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Sub-ohmic two-level system representation of the Kondo effect

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It has been recently shown that the particle-hole symmetric Anderson impurity model can be mapped onto a Z_2 slave-spin theory without any need of additional constraints. Here we prove by means of Numerical Renormalization Group that the slave-spin behaves in this model like a two-level system coupled to a sub-ohmic dissipative environment. It follows that the Z_2 symmetry gets spontaneously broken at zero temperature, which we find can be identified with the on-set of Kondo coherence, being the Kondo temperature proportional to the square of the order parameter. Since the model is numerically solvable, the results are very enlightening on the role of quantum fluctuations beyond mean field in the context of slave-boson approaches to correlated electron models, an issue that has been attracting interest since the 80's. Finally, our results suggest as a by-product that the paramagnetic metal phase of the Hubbard model at half-filling, in infinite coordination lattices and at zero temperature, as described for instance by Dynamical Mean Field Theory, corresponds to a slave-spin theory with a spontaneous breakdown of a local Z_2 gauge symmetry.

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Mott's localization, and all its annexes like the local moment formation and the Kondo effect, is a phenomenon that escapes any mean-field single-particle description since it directly affects only part of the electrons' degrees of freedom, namely their charge. This is unfortunate because mean-field theory is the simplest and straightest way to approach interacting many-body systems. A trick to circumvent this difficulty, which has provided lots of physical insights along the years, is to artificially enlarge the Hilbert space adding new degrees of freedom that aim to describe just the electron charge configurations, supplemented by local constraints that project the enlarged Hilbert space onto the physical one. The final scope is to make Mott's localization accessible already at the mean-field level. The most famous realization of this work-programme is the so-called *slave boson* technique, originally introduced to describe Anderson and Kondo models for f -electron systems.^{1,2} A delicate issue of the slave-boson theory is that the mean-field treatment, although providing quite satisfactory results, explicitly breaks a local $U(1)$ gauge symmetry, which cannot be broken hence requires going beyond mean-field to be restored.³⁻⁵ More recently, novel approaches have been proposed in the attempt of reducing the dimension of the enlarged Hilbert space, hence the redundancy of the representation, still maintaining the nice feature of making Mott localization accessible at the mean-field level.⁶⁻⁸ For instance, in Ref. 8 it has been shown that it is sufficient to introduce additional slave Ising variables on each site, namely just two level systems rather than infinite level ones as in the original slave-boson technique, to account at the mean-field level for a Mott transition in the half-filled Hubbard model. In this new representation the continuous $U(1)$ local gauge symmetry of the slave-boson theory is replaced by a discrete Z_2 one. Alike in the slave-boson theory, the Z_2 slave-spin formulation

must be supplemented by a constraint that projects the enlarged Hilbert space onto the physical one. Remarkably, it has been shown in Ref. 9 that the constraint is unnecessary in the case of an Anderson impurity model at particle-hole symmetry, and, equivalently, of a Hubbard model at half-filling in the limit of infinite coordination lattices, which can be mapped¹⁰ onto an impurity model self-consistently coupled to a bath. Specifically, given the Anderson impurity Hamiltonian

$$\begin{aligned} \mathcal{H}_{\text{AIM}} &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \\ &+ \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} \left(d_\sigma^\dagger c_{\mathbf{k}\sigma} + H.c. \right) + \frac{U}{2} (n_d - 1)^2 \\ &\equiv \mathcal{H}_{\text{bath}} + \mathcal{H}_{\text{hyb}} + \frac{U}{2} (n_d - 1)^2, \end{aligned} \quad (1)$$

where $c_{\mathbf{k}\sigma}^\dagger$ creates a conduction electron while d_σ^\dagger an impurity one, with $n_d = \sum_\sigma d_\sigma^\dagger d_\sigma$, and the Ising plus electron model

$$\mathcal{H}_{Z_2} = \mathcal{H}_{\text{bath}} + \sigma^x \mathcal{H}_{\text{hyb}} + \frac{U}{4} (1 - \sigma^z), \quad (2)$$

where σ^a , $a = x, y, z$, are Pauli matrices, it follows that at particle-hole symmetry the following identity holds:⁹

$$Z_{\text{AIM}} \equiv \text{Tr} \left(e^{-\beta \mathcal{H}_{\text{AIM}}} \right) = \frac{1}{2} Z_{Z_2} \equiv \frac{1}{2} \text{Tr} \left(e^{-\beta \mathcal{H}_{Z_2}} \right). \quad (3)$$

The Ising operator σ^z in (2) can be identified with the electron operator $1 - 2(n_d - 1)^2$, which has value +1 if $n_d = 1$ and -1 if $n_d = 0, 2$, hence it describes charge fluctuations. Furthermore, the mixed operator $\sigma^x d_\sigma$ actually represents the physical impurity annihilation operator. At zero temperature, the two Hamiltonians (1)

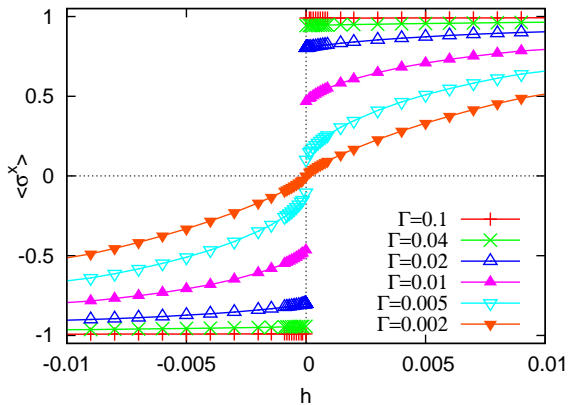


FIG. 1: The average value $\langle \sigma^x \rangle$ as a function of the external symmetry breaking field h for several values of Γ and $U = 0.1$.

and (2) must therefore have the same ground state energy. It can be readily shown that a mean-field factorized wavefunction $|\Psi\rangle = |\text{Ising}\rangle \times |\text{electrons}\rangle$ for the model (2) allows to reproduce all mean-field results of the slave-boson mean-field approach to the Anderson impurity Hamiltonian (1). In fact, if we assume that $\langle \text{Ising} | \sigma^z | \text{Ising} \rangle = \cos \theta$ and $\langle \text{Ising} | \sigma^x | \text{Ising} \rangle = \sin \theta$, then the electronic wavefunction must be the ground state of the resonant level Hamiltonian

$$\mathcal{H}_* = \mathcal{H}_{\text{bath}} + \sin \theta \mathcal{H}_{\text{hyb}} + \frac{U}{4} (1 - \cos \theta), \quad (4)$$

with energy $E(\theta)$ and hybridization width $\Gamma_* = \sin^2 \theta \Gamma$, lower than its bare value Γ . Minimization of $E(\theta)$ leads to the same result as obtained by slave-boson mean-field theory.¹¹ For instance, if we assume that $\Gamma(\epsilon) = \Gamma$ for $\epsilon \in [-D, D]$ and zero otherwise, assumption that we shall make hereafter taking $D = 1$ our unit of energy, then, for $U \gg \Gamma$, we find that the known mean-field result

$$\sin^2 \theta = \frac{1}{\Gamma} \exp\left(-\frac{\pi U}{16\Gamma}\right). \quad (5)$$

By analogy with slave bosons, it is tempting to interpret the finite value of $\sin \theta$ as manifestation of Kondo coherence, and the impurity operator d_σ in (2) as the coherent quasiparticle with weight $\sin^2 \theta$. In fact, within mean field the spectral function $A_{d_\sigma}(\epsilon)$ of the physical electron $\sigma^x d_\sigma$ is simply the convolution of the spectral functions of the resonant level, $A_d(\epsilon)$ and of the Ising operator σ^x ,

$$A_\sigma(\epsilon) = \sin^2 \theta \delta(\epsilon) + \frac{\cos^2 \theta}{2} \left(\delta(\epsilon - \Omega) + \delta(\epsilon + \Omega) \right), \quad (6)$$

where $\Omega = U/2 \cos \theta$ is the effective Zeeman splitting of the Ising spin. Specifically, one finds that

$$\begin{aligned} A_{d_\sigma}(\epsilon) &\rightarrow (A_d * A_\sigma)(\epsilon) = \sin^2 \theta A_d(\epsilon) \\ &+ \frac{\cos^2 \theta}{2} \left(\theta(\epsilon - \Omega) A_d(\epsilon - \Omega) + \theta(-\epsilon - \Omega) A_d(\epsilon + \Omega) \right), \end{aligned} \quad (7)$$

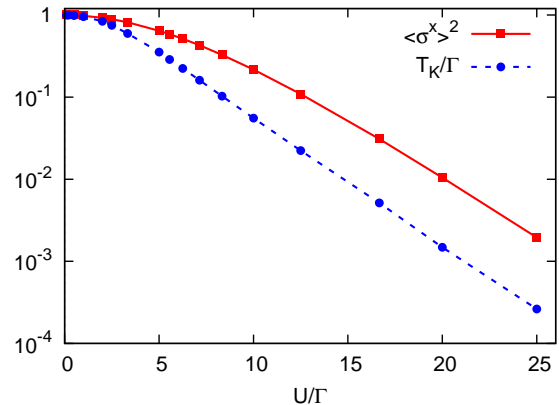


FIG. 2: Square of the symmetry breaking order parameter and of T_K/Γ plot in logarithmic scale versus U/Γ . Note the linear behavior at large U/Γ .

The mean-field expression of $A_{d_\sigma}(\epsilon)$ displays a low energy resonance with width Γ_* and weight $\sin^2 \theta$, the rest of its weight being concentrated in two symmetric peaks at energies $\pm \Omega$. It is quite reasonable to regard these latter as the Hubbard side-bands and instead the central peak as the Abrikosov-Suhl resonance, hence Γ_* the Kondo temperature T_K . However, while the mean field result predicts that the Hubbard bands are broadened on the same scale Γ_* as the central resonance, in reality their width is controlled by the bare Γ .

Another questionable aspect of the mean field solution with $\langle \sigma^x \rangle \neq 0$ is that it explicitly breaks the discrete symmetry of (2): $d_\sigma \rightarrow -d_\sigma$ and $\sigma^x \rightarrow -\sigma^x$. Therefore, just like in the conventional slave-boson approach,³ we may wonder how reliable is mean field. We are going to show that, unlike in slave-boson theory, the breaking of the discrete Z_2 symmetry of (2) is not an artifact of mean-field but does spontaneously occur in the actual ground state.

We start noticing that the model (2) resembles a two-level system coupled to a dissipative bath,¹² where the two levels are the states with $\sigma^x = \pm 1$ and the tunneling is provided by σ^z . In reality, the two models are not rigorously equivalent, since the hybridization operator \mathcal{H}_{hyb} does not behave exactly like the coupling to a dissipative bath of bosons. However, if we judge solely from the low frequency behavior of the dissipative-bath spectral function, $J(\omega) \sim \omega^s$,¹² we should conclude that the model (2) behaves like a spin-boson Hamiltonian with an extremely sub-ohmic dissipation, $s = 0$. In such a case, we expect the tunneling to be irrelevant at low energy, hence unable to split the degeneracy of the two levels. This conclusion is remarkable because it means that the mean field result is more correct than we would have expected; the Z_2 symmetry is spontaneously broken at zero temperature. There is still another aspect that we find worth mentioning. In reality, the Anderson impurity model (1) can be mapped into another spin-boson model¹³ with the role of the spin being played now by the physical spin of the

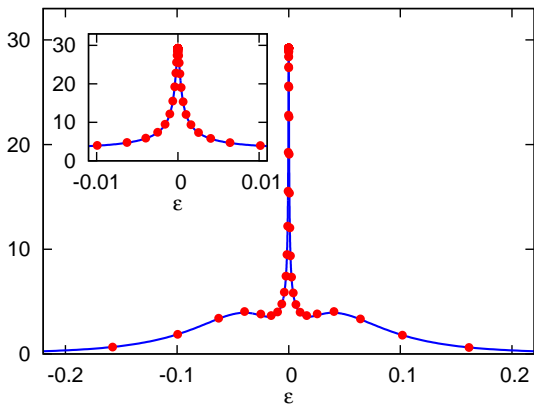


FIG. 3: Spectral function of the physical impurity electron operator, $\sigma^x d_\sigma$, at $U = 0.1$ and $\Gamma = 0.01$. The dots are the values of the impurity spectral function as calculated directly by the Anderson impurity model (1). We just plot few of these points, since the two spectral functions are just coincident.

impurity, rather than by the charge as in (2). In this alternative and more familiar representation, the bath is however ohmic and leads to incoherent delocalization of the physical spin, once again the Kondo effect. We find quite amusing that the Kondo effect, known to occur in the Anderson impurity model (1) with constant Γ , happens to be described by two complementary spin-boson models, in one of which it corresponds to delocalization while in the other, the model Eq. (2), to localization.

The above speculation can be supported by actual calculations, affordable because of the reduced dimension of the Hilbert space as opposed to conventional slave bosons. In particular, we shall consider both the Anderson impurity model, Eq. (1), and the model (2), and study them by means of the Numerical Renormalization Group (NRG).¹⁴

The first task we undertake is to confirm that spontaneous breaking of Z_2 does occur in model (2). We hence add to \mathcal{H}_{Z_2} a symmetry breaking perturbation $-h\sigma^x$, and calculate the average $\langle\sigma^x\rangle$ as function of h . The results are shown in Fig. 1, where it is evident the characteristic behavior of a symmetry broken phase. The asymptotic value of $\langle\sigma^x\rangle$ as $h \rightarrow 0^+$ can be considered as the zero-field order parameter. In Fig. 2 we plot $\langle\sigma^x\rangle^2$ as well the actual Kondo temperature in units of Γ of the Anderson impurity model (1) on a logarithmic scale as function of U/Γ . We showed that within mean field these two quantities coincide, but in reality they do not, see Fig. 2, even though the linear slope at large U/Γ is the same, and twice as bigger as the mean field value $-\pi U/16\Gamma$, Eq. (5). This simply means that mean field as usual overestimates the value of the symmetry breaking order parameter, hence of T_K .

The next important step is showing that gauge invariant quantities in both models (1) and (2) are indeed the same. We then calculate the impurity spectral function of the Anderson impurity model and compare it with the

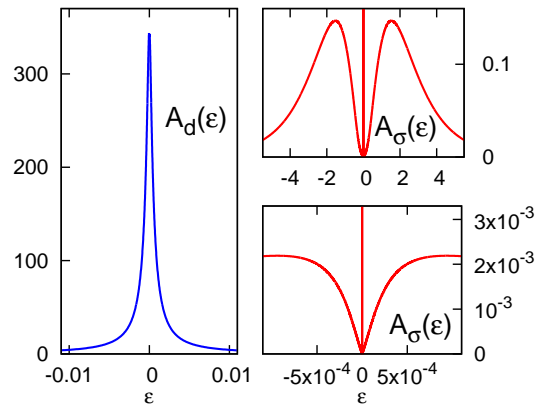


FIG. 4: Left panel: Spectral function of the impurity operator d_σ . Right panel: Spectral function of the Ising operator σ^x , on a large scale, top, and zoomed close to zero energy, bottom. The parameter that are used are $U = 0.1$ and $\Gamma = 0.01$ in units of the conduction electron half-bandwidth.

spectral function of the physical electron $\sigma^x d_\sigma$ in model (2). The two quantities are found to be practically indistinguishable from each other, see Fig. 3, thus confirming the validity of the mapping.

We previously showed that within mean field theory, the spectral function of the physical electron $A_{d\sigma}(\epsilon)$ is approximated by the convolution between the spectral functions $A_\sigma(\epsilon)$ of σ^x , whose mean field expression is given in Eq. (6), and $A_d(\epsilon)$ of d_σ , in mean field simply the spectral function of a resonant level model of width $\sin^2\theta\Gamma$. The actual NRG $A_d(\epsilon)$ is found not to differ much from the mean field result; it is still made up of a single resonance at the chemical potential, see Fig. 4, of width the true Kondo temperature. Instead, $A_\sigma(\epsilon)$ is substantially different from mean field, see Fig. 4. It still displays a δ -peak at $\epsilon = 0$ with weight $\langle\sigma^x\rangle^2$, even though not exactly coincident with the value extracted in the zero-field limit, see the comment below. However, the finite energy peaks shift at much higher energy, around the edge of the particle-hole continuum, and get quite broadened. In addition, a tiny linear in ϵ component appears at low energy, which resembles much the particle-hole spectrum of the resonant level since the linear behavior stops just around the Kondo temperature. This result shows that quantum fluctuations couple strongly the Ising spin with the electrons, providing a very short lifetime to the Ising spin-flip excitations. Although NRG, at least in the version we use, is not expected to be very accurate at high energy, especially in such a case of a sub-ohmic bath,¹⁵ we believe that the gross features of $A_\sigma(\epsilon)$ that we find, e.g. the very broad incoherent background peaked at high energy, are true.

We observe that the spectral function $A_{d\sigma}(\epsilon)$ of the physical electron $\sigma^x d_\sigma$, shown in Fig. 3, can be generally written as

$$A_{d\sigma}(\epsilon) = \int d\omega A_d(\epsilon - \omega) A_\sigma(\omega) K(\omega, \epsilon), \quad (8)$$

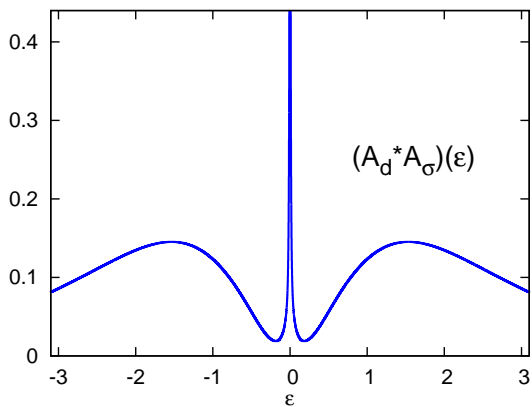


FIG. 5: Convolution of the spectral functions $A_\sigma(\epsilon)$ and $A_d(\epsilon)$ for $U = 0.1$ and $\Gamma = 0.01$. Note the absence of Hubbard bands, which should be appear at $\sim \pm U/2 = 0.05$ but are hidden below the broad background peaked around the particle-hole band edge at energy $\sim \pm 2D = \pm 2$.

where the kernel $K(\omega, \epsilon)$ amounts for all vertex corrections. In Fig. 5 we show the simple convolution of $A_d(\epsilon)$ and $A_\sigma(\omega)$, which, compared with the correct result in Fig. 3, could provide a rough estimate of vertex corrections. We notice that, while the Abrikosov-Suhl resonance is reproduced quite well also by the convolution, the Hubbard side-bands are completely masked by the broad background of $A_\sigma(\epsilon)$, see Fig. 4. This implies that

vertex corrections play a major role at high energy, filtering out that high-energy background and letting the Hubbard bands emerge.

In conclusion, we have shown several amusing features of the Z_2 slave-spin representation of the particle-hole symmetric Anderson impurity model that, unlike its slave-boson analogous, can be exactly solved by NRG. Specifically, we have shown that in this language the Kondo effect corresponds to spontaneous breaking of a local discrete Z_2 symmetry, that does survive quantum fluctuations.

We end by mentioning that, as a byproduct, our result suggests that the zero-temperature paramagnetic metal phase of the half-filled Hubbard model, in the limit of infinite lattice-coordination,¹⁰ can be regarded within the Z_2 slave-spin representation^{8,9} as a phase where a local Z_2 gauge symmetry is spontaneously broken. Conversely, the zero-temperature Mott metal-to-insulator transition would correspond to the restoration of the Z_2 symmetry. We note that this result does not violate Elitzur's theorem,¹⁶ because of the infinite lattice-coordination limit.¹⁷ However, we expect that the local Z_2 gauge symmetry should be recovered at any finite temperature, since a sub-ohmic dissipative two-level system is known to delocalize at any finite temperature.¹²

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