Disorder screening near the Mott–Anderson transition

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Abstract

Correlation-driven screening of disorder is studied within the typical-medium dynamical mean-field theory (TMT–DMFT) of the Mott–Anderson transition. In the strongly correlated regime, the site energies ε_R^i characterizing the effective disorder potential are strongly renormalized due to the phenomenon of Kondo pinning. This effect produces very strong screening when the interaction U is stronger than disorder W, but applies only to a fraction of the sites in the opposite limit ($U < W$).
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1. Introduction

Theories that are able to capture both the Mott [1] and the Anderson [2] mechanisms for electron localization have remained elusive despite many years of effort. An attractive approach to this difficult problem has recently been proposed by combining the dynamical mean-field theory (DMFT) [3] of the Mott transition and the typical-medium theory (TMT) [4] of Anderson localization. This new formulation of the Mott–Anderson problem has been explored in recent work by Vollhardt and collaborators [5] using numerical renormalization-group methods, but the precise mechanism for the critical behavior of this model remains to be elucidated. Here we examine the mechanism for disorder screening within this theory, which explains several aspects of the results found in Ref. [5].

Within TMT–DMFT, a lattice problem is mapped onto an ensemble of single-impurities problems, which are embedded in a self-consistently determined bath. Recent work of Ref. [6] examined the behavior of a collection of single-impurity models in the situation where the bath seen by the impurities was chosen to mimic the approach to the Mott–Anderson transition. In this work, the impurity quasiparticle weight Z_i was shown to present a scaling behavior as a function of the on-site energy ε_i and the distance t to the transition. These findings, however, are not sufficient to address the disorder screening behavior of the model, which requires the description of the renormalized disorder potential. In this paper, we demonstrate that a scaling procedure similar to that presented in Ref. [6] can also be carried on for the renormalized energy ε_R^i.

2. Renormalization of the disorder potential

We consider a collection of Anderson impurity models [6] with on-site repulsion U, on-site energies ε_i, and the total spectral weight t of the cavity field. Within TMT–DMFT, $t \to 0$ as the metal–insulator transition is approached, being a measure of the distance to the transition. Without loss of generality [6], we consider a featureless model bath with non-vanishing spectral weight for $-t/2 < \omega < t/2$ and zero otherwise. Our goal is to describe the statistics of the renormalized site energies in the limit $t \to 0$.

The impurity models were solved at zero temperature using the SB4 method [7,6], which provides a parametrization of the low-energy (quasiparticle) part of the local

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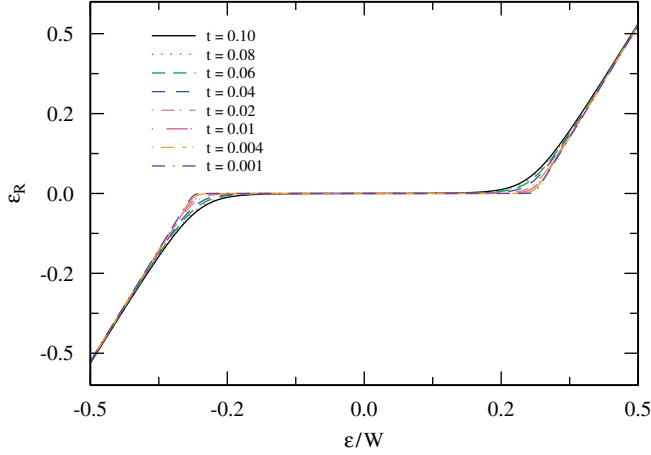E-mail address:* aguiar@fisica.ufmg.br (M.C.O. Aguiar).

Fig. 1. Renormalized energy ε_R as a function of the on-site energy ε for a collection of single-impurity problems close to the Mott–Anderson transition ($t \to 0$). The parameters used were $U = 1.75$ and $W = 2.8$.

Green's function, given by

$$G_i(\omega_n) = \frac{Z_i}{i\omega_n - \varepsilon_R^i - Z_i \Delta(\omega_n)}. \tag{1}$$

Here Z_i is the local quasiparticle weight and ε_R^i is the renormalized site energy. The details of the calculations mirror those of Ref. [6].

The results for the renormalized energy ε_R^i as a function of $-W/2 < \varepsilon_i < W/2$, in the vicinity of the Mott–Anderson transition ($t \to 0$), are shown in Fig. 1. As in Ref. [6], we find two-fluid behavior, where sites with $|\varepsilon_i| < U/2$ turn into local magnetic moments, corresponding to "Kondo pinning" [8] $\varepsilon_R^i \to 0$. For the remaining sites, $\varepsilon_R^i \to \varepsilon_i + U/2$ or $\varepsilon_R^i \to \varepsilon_i - U/2$, as they become, respectively, doubly occupied (those with $\varepsilon_i < -U/2$) or empty (those with $\varepsilon_i > U/2$). We should emphasize that such two-fluid behavior thus emerges only for sufficiently strong disorder, such that $U < W$. Otherwise all sites turn into local magnetic moments, and the Mott transition for moderate disorder retains a character similar to that found within the standard DMFT approach [8].

3. Scaling analysis

These results can alternatively be presented in a scaling form as shown in Fig. 2. Here we show that it is possible to collapse the family of curves $\varepsilon_R(t, \delta\varepsilon)/t^{0.5}$, where $\delta\varepsilon = (\varepsilon_i - \varepsilon^*)/\varepsilon^*$ and $\varepsilon^* = U/2$, onto a single universal scaling function $\varepsilon_R(t, \delta\varepsilon)/t^{0.5} = f[t/t^*(\delta\varepsilon)]$ with two branches, one for $\varepsilon_i < \varepsilon^*$ and other for $\varepsilon_i > \varepsilon^*$. In agreement with Ref. [6] (inset of Fig. 2), the crossover scale $t^*(\delta\varepsilon) \sim |\delta\varepsilon|^\phi$, with exponent $\phi = 2$. In the limit $t \to 0$, we find that the branch corresponding to $\varepsilon_i < \varepsilon^*$ has the asymptotic form $f(x) \sim x^{3/2}$ (here $x = t/t^*(\delta\varepsilon)$), corresponding to $\varepsilon_R(t) \sim t^2$. Similarly, for $\varepsilon_i > \varepsilon^*$, $f(x) \sim x^{-1/2}$ corresponding to $\varepsilon_R(t) \sim$ constant. For $x \gg 1$ the two branches merge, viz. $f(x) \sim A \pm B^\pm x^{-0.5}$.
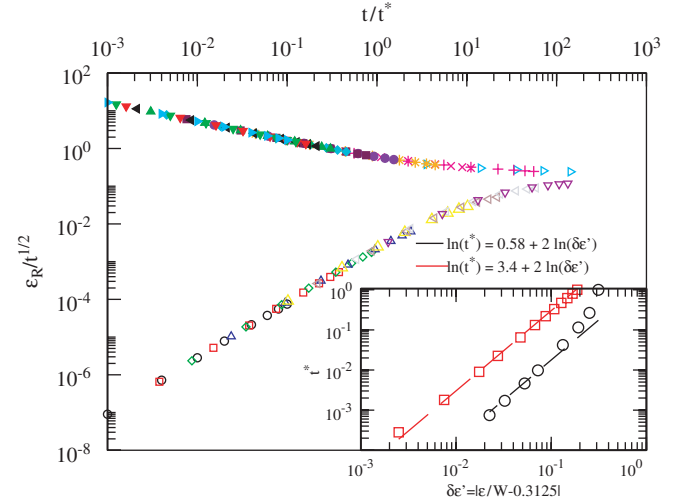

Fig. 2. Scaled renormalized energy $\varepsilon_R/t^{1/2}$ as a function of $t/t^*(\delta\varepsilon)$ showing that the results for different (and positive) ε can be collapsed onto a single scaling function with two branches. Different symbols correspond to different ε; the upper (bottom) branch contains results for $\varepsilon > U/2$ ($\varepsilon < U/2$). The inset shows the scaling parameter t^* as a function of $|\varepsilon/W - 0.3125|$ for the upper (squares) and bottom (circles) branches. The parameters used were $U = 1.75$ and $W = 2.8$.
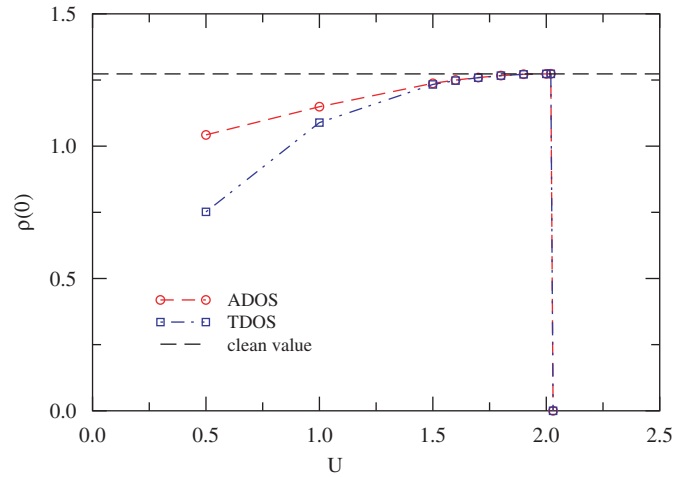

Fig. 3. Arithmetic and geometric density-of-states (ADOS and TDOS, respectively) at the Fermi level as a function of U, for $W = 1.5$, when the TMT–DMFT self-consistent loop is performed.

4. Disorder screening

Within TMT–DMFT, the Anderson localization effects are manifested by the reduction of the typical density of states (TDOS), since the (algebraic) average (ADOS) remains finite even in an Anderson insulator. When disorder is strongly screened due to the correlation effects, the two quantities should not differ much, as illustrated by the results of Fig. 3. Here we present the results of the fully self-consistent solution, as the Mott-like transition is approached by increasing U for $W = 1.5$. Close to the transition, both averages approach the clean limit (dashed line), indicating a strong screening effect. These results are

consistent with those found in the numerical renormalization-group solution of the TMT–DMFT equation of Ref. [5] .

As discussed above, strong disorder screening is expected near the Mott-like transition ($U > W$), which indeed corresponds to the mechanism responsible for the results in Fig. 3. When the transition is approached at strong disorder ($U < W$) (not shown), strong screening effects are found only for a fractions of the sites (i.e. of the volume of the sample), indicating different critical behavior at the Mott–Anderson transition. The details of the critical behavior in this case will be discussed elsewhere.

Acknowledgments

References

[1] N.F. Mott, Metal–insulator Transitions, Taylor & Francis, London, 1974.
[2] P.W. Anderson, Phys. Rev. 109 (1958) 1498.
[3] A. Georges, et al., Rev. Mod. Phys. 68 (1996) 13.
[4] V. Dobrosavljević, et al., Europhys. Lett. 62 (2003) 76.
[5] K. Byczuk, et al., Phys. Rev. Lett. 94 (2005) 056404.
[6] M.C.O. Aguiar, et al., Phys. Rev. B 73 (2006) 115117.
[7] G. Kotliar, A.E. Ruckenstein, Phys. Rev. Lett. 57 (1986) 1362.
[8] D. Tanasković, et al., Phys. Rev. Lett. 91 (2003) 066603.