LOCAL PSEUDOGAPS AND FREE MAGNETIC MOMENTS AT THE ANDERSON METAL-INSULATOR TRANSITION: NUMERICAL SIMULATION USING POWER-LAW BAND RANDOM MATRICES

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At the Anderson metal-insulator transition the eigenstates develop multifractal fluctuations. Therefore their properties are intermediate between being extended and localized. As a result these wave functions are power-law correlated, which causes a substantial suppression of the local density of states at some random positions, resembling random local pseudogaps at the Fermi energy. Consequently the Kondo screening of magnetic moments is suppressed when a magnetic impurity happens to be at such a position. Due to these unscreened magnetic moments the critical exponents and multifractal dimensions at the metal-insulator transition take their smaller, unitary ensemble values for exchange couplings not exceeding a certain critical value $J^* \approx .3D$, where D is the band width. Here we present numerical calculations of the distribution of Kondo temperatures for the critical Power-law Band Random Matrix (PBRM) ensemble, whose properties are similar to that of the Anderson transition with the advantage of using a continuous parameter for tuning the generalized multifractal dimensions of the eigenstates.

Keywords: Kondo effect; Anderson localization; multifractality.

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1. Introduction

The disorder driven Anderson metal-insulator transition (AMIT) continues to be an interesting topic of current condensed matter physics^{1,2,3}. The complex structure of the eigenstates right at the transition point has also been discussed and investigated

intensively (see Ref. 3 for details). Despite of many numerical investigations over the past decades the experimental relevance of the multifractal nature of these states has been shown clearly only recently in magnetic semiconductors⁴, in ultrasound experiments⁵ or STM probing of states at the quantum-Hall transition⁶.

The interplay of these unusual, multifractal states with other degrees of freedom have been brought to the focus over the past years. For example this is the key feature in a recent study of the enhancement of the critical transition temperature to the superconducting state⁷. The impact of interaction on dephasing effects in the presence of multifractality has been investigated in Ref. 8.

In the present work we provide numerical evidence of the intimate interplay of two famous, low-temperature, universal phenomena, the Kondo effect and the Anderson metal-insulator transition along the results presented in Ref. 9. We study the coupling of a single impurity placed in a host at the Anderson transition. The host is modeled by a random matrix termed as power-law band random matrix (PBRM). The isolated sample of length L is represented by an $L \times L$ real symmetric (time reversal invariant) matrix whose entries are randomly drawn from a normal distribution with zero mean, $\langle H_{ij}^0 \rangle = 0$, and a variance depending on the distance of the matrix element from the diagonal as³

$$\langle (H_{ij}^0)^2 \rangle = \frac{1}{2} \frac{\delta_{ij} + 1}{1 + [\sin(\pi|i-j|/L)/(\pi b/L)]^{2\alpha}}, \quad (1)$$

where b and α are parameters of the model. In order to reduce finite size effects this expression already incorporates periodic boundary conditions, where Eq. (1) is known as the periodic PBRM model. Nevertheless, for sites far away from each other and the border, i.e., if $1 \ll |i-j| \ll N$, the variance decays with a power law

$$\langle (H_{ij}^0)^2 \rangle \sim \left(\frac{b}{|i-j|} \right)^{2\alpha}. \quad (2)$$

Field-theoretical considerations and detailed numerical investigations verified³ that the PBRM model undergoes a transition at $\alpha = 1$ from delocalized states for $\alpha < 1$ to localized states for $\alpha > 1$. This transition shows almost all the key features of the AMIT, including multifractality of eigenfunctions and non-trivial spectral statistics at the critical point. However, the PBRM model does not reproduce mobility edges separating localized and extended states that emerge in the case of the conventional Anderson problem. An important point for the PBRM model, however, is the additional parameter b , which provides a continuous variation of the properties of the eigenstates, as well, as the spectral fluctuations by changing this parameter from zero to infinity. Hence setting $\alpha = 1$ we have a critical line as $0 < b < \infty$, where the limit of $b \gg 1$ corresponds to "metallic-like" behavior which is termed as weak-multifractality while the other limit of $b \ll 1$ shows "insulator-like" behavior that is known as strong-multifractality.

As for the magnetic impurity in such a disordered host we take the model described in^{11,12,13}. The host is represented by the PBRM model described above

with the choice of $\alpha = 1$. The parameter b is chosen over a wide range: $0.05 < b < 50.0$. The magnetic impurity is placed at every site and the effective Hamiltonian of the coupled system reads as

$$H = H^0 + J\vec{S}\vec{s}(0), \quad (3)$$

where H^0 stands for the electronic system in the disordered potential represented by Eq. (1) and the second term describes the $s - d$ contact interaction between the magnetic impurity, $\vec{S}$, coupled antiferromagnetically to the spin-density of the electronic system, $\vec{s}(0)$, at the place of the impurity. Parameter J is the strength of this coupling.

The Kondo temperature, T_K is defined using the perturbative ‘one-loop’ Nagaoka-Suhl formula¹⁴

$$\frac{1}{J} = \frac{1}{2N} \sum_{n=1}^N \frac{L^d |\psi_n(\mathbf{r})|^2}{|E_n - E_F|} \tanh\left(\frac{E_n - E_F}{2T_K}\right), \quad (4)$$

where $N \sim L^d$ is the number of states in the band of width D , E_F is the Fermi energy, and $|\psi_n(0)|^2$ is the probability density of the n th eigenstate at the position of the impurity with eigenvalue E_n . Unscreened, free magnetic moments may exist at such positions, where Eq. (4) does have a solution setting $T_K = 0$ if $J < J_c$, where

$$\frac{1}{J_c} = \frac{1}{2N} \sum_{n=1}^N \frac{L^d |\psi_n(\mathbf{r})|^2}{|E_n - E_F|}, \quad (5)$$

For a clean metallic system with a flat band, $J_c \sim D/\ln N$, vanishing logarithmically with N , leaving no free moments for any finite J . On the other hand, if the energy eigenstates at the Fermi energy become localized with a localization length ξ , finite local gaps of order $\Delta_I = (\rho \xi^d)^{-1}$ appear at the Fermi energy, cutting off the Kondo renormalization¹⁵ (ρ , average density of states). Therefore, there are with certainty free moments whenever $\Delta_I \gg T_K$, or, equivalently, $J \ll J_c^A \sim D/\ln N_I$, where $N_I = D/\Delta_I$ is the number of localized states with a finite wave function amplitude at the magnetic impurity site.

Therefore in search for the existence of free magnetic moments, first we plot the distribution of the maximum of $1/J_c = \rho_{eff}$ which also serves as a lower cutoff for the coupling constant, J_c , for the formation of the Kondo effect¹³. The quantity is the effective, weighted local density of states (LDOS).

$$\rho_{eff} = \frac{1}{2} \sum_{n=1}^N \frac{|\psi_i|^2}{|E_n - E_F|}. \quad (6)$$

Apparently as seen in Fig. 1 in our case the minimum of ρ_{eff} depends on system size in contrast to the findings of 13 (cf. Fig. 5 Inset).

In our previous paper⁹, we have derived expressions concerning the critical value of the coupling constant, J_c ,

$$J_c/D = \sqrt{1 - d_2(b)}, \quad (7)$$

This is the critical value of the exchange coupling at which $\sqrt{N}$ magnetic moments remain free. The quantity, d_2 appearing in this formula is called the correlation dimension and plays an important role in many different features of the AMIT³.

In order to check this relation numerically, we calculated $P(1/J_c)$ for several values of b different system sizes. The results for the case of strong multifractality ($b = 0.1$) are shown in Fig. 1. From those data, we extracted the largest value of J_c beyond which the distribution drops to zero with a Gaussian tail. The resulting J_c as function of b is plotted for different system sizes in Fig. 2. For large system sizes, J_c/D converges to unity at $b = 0$ and decays with a power-law for growing b ,

Fig. 1. (Color online) The distribution of $\rho_{eff} \equiv D/J_c$ for $b = 0.1$ for various sizes L . The $\ln \rho_{eff}$ has been rescaled by its mean, m , and variance σ . In the inset the distributions are given as a function of the unscaled variable. Note that the distribution shifts to large values as the system size is increased.

Fig. 2. (Color online) J_c/D , as function of b for various system sizes L . Red solid line: analytical result, Eq. (7).

in good agreement with the analytical result of Eq. (7). As also published in Ref. 9 we found the density of free magnetic moments compared to the total number of magnetic impurities. The results of Ref. 9 have been applied for the case of the critical PRBM, by substituting in

$$P_{\text{FM}} = \frac{n_{\text{FM}}}{n_{\text{M}}} = \text{Erfc} \left(\sqrt{\frac{\ln \xi}{2(1 - d_2(b))}} \frac{J}{D} \right), \quad (8)$$

$\xi \rightarrow L$, which is plotted in Fig. 3 together with the numerical results as function of J/D for various values of parameter b . The probability of finding no solution to Eq. (4) as presented in Fig. 3 seems to be very similar to the one obtained in Ref. 13 (cf. Fig. 4a). In Fig. 3 we show the numerical results for $L = 1024$ and apparently the parameter b produces a similar effect as $1/W$ for the conventional Anderson problem.

Fig. 3. (Color online) The portion of free magnetic moments $P_{\text{FM}} = n_{\text{FM}}/n_{\text{M}}$, as function of exchange coupling J/D , for various values of b for size $N = 1024$. The analytical result, Eq. (8), $\xi \rightarrow L$ and $d = 1$, is plotted for comparison. Inset: a typical plot of the local density of states at a site where the magnetic moment remains unscreened.

Fig. 4. (Color online) The distribution of the local Kondo temperatures, T_K in arbitrary units, $P(T_K)$ for exchange coupling strengths (a) $J/D = 0.2$, (b) $J/D = 0.9$ for various sizes L using $b = 0.5$.

As it is plotted in the inset of Fig. 3, we can clearly see that for intermediate values of b , the power-law wavefunction correlations yield a finite probability of having a pseudogap with an exponent related to the correlation dimension as d_2 .

Finally in Fig. 4 we plot the evolution of the full distribution of the probability density function of the Kondo temperatures, $P(T_K)$, obtained from the solution of Eq. (4) inserting a magnetic impurity at every single site as parameters, b and J change. The bimodal character of $P(T_K)$ is prominent for low value of J/D , while a smearing of the Kondo temperature is detected in the case of strong exchange coupling. The mean and the variance of T_K depend strongly on N .

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References

1. P. W. Anderson, *Phys. Rev.* **109**, 1492 (1958).
2. D. Belitz and T. R. Kirkpatrick, *Rev. Mod. Phys.* **66**, 261 (1994).
3. F. Evers and A. D. Mirlin, *Rev. Mod. Phys.* **80**, 1355 (2008).
4. A. Richardella, *et al. Science* **327**, 665 (2010).
5. S. Faez, *et al.*, *Phys. Rev. Lett.* **103**, 155703 (2009).
6. K. Hashimoto, *et al.*, *Phys. Rev. Lett.* **101**, 256802 (2008).
7. M. V. Feigel'man, *et al. Phys. Rev. Lett.* **98**, 027001 (2007); M. V. Feigel'man, *et al. Annals of Physics* **325**, 1368 (2010); I.S. Burmistrov, *et al.* arXiv:1102.3323.
8. I.S. Burmistrov, *et al. Ann. Phys.* **326** 1457 (2011).
9. S. Kettemann, E. R. Mucciolo, and I. Varga, *Phys. Rev. Lett.* **103**, 126401 (2009).
10. A. D. Mirlin, F. Evers, I. V. Gornyi, P. M. Ostrovsky, in "50 Years of Anderson Localization", ed. by E. Abrahams (World Scientific, 2010), Chapter 6, pp. 107-150; *Int. J. Mod. Phys. B* **24**, 1577 (2010).
11. S. Kettemann and E. R. Mucciolo, *JETP Lett.* **83**, 240 (2006) [*Pis'ma v ZhETF* **83**, 284 (2006)]; *Phys. Rev. B* **75**, 184407 (2007).
12. P. S. Cornaglia, D. R. Grempel, and C. A. Balseiro, *Phys. Rev. Lett.* **96**, 117209 (2006).
13. A. Zhuravlev *et al.*, *Phys. Rev. Lett.* **99**, 247202 (2007).
14. Y. Nagaoka, *Phys. Rev.* **138**, 1112 (1965); H. Suhl, *Phys. Rev.* **138**, 515 (1965).
15. S. Kettemann and M. E. Raikh, *Phys. Rev. Lett.* **90**, 146601 (2003).