.J. Millis, Physica B 259–261 (1999) 1169.
[24] P. Nozières, A. Blandin, J. Phys. 41 (1980) 193.
[25] D.L. Cox, Phys. Rev. Lett. 59 (1987) 1240.
[26] M. Jarrell, H.B. Pang, D.L. Cox, K.H. Luk, Phys. Rev. Lett. 77 (1996) 1612.
[27] M. Jarrell, H.B. Pang, D.L. Cox, F. Anders, Physica B 230 (1997) 557.
[28] H. Amitsuka, T. Sakakibara, J. Phys. Soc. Japan 63 (1994) 736.
[29] A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg, Rev. Mod. Phys. 68 (1996) 13.
[30] A.H. Castro Neto, G.E. Castilla, B.A. Jones, Phys. Rev. Lett. 81 (1997) 3531.
[31] A.H. Castro Neto, cond-mat/9911092.
[32] A. H. Castro Neto, B.A. Jones, cond-mat/0003085.
[33] C.H. Booth, D.E. MacLaughlin, R.H. Heffner, R. Chau, M.B. Maple, G.H. Kwei, Phys. Rev. Lett. 81 (1998) 3960.
[34] E. Miranda, V. Dobrosavljević, unpublished.
[35] V. Dobrosavljević, G. Kotliar, Phys. Rev. Lett. 78 (1997) 3943.
[36] V. Dobrosavljević, G. Kotliar, Philos. Trans. Roy. Soc. London A 356 (1998) 1.
[37] V. Janis, D. Vollhardt, Phys. Rev. B 46 (1992) 15712.
[38] V. Dobrosavljević, G. Kotliar, Phys. Rev. Lett. 71 (1993) 3218.
[39] V. Dobrosavljević, G. Kotliar, Phys. Rev. B 50 (1994) 1430.
[40] R. Abou-Chacra, P.W. Anderson, D.J. Thouless, J. Phys. C 6 (1973) 1734.
[41] S. Barnes, J. Phys. F 7 (1977) 2637.
[42] N. Read, D.M. Newns, J. Phys. C 16 (1983) L1055.
[43] P. Coleman, Phys. Rev. B 35 (1987) 5072.
[44] M.C. de Andrade et al., Phys. Rev. Lett 81 (1998) 5620.
[45] R.B. Griffiths, Phys. Rev. Lett 23 (1969) 17.