Unbinding slave spins in the Anderson impurity model

Manumitting slave-spins in the Anderson impurity model

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(Dated: October 31, 2017)

We show that a generic single-orbital Anderson impurity model, lacking for instance any kind of particle-hole symmetry, can be exactly mapped without any constraint onto a resonant level model coupled to two Ising variables, which reduce to one if the hybridisation is particle-hole symmetric. The mean-field solution of this model is found to be stable to unphysical spontaneous magnetisation of the impurity, unlike the saddle-point solution in the standard slave-boson representation. Remarkably, the mean-field estimate of the Wilson ratio approaches the exact value $R_{\rm W} = 2$ in the Kondo regime.

PACS numbers: 71.10.Fd,71.30.+h,05.30.Rt

I. INTRODUCTION

Within any approximate technique based on independent particles, as e.g. Hartree-Fock, the electron's quantum numbers, i.e. its charge, spin and, eventually, orbital component, are inevitably all entangled into single-particle excitations. This is ultimately the reason why such independent-particle schemes fail in correlated electron systems where charge degrees of freedom are instead well separated in energy from spin and orbital ones.

An efficient and popular trick to disentangle charge from other degrees of freedom is to enlarge the Hilbert space adding auxiliary particles *slaves* to the physical charge excitations. There are by now various implementations of such trick, starting from the elder slave-boson theory[1–3] to more recent slave-spin[4–6] and slave-rotor[7] ones. Those auxiliary particles are held in slavery by a product of local constraints that project the enlarged Hilbert space $\mathscr{H}_*$ onto the physical subspace $\mathscr{H}$, and concurrently the effective Hamiltonian H_* of the electrons plus the auxiliary particles onto the original electron-only one, H. As common in such cases, H_* possesses local gauge invariance that translates into local conserved quantities. The constraints simply fix the values that those conserved quantities must have in the physical subspace.

The big advantage of this apparently more cumbersome approach is that a mean-field decoupling of the electrons from the slave particles naturally provides the desired disentanglement of charge from all other degrees of freedom, thus allowing the access to phenomena like Mott's localisation[3] otherwise inaccessible by mean-field in the original electron-only representation.

The problem with mean field in slave-particle theories is that the constraints are only satisfied *on average*, which brings about unphysical gauge-symmetry breaking, i.e. mean-field solutions mixing the physical subspace with the non-physical one. There is actually an exception where the constraint is not required: a particle-hole (p-h) symmetric single-orbital Anderson impurity model (AIM) that is represented in terms of a resonant level coupled to a two-level system, one level corresponding to the impurity being singly occupied and the other to the impurity being empty or doubly occupied. Because of p-h symmetry, the partition function within the physical subspace is equal[8] to that in the unphysical one, so that the former is just half of the partition function calculated in the whole enlarged Hilbert space without any restriction. In this representation the Hamiltonian possesses a local Z_2 gauge symmetry, which is spontaneously broken at zero temperature[9] since the model effectively corresponds to a two-level system in a sub-ohmic bath[10]. Therefore the symmetry breaking is here not a spurious result of mean field but a real feature of the model. Since a p-h symmetric Hubbard model in infinitely coordinated lattices maps within dynamical mean-field theory (DMFT)[11] just onto that same AIM, one can show[8] that the free energy of the lattice model can be straightforwardly obtained by that of its Z_2 slave spin representation[5,6] without imposing any constraint. One remarkable consequence of such mapping is that the metallic phase of the Hubbard model translates into a phase where the local Z_2 gauge symmetry breaks spontaneously[12], which is not prohibited when the lattice coordination number is infinite[13], whereas the symmetry is restored in the Mott insulator. This mapping thus endows the Mott transition of a genuine order parameter. More recently, a similar trick of exploiting particle-hole symmetry to get rid of the local constraints was used[14] to derive a Landau-Ginzburg theory of the orbital-selective Mott transition in a two-band Hubbard model at half-filling.

In view of the above promising results, it is worth exploring whether it is still possible to get rid of the constraints away from particle-hole symmetry, which is precisely the goal of the present work.

II. THE MODEL

We consider the single-orbital AIM

$$H = \sum_{\mathbf{k}\sigma} \left[\epsilon_{\mathbf{k}\sigma}\, c^\dagger_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} + T_{\mathbf{k}\sigma} \Big(d^\dagger_\sigma\, c_{\mathbf{k}\sigma} + c^\dagger_{\mathbf{k}\sigma}\, d_\sigma \Big) \right] - \frac{U}{4}\,\Omega - \mu\big(n_\uparrow + n_\downarrow - 1\big) - h\big(n_\uparrow - n_\downarrow\big)\,, \tag{1}$$

where $n_\sigma = d^\dagger_\sigma d_\sigma$ and

$$\Omega = \Omega^\dagger = \Omega^{-1} = -\big(2n_\uparrow - 1\big)\big(2n_\downarrow - 1\big)\,, \qquad (2)$$

such that $\Omega\, d_\sigma\, \Omega = -d_\sigma$. We assume generically spin-dependent and p-h non-symmetric hybridisation amplitudes $T_{\mathbf{k}\sigma}$. By contrast, we can always consider, without loss of generality, a p-h symmetric spectrum $\epsilon_{\mathbf{k}\sigma}$, which implies the existence of a one-to-one correspondence between spin-dependent pairs of momenta, $\mathbf{k}$ and $\mathbf{p} = \mathbf{C}_\sigma(\mathbf{k})$, such that $\epsilon_{\mathbf{k}\sigma} = -\epsilon_{\mathbf{p}\sigma}$. For convenience we define for all $\mathbf{k}$ such that $\epsilon_{\mathbf{k}} < 0$ the following combinations of fermionic operators

$$c_{1(2)\mathbf{k}\sigma} = \Big(c_{\mathbf{k}\sigma} \pm c_{\mathbf{C}_\sigma(\mathbf{k})\sigma}\Big)/\sqrt{2}\,, \qquad (3)$$

as well as of hybridisation amplitudes

$$V_{1(2)\mathbf{k}\sigma} = \Big(T_{\mathbf{k}\sigma} \pm T_{\mathbf{C}_\sigma(\mathbf{k})\sigma}\Big)/\sqrt{2}\,, \qquad (4)$$

so that the Hamiltonian can be rewritten as

$$\begin{aligned} H(U,\mu,h,V_{2\uparrow},V_{2\downarrow}) &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma}\Big(c^\dagger_{1\mathbf{k}\sigma}\, c_{2\mathbf{k}\sigma} + H.c.\Big) \\ &+ \sum_{\mathbf{k}\sigma}\sum_{a=1}^{2} V_{a\mathbf{k}\sigma}\Big(d^\dagger_\sigma\, c_{a\mathbf{k}\sigma} + H.c.\Big) \\ &- \frac{U}{4}\,\Omega - \mu\big(n_\uparrow + n_\downarrow - 1\big) - h\big(n_\uparrow - n_\downarrow\big)\,, \end{aligned} \qquad (5)$$

where we denote the sets of $V_{2\mathbf{k}\sigma}$ shortly as $V_{2\sigma}$, and hereafter $\mathbf{k}$ is restricted to $\epsilon_{\mathbf{k}\sigma} < 0$.
Under a spin-σ particle-hole transformation

$$\mathcal{C}_\sigma : \left(d_\sigma \to d^\dagger_\sigma \cup \prod_{\mathbf{k}} \left(c_{1\mathbf{k}\sigma} \to -c^\dagger_{1\mathbf{k}\sigma} \cup c_{2\mathbf{k}\sigma} \to c^\dagger_{2\mathbf{k}\sigma}\right)\right), \qquad (6)$$

the Hamiltonian parameters change as follows

$$\begin{aligned} &U \to -U\,, \qquad \mu \to \mp h\,, \qquad h \to \mp \mu\,, \\ &V_{2\uparrow} \to \mp V_{2\uparrow}\,, \quad V_{2\downarrow} \to \pm V_{2\downarrow}\,, \end{aligned} \qquad (7)$$

while $V_{1\mathbf{k}\sigma}$ and $\epsilon_{\mathbf{k}\sigma}$ stay invariant. The two signs here refer to the action of $\mathcal{C}_\uparrow$ and $\mathcal{C}_\downarrow$, respectively. Since the partition function $Z(U,\mu,h,V_{2\uparrow},V_{2\downarrow})$ is invariant under any unitary transformation, then

$$\begin{aligned} Z(U,\mu,h,V_{2\uparrow},V_{2\downarrow}) &= Z(-U,-h,-\mu,-V_{2\uparrow},V_{2\downarrow}) \\ &= Z(-U,h,\mu,V_{2\uparrow},-V_{2\downarrow}) \\ &= Z(U,-\mu,-h,-V_{2\uparrow},-V_{2\downarrow})\,. \end{aligned} \qquad (8)$$

III. MAPPING WITHIN THE SLAVE-SPIN REPRESENTATION

In Ref. 4 a new slave-particle representation of Hubbard-like models was introduced, which in our case consists in associating to each impurity-electron species d_σ an auxiliary Ising variable τ^a_σ, $a = x, y, z$. The Hamiltonian in such enlarged Hilbert space can be written as

$$\begin{aligned} H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow}) = \sum_{\mathbf{k}\sigma} \Big[&\epsilon_{\mathbf{k}\sigma}\Big(c^\dagger_{1\mathbf{k}\sigma}\, c_{2\mathbf{k}\sigma} + H.c.\Big) \\ &+ \tau^x_\sigma\, V_{1\mathbf{k}\sigma}\Big(d^\dagger_\sigma\, c_{1\mathbf{k}\sigma} + H.c.\Big) \\ &+ i\,\tau^y_\sigma\, V_{2\mathbf{k}\sigma}\Big(d^\dagger_\sigma\, c_{2\mathbf{k}\sigma} - H.c.\Big)\Big] \\ &+ \frac{U}{4}\,\tau^z_\uparrow\,\tau^z_\downarrow - \frac{\mu}{2}\big(\tau^z_\uparrow + \tau^z_\downarrow\big) - \frac{h}{2}\big(\tau^z_\uparrow - \tau^z_\downarrow\big)\,. \end{aligned} \qquad (9)$$

This model maps onto the original Hamiltonian Eq.(5) in a specified *physical* subspace $\mathscr{H}$ of the enlarged Hilbert space $\mathscr{H}_*$. We introduce the two commuting operators

$$\mathcal{P}_\uparrow = \tau^z_\uparrow\,\big(2n_\uparrow - 1\big)\,, \qquad \mathcal{P}_\downarrow = \tau^z_\downarrow\,\big(2n_\downarrow - 1\big)\,, \qquad (10)$$

which have eigenvalues $p_\sigma = \pm 1$ and can thus be regarded as *parity* operators. The Hamiltonian (9) commutes with both $\mathcal{P}_\uparrow$ and $\mathcal{P}_\downarrow$, so that each eigenstate of H_2 can also be chosen as eigenstate of $\mathcal{P}_\sigma$ with eigenvalues p_σ, $\sigma = \uparrow, \downarrow$. The physical subspace $\mathscr{H}$ comprises all states even under parity, i.e. with $p_\sigma = +1$. The projector onto $\mathscr{H}$ is thus

$$\mathbb{P} = \mathbb{P}_\uparrow\,\mathbb{P}_\downarrow = \frac{1}{2}\Big(1 + \mathcal{P}_\uparrow\Big)\;\frac{1}{2}\Big(1 + \mathcal{P}_\downarrow\Big)\,, \qquad (11)$$

and corresponds to the operator equivalence

$$\tau^z_\sigma \equiv \big(2n_\sigma - 1\big)\,, \qquad (12)$$

which is just the slave-spin constraint[4]. We observe that the hybridisation with the operators $c_{2\mathbf{k}\sigma}$ might seem at odds with the original representation $d_\sigma \to \tau^x_\sigma\, d_\sigma$ in Ref. 4, but in reality it is not since in the physical subspace $\tau^x_\sigma\, d^\dagger_\sigma \equiv i\tau^y_\sigma\, d^\dagger_\sigma$. We shall prefer the expression Eq. (9) of the slave-spin Hamiltonian, since here the role of the p-h symmetry transformation $\mathcal{C}_\sigma$ is simply played by τ^x_σ. Indeed the equivalences below hold straightforwardly

$$\begin{aligned} &H_2(-U,h,\mu,V_{2\uparrow},-V_{2\downarrow}) = \tau^x_\downarrow\, H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow})\,\tau^x_\downarrow\,, \\ &H_2(-U,-h,-\mu,-V_{2\uparrow},V_{2\downarrow}) = \tau^x_\uparrow\, H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow})\,\tau^x_\uparrow\,, \\ &H_2(U,-\mu,-h,-V_{2\uparrow},-V_{2\downarrow}) = \\ &\qquad\qquad \tau^x_\uparrow\,\tau^x_\downarrow\, H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow})\,\tau^x_\downarrow\,\tau^x_\uparrow, \end{aligned}$$

so that, through Eq. (8), we find that

$$\begin{aligned} Z(U,\mu,h,V_{2\uparrow},V_{2\downarrow}) &= \mathrm{Tr}\Big(\mathrm{e}^{-\beta H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow})}\;\mathbb{P}\Big) \\ &= \mathrm{Tr}\Big(\tau^x_\downarrow\,\mathrm{e}^{-\beta H_1(U,\mu,h,V_{2\uparrow},V_{2\downarrow})}\,\tau^x_\downarrow\,\mathbb{P}\Big) \\ &= \mathrm{Tr}\Big(\tau^x_\uparrow\,\mathrm{e}^{-\beta H_1(U,\mu,h,V_{2\uparrow},V_{2\downarrow})}\,\tau^x_\uparrow\,\mathbb{P}\Big) \\ &= \mathrm{Tr}\Big(\tau^x_\uparrow\,\tau^x_\downarrow\,\mathrm{e}^{-\beta H_1(U,\mu,h,V_{2\uparrow},V_{2\downarrow})}\,\tau^x_\downarrow\,\tau^x_\uparrow\,\mathbb{P}\Big)\,. \end{aligned} \qquad (13)$$

Since $1 = \mathbb{P} + \tau^x_\uparrow \mathbb{P} \tau^x_\uparrow + \tau^x_\downarrow \mathbb{P} \tau^x_\downarrow + \tau^x_\uparrow \tau^x_\downarrow \mathbb{P} \tau^x_\downarrow \tau^x_\uparrow$, it readily follows that

$$Z(U,\mu,h,V_{2\uparrow},V_{2\downarrow}) = \frac{1}{4}\,\mathrm{Tr}\Big(\mathrm{e}^{-\beta H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow})}\Big)\,. \quad (14)$$

The Eq. (14) is our main result. It states that the partition function of the original impurity model (5) can be calculated *without any constraint* through the partition function of the model (9).
Following the same line of reasoning, we can demonstrate that also the physical single-particle Green's functions in imaginary time τ of the impurity can be calculated through the Green's functions of the composite operators $\tau^x_\sigma\, d_\sigma$ and $\tau^y_\sigma\, d_\sigma$ in the slave-spin representation without constraints. In particular (details can be found in the Supplemental Material[15])

$$\begin{aligned}\mathcal{G}_\sigma(\tau) &= -\big\langle\, \mathrm{T}\Big(d_\sigma(\tau)\, d^\dagger_\sigma(0)\Big)\,\big\rangle \\ &= -\big\langle\, \mathrm{T}\Big(\tau^x_\sigma(\tau)\, d_\sigma(\tau)\, \tau^+_\sigma(0)\, d^\dagger_\sigma(0)\Big)\,\big\rangle_2\,,\end{aligned} \quad (15)$$

where $\tau^+_\sigma = \tau^x_\sigma + i\tau^y_\sigma$, and $\langle \ldots \rangle_2$ denotes the thermal average with the Boltzmann distribution of H_2 in Eq. (9) and with the operators propagating in imaginary time with that same Hamiltonian.

A. An equivalent representation

The Hamiltonian Eq. (9) lacks a clear separation between charge and spin degrees of freedom that is desirable above all when the interaction U is large. The latter is coupled to the combination $\tau^z_\uparrow \tau^z_\downarrow$, which is therefore the actual operator that controls the large-U freezing of valence fluctuations. Since $\tau^z_\uparrow \tau^z_\downarrow$ is still an Ising variable, with value ± 1, we can exploit a convenient change of variables and define, following Ref. 16,

$$\begin{aligned} &\tau^z_\uparrow \tau^z_\downarrow = -\sigma^z\,, \quad \tau^z_\uparrow = \tau^z\,, \qquad \tau^z_\downarrow = -\tau^z\,\sigma^z\,, \\ &\qquad\qquad \tau^x_\uparrow = \tau^x\,\sigma^x\,, \quad \tau^x_\downarrow = \sigma^x\,, \\ &\qquad\qquad \tau^y_\uparrow = \tau^y\,\sigma^x\,, \quad \tau^y_\downarrow = -\tau^z\,\sigma^y\,. \end{aligned} \quad (16)$$

After this transformation, Eq. (9) changes into

$$\begin{aligned} H_2(U,\mu,h,V_{2\uparrow},V_{2\downarrow}) = &\sum_{\mathbf{k}\sigma}\Bigg[\epsilon_{\mathbf{k}\sigma}\Big(c^\dagger_{1\mathbf{k}\sigma}\, c_{2\mathbf{k}\sigma} + H.c.\Big) \\ &+\sigma^x\big(\tau^x\,\delta_{\sigma\uparrow} + \delta_{\sigma\downarrow}\big)\, V_{1\mathbf{k}\sigma}\Big(d^\dagger_\sigma\, c_{1\mathbf{k}\sigma} + H.c.\Big) \\ &+i\,\big(\tau^y\,\sigma^x\,\delta_{\sigma\uparrow} - \tau^z\,\sigma^y\,\delta_{\sigma\downarrow}\big)\, V_{2\mathbf{k}\sigma}\Big(d^\dagger_\sigma\, c_{2\mathbf{k}\sigma} - H.c.\Big)\Bigg] \\ &-\frac{U}{4}\,\sigma^z - \Big[\frac{\mu}{2}\big(1-\sigma^z\big) + \frac{h}{2}\big(1+\sigma^z\big)\Big]\,\tau^z\,, \end{aligned} \quad (17)$$

where $\delta_{\sigma\sigma'}$ is the Kronecker delta. Eq. (17) notably simplifies when $V_{2\sigma} = 0$. In this case $\mathcal{P}_\uparrow = \tau^z\,\big(2n_\uparrow - 1\big)$, with eigenvalues $p_\uparrow = \pm 1$, is conserved, and moreover the two subspaces with $p_\uparrow = \pm 1$ are actually related by the p-h transformation $\mathcal{C}_\uparrow$ Eq. (6). Therefore, following exactly the same steps as before but in the reverse order, we conclude that the partition function of the original model Eq. (5) at $V_{2\sigma} = 0$ can be calculated as

$$Z(U,\mu,h,0,0) = \frac{1}{2}\,\mathrm{Tr}\Big(\mathrm{e}^{-\beta H_1(U,\mu,h)}\Big)\,, \quad (18)$$

where

$$\begin{aligned} H_1(U,\mu,h) = &\sum_{\mathbf{k}\sigma}\Bigg[\epsilon_{\mathbf{k}\sigma}\Big(c^\dagger_{1\mathbf{k}\sigma}\, c_{2\mathbf{k}\sigma} + H.c.\Big) \\ &+\sigma^x\, V_{1\mathbf{k}\sigma}\Big(d^\dagger_\sigma\, c_{1\mathbf{k}\sigma} + H.c.\Big)\Bigg] \\ &-\frac{U}{4}\,\sigma^z - \Big[\frac{\mu}{2}\big(1-\sigma^z\big) + \frac{h}{2}\big(1+\sigma^z\big)\Big]\,\big(2n_\uparrow - 1\big)\,, \end{aligned} \quad (19)$$

involves now a single auxiliary Ising variable. The mapping Eq. (18) with the Hamiltonian (19) generalises the results obtained in Ref. 8 in the presence of a chemical shift of the impurity level, both spin independent and dependent.

B. Extension to multi-orbital impurity models

The mapping in Sec. III can be straightforwardly extended to a multi-orbital impurity model with Hamiltonian

$$\begin{aligned} H = H_{\mathrm{imp}} &+ \sum_{\mathbf{k}\sigma}\sum_{\alpha=1}^{M} \epsilon_{\alpha\mathbf{k}\sigma}\,\Big(c^\dagger_{1\alpha\mathbf{k}\sigma}\, c_{2\alpha\mathbf{k}\sigma} + H.c.\Big) \\ &+ \sum_{\mathbf{k}\sigma}\sum_{a=1}^{2}\sum_{\alpha=1}^{M} V_{a\alpha\mathbf{k}\sigma}\Big(d^\dagger_{\alpha\sigma}\, c_{a\alpha\mathbf{k}\sigma} + H.c.\Big)\,, \end{aligned} \quad (20)$$

in the simple and not very realistic case where the isolated impurity Hamiltonian H_{imp} involves only the occupation numbers $n_{\alpha\sigma} = d^\dagger_{\alpha\sigma}\, d_{\alpha\sigma}$, where $\alpha = 1,\ldots,M$ is the orbital index, i.e. $H_{\mathrm{imp}} = H_{\mathrm{imp}}\Big(\{n_{\alpha\sigma}\}\Big)$, does not include Coulomb exchange terms. In this circumstance we can exploit the p-h transformations Eq. (6) for each orbital species and follows exactly the same reasoning as in Sec. III to show that the partition function Z of the Hamiltonian (20) can be calculated through

$$Z = \left(\frac{1}{2}\right)^{2M}\,\mathrm{Tr}\Big(\mathrm{e}^{-\beta H_*}\Big)\,, \quad (21)$$

where

$$\begin{aligned} H_* \;=\; &H_{\mathrm{imp}}\big(\{\tau^z_{\alpha\sigma}\}\big) + \sum_{\alpha\mathbf{k}\sigma}\epsilon_{\mathbf{k}\alpha\sigma}\Big(c^\dagger_{1\alpha\mathbf{k}\sigma}\, c_{2\alpha\mathbf{k}\sigma} + H.c.\Big) \\ &+\sum_{\alpha\mathbf{k}\sigma}\Bigg[\tau^x_{a\sigma}\, V_{1\mathbf{k}a\sigma}\Big(d^\dagger_{a\sigma}\, c_{1\mathbf{k}a\sigma} + H.c.\Big) \\ &+i\tau^y_{a\sigma}\, V_{2\mathbf{k}a\sigma}\Big(d^\dagger_{a\sigma}\, c_{2\mathbf{k}a\sigma} - H.c.\Big)\Bigg]\,. \end{aligned} \quad (22)$$

IV. MEAN FIELD SOLUTION

To highlight the importance of a mapping without constraints, we here study the simple case where the bath and the hybridisation are both p-h invariant and the only source of p-h asymmetry is either a Zeeman splitting h or a chemical shift μ of the impurity level. The Hamiltonian is therefore that in Eq. (5) at finite $h \gtrsim 0$ but $\mu = 0$, or vice versa, with $V_{2\mathbf{k}\sigma} = 0$ and spin-independent $\epsilon_{\mathbf{k}\sigma} = \epsilon_{\mathbf{k}}$ and $V_{1\mathbf{k}\sigma} = V_{\mathbf{k}}$.

We mention that the mean-field approach to the standard slave-boson representation of such Hamiltonian at $h = \mu = 0$ erroneously yields at large U a negative magnetic susceptibility $\chi_{\rm imp} < 0$, see Supplemental Materials[15] for details, signalling instability of the paramagnetic solution towards spontaneous spin polarisation[17]. This is the tangible evidence that imposing the constraint *on average* may lead to wrong results.

Let us consider instead our mapping onto the equivalent Hamiltonians (17) and (19), which do not require any constraint to be imposed. The simplest mean-field approach consists in approximating the ground state wavefunction with a factorised one product of a fermionic part $|\,\Psi\rangle$ times an Ising one $|\,\Phi\rangle$. However, such an approximation is physically sound as long as the two subsystems are controlled by well separated energy scales, otherwise we have no guarantee that the fluctuations beyond mean field are negligible. This is indeed realised in model (19) when U is large. On the contrary, a sharp distinction of energy scales is absent in the equivalent representation Eq. (17), where, after mean-field decoupling, the Ising sector $\big(\boldsymbol{\tau},\boldsymbol{\sigma}\big) \equiv \big(\boldsymbol{\tau}_\uparrow,\boldsymbol{\tau}_\downarrow\big)$ always contains excitation energies within the resonant level spectral width. Therefore, even though Eq. (17) is equivalent to Eq. (19), the mean-field approximation is only justified in the latter model and when U is large, which we shall consider hereafter.

Within mean-field applied to model (17), if we denote as

$$\sin\theta = \langle\Phi|\,\sigma^x\,|\Phi\rangle\,, \qquad \cos\theta = \langle\Phi|\,\sigma^z\,|\Phi\rangle\,, \tag{23}$$

then the optimal $|\,\Psi\rangle$ is the ground state of the Hamiltonian

$$H_* \;=\; \sum_{\mathbf{k}\sigma}\left[\epsilon_{\mathbf{k}\sigma}\,c^\dagger_{\mathbf{k}\sigma}\,c_{\mathbf{k}\sigma} + \sin\theta\,V_{\mathbf{k}}\Big(d^\dagger_\sigma\,c_{\mathbf{k}\sigma} + c^\dagger_{\mathbf{k}\sigma}\,d_\sigma\Big)\right] - \epsilon\,\big(1\pm\cos\theta\big)\left(n_\uparrow - \frac{1}{2}\right),$$

where the plus sign applies to $\epsilon = h$, while the minus to $\epsilon = \mu$. Assuming, as usual, that the hybridisation function $\Delta(\omega)$ with the bath can be approximated as

$$\Delta(\omega) = \sum_{\mathbf{k}}\,\frac{V^2_{\mathbf{k}}}{\omega - \epsilon_{\mathbf{k}} + i0^+} \simeq -i\,\Gamma_0\,\theta\big(D - |\omega|\big)\,, \tag{24}$$

where the cut-off D is of the order of the conduction bandwidth, we readily find that

$$E_*(\theta) \equiv \langle\Psi|\,H_*\,|\Psi\rangle = E_0 - \epsilon_\uparrow(\theta)\,\left(n_\uparrow(\theta) - \frac{1}{2}\right) - \frac{\Gamma(\theta)}{\pi}\left[\ln\frac{\mathrm{e}D}{\Gamma(\theta)} + \ln\frac{\mathrm{e}D}{\sqrt{\epsilon_\uparrow(\theta)^2 + \Gamma(\theta)^2}}\right], \tag{25}$$

where E_0 is the bath-energy in the absence of impurity, $\Gamma(\theta) = \sin^2\theta\,\Gamma_0$ and

$$\epsilon_\uparrow(\theta) = \epsilon\,\big(1\pm\cos\theta\big)\,, \quad n_\uparrow(\theta) - \frac{1}{2} = \frac{1}{\pi}\,\tan^{-1}\frac{\epsilon_\uparrow(\theta)}{\Gamma(\theta)}\,.$$

The variational energy is therefore

$$E(\theta) = \langle\Phi|\,\langle\Psi|\,H_1(U,0,h)\,|\Psi\rangle\,|\Phi\rangle = E_*(\theta) - \frac{U}{4}\,\cos\theta\,,$$

which we still have to minimise with respect to θ. It is more convenient to use $\Gamma = \Gamma\big(\theta(\Gamma)\big)$ as variational parameter, which leads to the saddle-point equation

$$0 = \frac{\partial E(\Gamma)}{\partial\Gamma} = -\frac{1}{\pi}\left[\ln\frac{D}{\Gamma} + \ln\frac{D}{\sqrt{\epsilon_\uparrow\big(\theta(\Gamma)\big)^2 + \Gamma^2}}\right] + \left(\frac{U}{4} \pm \frac{\epsilon}{\pi}\,\tan^{-1}\frac{\epsilon_\uparrow\big(\theta(\Gamma)\big)}{\Gamma}\right)\frac{1}{2}\,\frac{1}{\sqrt{\Gamma_0^2 - \Gamma_0\,\Gamma}}\,. \tag{26}$$

For large U the solution of Eq. (26) at $\epsilon \ll \Gamma$ reads

$$\Gamma(\epsilon) \simeq \Gamma(0) - \frac{\epsilon^2}{4\Gamma(0)}\left(1 \pm \sqrt{1 - \Gamma(0)/\Gamma_0}\,\right)^2, \tag{27}$$

where $\Gamma(0) \simeq D\,\exp\big[-\pi U/16\Gamma_0\big]$ is the same as in slave-boson mean-field theory, and can be associated with the Kondo temperature T_K, though overestimated with respect to its actual value[9]. The susceptibility to the field ϵ readily follows

$$-\frac{\partial^2 E}{\partial\epsilon^2}\Big|_{\epsilon=0} \simeq \frac{1}{\pi\Gamma(0)}\left(1 \pm \sqrt{1 - \Gamma(0)/\Gamma_0}\,\right)^2. \tag{28}$$

Since $\Gamma_0 \gg \Gamma(0)$ for $U \gg \Gamma_0$, the impurity contribution to charge $\kappa_{\rm imp}$, $\epsilon = \mu$ and minus sign, and spin $\chi_{\rm imp}$, $\epsilon = h$ and plus sign, susceptibilities become

$$\kappa_{\rm imp} \simeq \frac{\Gamma(0)}{4\pi\Gamma_0^2} \simeq 0\,, \qquad \chi_{\rm imp} \simeq \frac{4}{\pi\Gamma(0)}\,\left(1 - \frac{\Gamma(0)}{2\Gamma_0}\right) \simeq \frac{4}{\pi\Gamma(0)}\,. \tag{29}$$

We emphasize that $\chi_{\rm imp}$ is positive, unlike in slave-boson mean-field theory. The impurity contribution to the specific heat at low temperature only comes from the fermionic degrees of freedom and reads explicitly

$$c_{\rm imp} \simeq \frac{2\pi^2}{3}\,\frac{T}{\pi\Gamma(0)}\,, \tag{30}$$

thus a Wilson ratio $R_W = 2$ at large U, in agreement with the exact value.
According to Nozières' Fermi liquid description of the Kondo effect[18], see also Ref. 19,

$$\kappa_{\rm imp} = 2\rho_* \left(1 - A^{\rm S}\right), \qquad \chi_{\rm imp} = 2\rho_* \left(1 - A^{\rm A}\right), \quad (31)$$

where $\rho_* = 1/\pi\Gamma(0) = Z\rho_0$ is the quasiparticle density of states at the chemical potential, as opposed to its *bare* value $\rho_0 = 1/\pi\Gamma_0$, with $Z = \sin^2\theta \ll 1$ the quasiparticle residue; while $A^{\rm S}$ and $A^{\rm A}$ the quasiparticle scattering amplitudes in the symmetric (S) and antisymmetric (A) channels, respectively. The mean-field results (29) are thus compatible at large U with

$$A^{\rm S} = -A^{\rm A} = 1\,, \quad (32)$$

which, together with Eq. (30), are the bases of Nozières' local Fermi liquid theory of the Kondo effect[18], which has been successfully exploited in very many contexts, not least to derive universal properties in transport across quantum dots[20,21]. We emphasise that the universal values in Eq. (32) simply follows from the expressions of the impurity charge and spin density vertices, the former proportional to $(1 - \sigma^z)$ and the latter to $(1 + \sigma^z)$, and the fact that, at large U, $\sigma^z \simeq 1$ with negligible fluctuations. As a result, the mean-field solution, $\sigma^z \to \langle\sigma^z\rangle$, already captures the leading vertex corrections, which is indeed remarkable. By contrast, the mean-field approximation does not allow recovering the non-universal corrections to the Kondo regime, which are polynomials in $1/U$ for large U[22,23]. These corrections are sub-leading in the spin susceptibility, but leading in the charge one, see Eq. (29).

We conclude by mentioning that the model Eq. (19) can be still viewed as a dissipative two-level system[10] in a sub-ohmic bath, as it was the case at $\epsilon = 0$[9]. Each potential well corresponds to a value of $\sigma^x = \pm 1$, while σ^z induces quantum tunnelling between the two wells. Localisation inside a well is signalled by a finite expectation value of σ^x, and also corresponds to spontaneous breakdown of the local Z_2 gauge symmetry $\sigma^x \to -\sigma^x$ and $d_\sigma \to -d_\sigma$. The Kondo temperature $T_K \sim \langle\sigma^x\rangle^2$ thus plays the role of a *bona fide* order parameter.
In this language, the field ϵ translates into an assisted tunnelling that does hamper localisation but, at least within mean-field, cannot impede it, as shown in Fig. 1 for the case of a Zeeman splitting $\epsilon = h$, where we plot the mean field values of $\Gamma(h) \sim \langle\sigma^x\rangle_h^2$ and magnetisation $m(h)$. We believe that the persistence of Z_2 gauge-symmetry breaking even in the presence of the assisted tunnelling is real and not just an artefact of mean field.

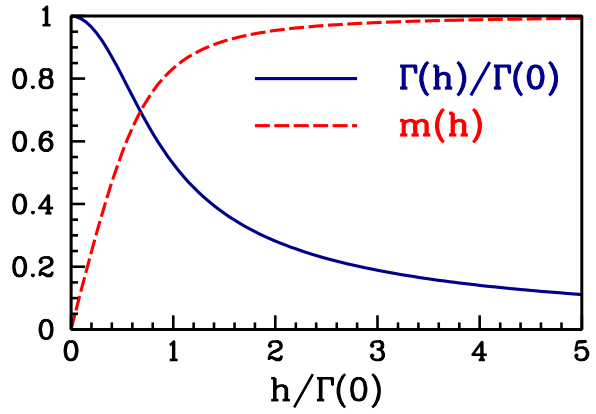

FIG. 1: Mean field values of the effective hybridisation width $\Gamma(h)$ and magnetisation $m(h)$ as function of the magnetic field h. The parameters are $U = 0.1$ and $\Gamma_0 = 1.96 \times 10^{-3}$ in units of the cutoff D, which correspond to $\Gamma(0) \equiv T_K \simeq 4.1 \times 10^{-5}$.

V. CONCLUSIONS

We have shown that a generic single-orbital Anderson impurity model can be mapped without any constraint onto a resonant level model coupled to two Ising spins, or just one in the simpler case when the hybridisation with the bath is particle-hole symmetric. The mean-field decoupling of electrons from the Ising variables is able to reproduce quite accurately the magnetic properties of the model even deep inside the large-U Kondo regime, specifically the finite susceptibility $\chi \sim 1/T_K$ and Wilson ratio $R_{\rm W} = 2$. By comparison, in the same Kondo regime conventional slave-boson mean-field theory yields a spin-polarised lowest energy solution that unphysically breaks spin $SU(2)$ symmetry.
We also demonstrate how single-particle Green's functions of the physical fermions can be calculated without constraints, which would for instance allow exploiting DMFT to study in the slave-spin representation[12] particle-hole non-symmetric Hubbard-like models in lattices with infinite coordination. This could in some cases be more convenient than directly working within the physical Hilbert space, though smaller, especially when one wants to prevent spontaneous symmetry breaking that usually accompanies a Mott transition, since the slave-spin Hamiltonian Eq. (9) is particle-hole symmetric in terms of the auxiliary fermions, despite the Hamiltonian of the physical electrons is not.

Acknowledgments

This work has been supported by the European Union under H2020 Framework Programs, ERC Advanced Grant No. 692670 "FIRSTORM".

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