Few-body nature of Kondo correlated ground states

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The quenching of degenerate impurity states in metals generally induces a long-range correlated quantum state known as the Kondo screening cloud. While a macroscopic number of particles clearly take part in forming this extended structure, assessing the number of truly entangled degrees of freedom requires a careful analysis of the relevant many-body wavefunction. For this purpose, we examine the natural single-particle orbitals that are eigenstates of the single-particle density (correlation) matrix for the ground state of two quantum impurity problems: the interacting resonant level model (IRLM) and the single impurity Anderson model (SIAM). As a simple and general probe for few-body versus many-body character we consider the rate of exponential decay of the correlation matrix eigenvalues towards inactive (fully empty or filled) orbitals. We find that this rate remains large in the physically most relevant region of parameter space, implying a few-body character. Genuine many-body correlations emerge only when the Kondo temperature becomes exponentially small, for instance near a quantum critical point. In addition, we demonstrate that a simple numerical diagonalization of the few-body problem restricted to the Fock space of the most correlated orbitals converges exponentially fast with respect to the number of orbitals, to the true ground state of the IRLM. We also show that finite size effects drastically affect the correlation spectrum, shedding light on an apparent paradox arising from previous studies on short chains.

I. INTRODUCTION

Strongly interacting quantum many-body systems constitute one of the most challenging problems in physics. The combination of a macroscopic number of particles with interactions that are relevant in the renormalization sense puts paid to strategies involving the most commonly used tools of quantum mechanics (perturbation theory, exact diagonalization). Over the past decades, advanced numerical methods have been tailored to reliably extract physical information of interacting fermion models, from the Numerical Renormalization Group (NRG) [1] and Density Matrix Renormalization Group [2] in low dimensions, to continuous time quantum Monte Carlo simulations [3] within the Dynamical Mean Field Theory [4] for higher connectivity lattices. While answering many physical questions, these methods have not yet fully characterized the link between strong correlations and physical complexity for generic quantum many-body systems.

Some classes of problems that are insurmountable by brute force can be tackled due to a hidden simplicity of the physically relevant states (e.g. ground and low-lying thermal states). Indeed, diagnostic tools such as entanglement measures [5] have shown that the Density Matrix Renormalization group [6–9] owes its success to the matrix-product state structure of ground states of locally interacting one dimensional lattices. Insights about entanglement between spatially distinct regions have subsequently lead to a deep understanding of the matrix and tensor product state structure of translationally invariant low-dimensional interacting ground states. The conceptual understanding of inhomogeneous systems is less complete, as is attested to by the ongoing work on many-body localization. [10] A simple starting point for studying non-uniform many-body states is the class of systems known as quantum impurity models [11, 12]: while strong interactions are limited to few local sites, scattering from electronic reservoirs generates complex quantum states showing long-range spatial entanglement, dubbed the Kondo screening cloud [13]. The question of quantifying the amount of correlations contained in such a non-local many-body impurity state has not yet been addressed exhaustively [14–16]. In this Article, we answer the question “How many of the particles in the Kondo cloud are correlated with each other or with the impurity in the quantum many-body sense?”

Given the central position that the Kondo problem occupies in many-body physics, it may seem the answer is obvious: many electrons become correlated. After all, the Kondo screening cloud is typically much larger than the Fermi wavelength and thus encompasses many conduction electrons. However, recent studies have come to a different and seemingly paradoxical conclusion [17, 18]. These works considered the one-body density matrix (also called the correlation matrix) [19–21] of the Kondo problem. Its eigenvectors define an optimal set of single-particle orbitals that are commonly referred to as “natural orbitals” in the quantum chemistry literature [22]. The associated eigenvalues are ground state occupation numbers for the natural orbitals. If an occupation number is close to zero or one, i.e. nearly empty of filled, the corresponding orbital is not involved in many-body correlations, and is therefore said to be inactive. The remaining orbitals are called active and host correlated particles. One study [18] found that there is a single active orbital that is “solely responsible for screening the impurity spin in both the weak and strong Kondo coupling regime”, and that the resulting singlet is disentangled from the rest of the system. The authors of another study [17] similarly report that they have identified “a dominant single
We will show that this proposed single-correlated-orbital picture at weak coupling is purely a finite size effect (here weak coupling means small exchange interaction, so that the Kondo temperature is exponentially low). Indeed, in the works quoted, systems consisting of at most a few hundred real-space lattice sites were studied. However, the Kondo length becomes quickly larger than this system size when the dimensionless Kondo coupling is reduced to values below unity. When this happens, Kondo correlations cannot fully develop, and many-body effects are dramatically reduced compared to the thermodynamic limit. Clearly, a systematic characterization of the active space of Kondo-correlated systems in the thermodynamic limit is still lacking, and this will be one important goal of our study. We point out that the question we are asking concerns how to express microscopically the ground state of the system in terms of the complete set of bare degrees of freedom, used to define the model. It is of course well-known that the effective description of excitations at energies sufficiently smaller than the Kondo temperature, is that of a Fermi liquid.

We have devised the following method to determine the number of particles taking part in ground state correlations. We use the NRG to calculate the correlation matrix of a fermionic quantum impurity model. We are particularly interested models that display Kondo correlations. The Wilson grid discretization [12] employed by NRG allows us to study systems with a real-space size that grows exponentially with the dimension of the single-particle Hilbert space. We are thus able to obtain results for the correlation matrix that are converged to the thermodynamic limit. We then use the eigenvectors of the correlation matrix to construct a trial state containing M active orbitals on top of an uncorrelated Fermi sea. At half-filling, minimizing the energy expectation value of the trial state is equivalent to exactly diagonalizing an M/2-particle problem in the subspace of active orbitals. The resulting variational energy is compared to the true ground state energy (very accurately calculated with NRG). If the energy difference is much less than the Kondo temperature, then the trial state is an accurate approximation to the true ground state. When this is the case, we conclude that at most M orbitals (M/2 particles) take part in correlations.

We have carried out the above procedure for the interacting resonant level model (IRLM) that displays bona fide Kondo correlations in its charge sector. What we find is surprising: while the picture of a single orbital screening the impurity (advocated in Refs.17 and 18) does not apply in general, neither does the pessimistic view that Kondo correlations involve a macroscopic number of electrons within the large screening cloud. For a realistic Kondo temperature of $10^{-3}$ of the ultraviolet scale set by the Fermi energy, we find that a trial state with only 7 correlated particles approximates the ground state energy to an accuracy of 1% of the Kondo temperature. Only when one reaches unrealistic regimes where the Kondo temperature becomes exponentially small, does the number of correlated particles in the ground state increase beyond a handful, making impractical a description in terms of natural orbitals. This observation suggests that Fermi liquid ground states of quantum impurity models in the thermodynamic limit are for practical purposes few-body in nature, thus neither single-body nor many-body, once reformulated in the optimal space of natural orbitals.

An important question concerns whether these results are a general feature of Kondo physics, or specific to the IRLM. Arguably, mapping the IRLM to the anisotropic Kondo model might yield a more correlated state than the IRLM ground state. Indeed since IRLM fermions are non-linear and non-polynomial functions of the bare fermions of the Kondo model, a few-body correlated IRLM ground state might translate into a truly many-body correlated ground state in the Kondo representation. For instance, the Toulouse point of the Kondo model is certainly non-trivial in the original Kondo framework, while it involves completely free fermions on the IRLM side. We have therefore also studied the Anderson impurity model (SIAM), that displays Kondo correlations in its spin sector.

Our study of the SIAM again reveals an exponential decay of the natural orbitals to full occupancy or vacancy for any finite Kondo temperature. Our conclusions are therefore not specific to the IRLM, and pertain to other quantum impurity models displaying a Fermi liquid ground state.

The rest of this Article is structured as follows. In Section II we introduce the IRLM, and discuss its equivalence to the single channel Kondo model. We also review general properties of the correlation matrix for quantum impurity models. In Section III, we examine numerical results for the correlation matrix spectrum, using systematic NRG calculations. Special attention is paid to finite size effects (extra technical details are given in several appendices). In Section IV, we propose a few-body Ansatz based on natural orbitals, which shows exponential convergence to the numerically exact multi-particle wavefunction describing our NRG results. Section VI contains our results for the correlation matrix of the SIAM, which shows that our conclusions are not specific to the IRLM. Section VI summarizes our main findings and identifies promising directions for future research.

## II. GENERALITIES ON THE CORRELATION MATRIX

A simple setting to probe Kondo correlated states is the interacting resonant level model [23] (IRLM):

$$
\mathcal{H} = U \left( d^\dagger d - \frac{1}{2} \right) \left( c^\dagger_0 c_0 - \frac{1}{2} \right) + V \left( d^\dagger c_0 + c^\dagger_0 d \right) + \sum_{i=1}^{N-2} t_i \left( c^\dagger_i c_{i-1} + c^\dagger_{i-1} c_i \right),
$$

(1)
involving spinless fermions on a tight binding chain of \( N \) sites (including the \( d \)-level as site \( i = -1 \)). Both Coulomb interaction \( U \) and tunneling \( V \) couple the resonant level \( d^l \) to the local orbital \( c^d_{ij} \) at the start of the chain. Despite the absence of spin degrees of freedom, the IRLM can be mapped onto the spin-anisotropic Kondo model [24–26]. The mapping is exact for energy scales below the ultraviolet scale set by the Fermi energy measured from the bottom of the band, provided the Kondo coupling times the density of states is sufficiently small, i.e. one is in the universal Kondo regime. The equivalence relies on spin-charge separation in the Kondo model, with only spin-density fluctuations coupling to the magnetic impurity. This subsystem is then bosonized and refermionized in terms of spinless fermions. The procedure was first outlined in [27]. For a recent review, including careful bookkeeping of phases generated by fermion exchange, see for instance [28]. This equivalence has been used in the past to study some delicate facets of the Kondo problem with high accuracy, for instance quench dynamics [29]. In the present context, the spinless nature of the IRLM facilitates the bookkeeping that is necessary to compute accurately the correlation matrix.

To introduce the correlation matrix, it is helpful to first consider the properties of uncorrelated fermionic states. These can be viewed as single Slater determinants, characterized by a set of one-particle orbitals \( q^i_m \) that are each either filled or empty. The orbitals are linear combinations of the physical orbitals \( c^d_{ij} \) used to construct the Hamiltonian, e.g. the lattice site basis, \( q^i_m = \sum_j U_{mj} c^d_{ij} \). Introducing the correlation matrix matrix of the physical orbitals \( Q_{ij} = \langle c^d_{ij} c^d_{ji} \rangle \), it is clear that for a Slater determinant one obtains \( \sum_{ij} U^*_{m_j} U_{n_i} Q_{ij} = \langle q^i_m q^i_n \rangle = \lambda_n \delta_{n,m} \) with \( \lambda_n = 0 \) or 1, depending whether orbital \( q^i_m \) is empty or filled. Note that \( Q \) is proportional to the one-particle reduced density matrix. Recent studies have used the correlation matrix as a tool to study quantum impurity problems [18–20]. For a general many-body state, the eigenvalues \( \lambda_n \) of the correlation matrix \( Q \) define occupancies between zero and one. The number of eigenvalues significantly different from zero or one provides a sensitive measure of correlations, while the associated eigenvectors of \( Q \) define the single-particle basis in which correlations are most economically represented [19]. It is worth pointing out that many NRG studies of impurity models focus on observables associated with the impurity degree of freedom only. The \( N \times N \) matrix elements \( Q_{i,j} = \langle c^d_{ij} c^d_{ji} \rangle \) (where \( i, j \in \{-1, 0, \ldots, N-2\} \) and \( c_{-1} \equiv d \)) involve observables in the environment \((i,j > -1)\) and observables that are hybridized between the impurity and the environment \((i = -1, j > -1, j = -1, i > -1)\). Calculating \( Q \) using NRG is therefore more involved than the standard NRG analysis of impurity problems.

Let us focus now on the general properties of the correlation matrix \( Q \). Clearly, its eigenvalues \( \lambda_n \) are independent of the choice of one-particle orbitals used in its definition. Since the eigenvalues \( \lambda_n = \langle q^i n | q^i n \rangle \) correspond to occupancies of the natural orbitals, they belong to the interval \([0,1]\). As mentioned before, the eigenvalues are either zero or one for a Slater determinant, and their departure from these trivial values signal that the associated orbitals participate in quantum many-body correlations. As a simple example, consider the Bell-like state:

\[
\Psi = \frac{1}{\sqrt{2}} \left( c^d_{1i} c^d_{2j} + c^d_{1j} c^d_{2i} \right) |\Phi\rangle
\]

with \(|\Phi\rangle\) a Slater determinant that does not involve orbitals \(i, j, k, l\) (considered distinct from each other). It is easy to check that for this state \( Q \) has four eigenvalues different from zero or one, that are all equal to 1/2. The IRLM Hamiltonian (1) manifests particle-hole symmetry \( H = P^\dagger HP \), where \( P \) is the unitary and hermitian particle-hole conjugation operator:

\[
P = \prod_{i=0}^{N-1} \left( c_{2i-1} - c^\dagger_{2i-1} \right) \left( c_{2i} + c^\dagger_{2i} \right),
\]

acting as \( P^\dagger c_i P = (-1)^i c^\dagger_i \) and \( P |0\rangle = c^\dagger_{0} \cdots c^\dagger_{N-2} |0\rangle \). Since \( P^2 = 1 \), the eigenvalues of \( P \) are \( \pm 1 \), and we have \( Q_{ij} = \delta_{ij} - (-1)^{i+j} Q_{ji} \), thus the diagonal entries of \( Q \) are all equal to 1/2. Furthermore the matrix elements of the Hamiltonian \( H \) are all real in the Fock-space basis built from \( c^\dagger_i \) operators and hence the expansion coefficients of the eigenstates of \( H \) in this basis are real too. This implies \( Q_{ij} = Q_{ji} \), and from the particle-hole symmetry of \( Q \), we conclude that \( Q_{ij} = 0 \) for \( i + j \) even and \( i \neq j \).

Owing to particle-hole symmetry the eigenvalues of \( Q \) then come in pairs \( 1/2 \pm r \).

![FIG. 1. Top panel: Spectrum of \( \tilde{Q} \) for the IRLM at various values of interaction \( U \) for \( V = 0.15 \), in units of the half bandwidth \( D = 1 \). The right side shows eigenvalues \( 0 < \lambda_n < 1/2 \), while the left side shows \( 1 - \lambda_n \) for \( 1/2 < \lambda_n < 1 \), thus exhibiting particle-hole symmetry explicitly. Apart from four strongly correlated orbitals on the plateau (around which the horizontal index \( n \) is centered), the rest of the eigenvalues decay exponentially fast towards either the empty and filled occupancies. In Appendix A it is demonstrated that these results are converged to the continuum and thermodynamic limit \( N \to \infty \), \( \Lambda \to 1 \).](image-url)
III. STUDY OF THE IRLM CORRELATION SPECTRUM

The relatively low computational cost to implement NRG for the IRLM makes it possible to track with high accuracy the flow of the $N^2$ operators $c_i^\dagger c_j$ needed for calculating $\hat{Q}$ with modest computational resources, provided the block-diagonal structure imposed by particle-number conservation is exploited to keep matrix dimensions manageable. Aiming to resolve $\hat{Q}$-eigenvalues that are exponentially small, we calculate the elements of $\hat{Q}$ to a very high precision, allowing up to thousands of kept states after truncation (see Appendix A for a detailed study of the convergence). The NRG implementation is based on the hopping amplitudes along the Wilson chain \[12]:

$$t_j = \frac{(1 + \Lambda^{-1}) (1 - \Lambda^{-j-1})}{2\sqrt{1 - \Lambda^{-2j-1}\sqrt{1 - \Lambda^{-2j-3}}} \Lambda^{-j/2} D},$$

so that $D = 1$ sets the half-bandwidth of the bath and also our Fermi energy. We present here calculations for the Wilson parameter $\Lambda = 1.5$ (a more systematic study is presented in Appendix A), tunneling $V = 0.15 D$, and up to $N = 180$ sites. The lowest energy at play is thus of the order $\Lambda^{-N/2} D \simeq 10^{-16} D$, ensuring convergence to the ground state for all practical purposes.

Fig. 1 displays the full eigenspectrum of $\hat{Q}$, showing on the left side $1 - \lambda_n$ for $1/2 < \lambda < 1$, and on the right side $\lambda_n$ for $0 < \lambda_n < 1/2$, so that particle-hole symmetry becomes apparent. Note that the eigenvalue index $n$ runs from $-N/2$ to $N/2$, excluding $n = 0$, in order to display more clearly the particle-hole conjugation. The general behavior of the particle-hole symmetrized spectrum is as follows. There is an approximate four-fold degeneracy of the highest eigenvalue $\lambda_{\text{max}} \equiv \lambda_1 = 1 - \lambda_{-1}$, indicating Bell-like entanglement between the four most correlated orbitals $q_1^0, q_2^0, q_1^1, q_2^1$ (from our chosen convention, the index $n$ is centered around most correlated orbitals). This is related to the fact that, at negative $U$, the impurity orbital and the first energy shell tend to be either both filled or both empty due to Coulomb attraction, and similarly, at positive $U$, if the impurity orbital is filled, the first energy shell tends to be empty, and vice versa. The other eigenvalues decay exponentially, $\lambda_n \simeq A e^{-x n}$ for $n > 2$ and $\lambda_n \simeq 1 - A e^{\mp x}$ for $n < -2$, with a decay rate $x$ that depends on interaction strength. We show in Appendix A that this exponential decay is not an artefact of the Wilson chain, and is robust in the continuum limit $\Lambda \rightarrow 1$. This behavior of the $\hat{Q}$-eigenvalues has previously been observed in studies of impurity models discretized on regular real space lattices \[18-20\]. We emphasize that the Kondo regime corresponds to $U < 0$ in the IRLM, and indeed the slower decay of the $\hat{Q}$-eigenvalues in Fig. 1 attests that this regime is more correlated than for $U > 0$.

The behavior of $\lambda_{\text{max}}$, the maximum eigenvalue of $\hat{Q}$ in the range $[0, 1/2]$, is displayed as a function of interaction $U$ in Fig. 2, showing that it remains small for all $U > 0$ (this is the weakly correlated sector of the IRLM), vanishes at $U = 0$ (the ground state is a Slater determinant, so that all eigenvalues are trivial), and increases sharply only for $-1.3 < U < -1.0$ due to the approach to the IRLM quantum critical point $U_c \simeq 1.3$ where the Kondo temperature vanishes. Our key observation is that the decay rate $x$ of the $\hat{Q}$-eigenvalues drops to small values only when the Kondo temperature becomes exponentially small, seemingly with a linear vanishing as $|U - U_c|$ (see middle panel), as also shown by the slow inverse logarithmic decrease of $x$ as a function of Kondo temperature (see bottom panel in Fig. 2). Thus, only the quantum critical regime corresponds to a true many-body state as opposed to a few correlated particles on top of an uncorrelated Fermi sea. Larger negative $U < -1.3$ leads to a discontinuous transition to a phase where particle-hole symmetry is broken (corresponding to the ferromagnetic phase of the Kondo Hamiltonian), involving clearly less
correlations due to a jump of the decay rate $x$ to finite values.

Our results are seemingly inconsistent with results for the Kondo model reported in [17, 18]. According to these studies, $x$ should become large close to the phase transition, whereas we find that it vanishes. To shed light on the apparent paradox, we show in Fig. 3 the spectrum of $Q$ as a function of the number $N$ of Wilson chain sites. The real space system size is $\Lambda^{N/2}$. Here we used $\Lambda = 2.25$ and picked a point $U = -1.2$ close to the critical point. For this choice, the Kondo length has the astronomically large value $1/T_K = 10^{13}$, which matches the system size when $N = 75$. In Appendix C we explain how the Kondo temperature $T_K$ is calculated.) For $N$ significantly smaller than 75, we see very quick exponential decay of the spectrum, corresponding to large $x$ and a ground state with few correlated particles. However, when $N$ increases beyond 75, the decay rate $x$ soon saturates to a small value, so that a large number of correlated particles participate in the true ground state in the thermodynamic limit. These finite size artifacts explain the results reported in [17, 18] where real space lattices with at most a few hundred sites were studied, leading to system sizes of the order of a hundred times the Fermi wavelength. The exponentially diverging Kondo length reaches this order of magnitude long before the weak coupling regime in the vicinity of the critical point is entered. In terms of IRLM parameters, a system size between $10^2$ and $10^3$ times the Fermi wavelength prevents a fully correlated ground state from forming for $U < -0.5$, and leads to a severe overestimate of the decay rate $x$ close to the critical point. Figure 3 clearly establishes that correlations increase when the Kondo cloud becomes more extended, in agreement with intuition.

A standard method for probing Kondo correlations is to perturb the system at the Kondo scale, and to see the effect this has on observables. For instance, a biasing potential $\epsilon_d d_i d_j$ in the IRLM, corresponding to a Zeeman splitting between the spin-up and spin-down states of the magnetic impurity in the Kondo model, prevents formation of the Kondo singlet. The occupancy $\langle d_i d_j \rangle$ (or equivalently the impurity magnetization) reveals significant symmetry breaking when $\epsilon_d$ reaches the Kondo scale. It is intuitively clear that the symmetry breaking in the ground state is a sign of reduced correlations, but the observable $\langle d_i d_j \rangle$ does not directly measure this – one can clearly modify the degree of correlations in the ground state without changing $\langle d_i d_j \rangle$ at half-filling ($\epsilon_d = 0$) when $U$ is changed. The spectrum of $Q$, on the other hand, directly measures correlations. In Fig. 4 we plot the decay rate $x$ of the $Q$-eigenvalues as a function of $\epsilon_d$. The calculation was performed for $U = -1.0$ and $V = 0.15$, which corresponds to $T_K = 1.87 \times 10^{-6}$. We used $\Lambda = 1.5$ which yields a decay rate $x$ that is converged to the $N \to \infty$, $\Lambda \to 1$ limit. For comparison, we also plot $\langle d_i d_j \rangle$ versus $\epsilon_d$ in an inset. We see that $x$ starts changing from its unperturbed value when $\epsilon_d$ exceeds the Kondo temperature. As $\epsilon_d$ increases further, $x$ increases monotonically, indicating that fewer and fewer correlated particles are present, the more severely singlet formation is prevented. In this way, the $Q$ matrix spectrum proves the picture suggested by the $d$-level occupancy $\langle d_i d_j \rangle$.

We now examine the spatial dispersion (along the Wilson chain) of the $Q$-matrix orbitals $q_{j,n} = \sum_i U_{ni} c_i^j$, by plotting the absolute value $|U_{ni}|$ of the eigenvectors obtained from the diagonalization of the matrix $Q_{ij}$ (this also displays particle-hole symmetry more clearly). Fig. 5 shows how correlations spread along the system for four values of the interaction $U$. It is clear from Fig. 5 that all the natural orbitals are highly non-local, and carry information mostly forward along the chain. The most correlated orbitals ($n = 1$ and $n = -1$) are predominantly...
localized near the impurity (site $i = -1$), as expected from the short range of the interaction, but develop also long tails that extend to large distances. For $U > 0$, the spatial structure of correlated orbitals is fairly insensitive to the interaction strength, showing that this regime remains weakly correlated. In contrast, for negative values of the interaction, as we go closer to the quantum critical point $U_c = -1.3$, correlated orbitals become more delocalized, due to the divergence of the Kondo length. In addition, more and more orbitals become entangled, due to the slower decay of the eigenvalues $\lambda_n$ in Fig. 1.

IV. FEW-BODY ANSATZ FROM NATURAL ORBITALS

Equipped with this construction of the natural orbitals of the $Q$-matrix, we establish our most surprising finding, namely that the ground state of the IRLM is few-body in nature for realistic (i.e. non exponentially vanishing) Kondo temperatures. This result is clearly suggested by the exponential decay of the $Q$-matrix eigenvalues in Fig. 1. Since most of the eigenvalues $\lambda_n$ are exponentially close to either zero or one, it seems a good approximation to assume that their associated orbitals are exactly uncorrelated, keeping a core of $M$ truly correlated orbitals within the ground state wave function (those orbitals correspond to the $M$ $\lambda_n$-eigenvalues that are closest to 1/2, and we choose $M$ to be even, which allows for a correlated sector that is exactly half-filled). Specifically, half of the $N - M$ uncorrelated orbitals (the ones that have their eigenvalues closest to 1) will be frozen and described by a Slater determinant $|\Psi_0\rangle = \prod_{n=-M}^{-M/2} q_n |0\rangle$ in the eigenorbitals of the correlation matrix computed by NRG. The other half of the uncorrelated orbitals (those with $\hat{Q}$-eigenvalues closest to 0) are taken as empty. We therefore write the full wave function as follows:

$$|\Psi_{\text{few}}\rangle = \sum_{\{N_n\}} \Psi(N_{-\frac{M}{2}}, \ldots, N_{\frac{M}{2}}) \prod_{n=-\frac{M}{2}}^{M} [q_n]^{N_n} |\Psi_0\rangle,$$

with $N_n = 0, 1$ the occupancy of correlated orbital $q_n^\dagger$, the summation restricted to occupations such that $\sum_{n=-M/2}^{M/2} N_n = M/2$, and $\Psi(N_{-\frac{M}{2}}, \ldots, N_{\frac{M}{2}})$ the complete few-body wave function in the correlated subspace.

The Hamiltonian can be re-expressed within the $q_n^\dagger$ orbitals, and then exactly divided into three pieces: $\mathcal{H} = H_{\text{corr}} + H_{\text{uncorr}} + H_{\text{mix}}$, depending on whether the indices $n$ act only within the correlated sector (first term), or only within the uncorrelated sector (second term), or mix both sectors (third term). Minimizing $\langle \Psi_{\text{few}} | \mathcal{H} | \Psi_{\text{few}} \rangle$ with respect to the few-body wave function $\Psi(N_{-\frac{M}{2}}, \ldots, N_{\frac{M}{2}})$ yields a variational energy equal to the ground state energy of the few-body Hamiltonian $\mathcal{H}_{\text{few}} = H_{\text{corr}} + \Pi (H_{\text{uncorr}} + H_{\text{mix}}) \Pi$, that acts on states in which electrons occupy correlated orbitals only, with $\Pi = \prod_{m=-\frac{M}{2}}^{-\frac{M}{2} - 1} q_m$. Within the Fock space constructed from correlated orbitals only, $\Pi \mathcal{H}_{\text{uncorr}} \Pi$ is a real number, while $\Pi \mathcal{H}_{\text{mix}} \Pi$ is a quadratic operator (see Appendix B for details). The optimal wavefunction $\Psi(N_{-\frac{M}{2}}, \ldots, N_{\frac{M}{2}})$ can be found by exact diagonalization of the few-body Hamiltonian $\mathcal{H}_{\text{few}}$, which we have done for increasing values of $M$.

The only relevant parameter of the few-body approximation is the number $M$ of kept correlated orbitals. Obviously, the limit $M \rightarrow N$ would lead to the exact wave function. We stress that all computations at finite $M$ are done in the thermodynamic limit, since the $N - M$ uncorrelated orbitals are fully accounted for in our Ansatz (5). These uncorrelated orbitals actually constitute a major part of the total energy, despite being evaluated in a single-particle picture. The difference between the computed few-body energy $E_{\text{few}} = \langle \Psi_{\text{few}} | \mathcal{H} | \Psi_{\text{few}} \rangle$ at fixed $M$ and the many-body ground state energy $E_{\text{NRG}}$ obtained from the converged NRG simulations is shown in Fig. 6. We find an exponential convergence of the few-body energy as a function of the number $M$ of correlated orbitals, as anticipated from the structure of the $Q$-matrix spectrum. Note that for the half-filling considered here, the number of truly interacting fermions is $M/2$. We see that an accuracy of 6 digits is obtained for 6 correlated orbitals.
(3 interacting particles) for all \( U > 0 \). For \( U < 0 \), the rate of convergence becomes slower the closer we come to the critical point, consistent with the increase in the number of \( \tilde{Q} \)-eigenvalues that are significantly different from zero or one. However, even at \( U = -1.0 \), where the Kondo temperature is \( 1.87 \times 10^{-6} \), 20 correlated orbitals (10 interacting particles) would give an accuracy better than 10% of the Kondo temperature. This clearly vindicates our claim that for practical purposes, the ground state of the Kondo problem is few-body and not many-body in nature, once expressed in the optimal set of natural orbitals. Only exponentially close to a quantum phase transition does a truly many-correlated-particle wave function emerge, as discussed previously for dissipative systems [30].

\[ \mathcal{H} = U \left( \hat{d}_i^\dagger \hat{d}_i^\uparrow - \frac{1}{2} \right) \left( \hat{d}_i^\dagger \hat{d}_i^\downarrow - \frac{1}{2} \right) + V \sum_{\sigma = \uparrow, \downarrow} \left( \hat{d}_i^\sigma \hat{c}_{0,\sigma} + \hat{c}_{0,\sigma}^\dagger \hat{d}_i^\sigma \right) + \sum_{\sigma = \uparrow, \downarrow} \sum_{i=1}^{N-2} t_i \left( \hat{c}_{i,\sigma}^\dagger \hat{c}_{i-1,\sigma} + \hat{c}_{i-1,\sigma}^\dagger \hat{c}_{i,\sigma} \right), \quad (6) \]

whose effective low-energy description in the strong interaction limit \( U \gg \Gamma = V^2/(2D) \) is the Kondo model, \( D \) being the half-bandwidth. Hamiltonian (6) is again discretized on the Wilson chain, and we used particle number as well as spin conservation to optimize the numerical simulations, as the spinfulness of the SIAM fermions doubles the dimension of the single-particle Hilbert space. Because the ground state is a spin singlet, \( \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} \rangle \propto \delta_{\sigma\sigma'} \) and \( \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma'} \rangle = \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \rangle \). Thus there is an extra two-fold degeneracy in the correlation matrix spectrum, as compared to the IRLM. The NRG calculation of the correlation matrix demands more computational resources than for the IRLM, but as we show in Appendix A, we succeeded in obtaining well-converged results. As for IRLM, we include the \( d \)-level fermions in the operators used to construct the correlation matrix, so that the limit \( U = 0 \) is strictly uncorrelated.

The top panel of Fig. 7 shows the correlation matrix spectrum, plotted in the same way as for the IRLM in Fig. 1. Beyond a central plateau, that still contains the four eigenvalues furthest from full occupancy or vacancy, we see degenerate pairs \( \lambda_{n\uparrow} = \lambda_{n\downarrow} \) that decay exponentially \( \lambda_{n\sigma} \sim \exp(-x|n|) \). In the bottom panel of Fig. 7, we show the extracted decay rate \( x \), as a function of the Kondo temperature \( T_K \) (the latter is calculated from the magnetic susceptibility of the impurity). We see a finite decay rate even at extremely low Kondo temperatures \( \sim 10^{-12} \) of the band width, and our results are consistent with \( x \) vanishing at zero Kondo coupling (\( U \to \infty \)).

The exponential decay of correlation matrix eigenvalues (natural orbital occupation numbers) to full occupancy or vacancy therefore is not a special feature of the IRLM representation of Kondo physics. Thus, also for the SIAM, the single-particle Hilbert space can be partitioned into an \( M \)-dimensional correlated sector, and a remainder that is uncorrelated. An ansatz that straightforwardly generalizes (5) can be constructed. Its accuracy is controlled by \( M \), and any desired accuracy can be obtained with an \( M \) that remains finite in the thermodynamic limit. Due to the fact that there is an extra degeneracy in the correlation matrix spectrum of the SIAM and also because for given \( T_K \), the decay rate \( x \) is roughly twice smaller for SIAM fermions than for IRLM fermions, a larger \( M \) will be required for the same accuracy at a given \( T_K \) than in the IRLM. As a practical matter, this limits the range of Kondo couplings for which few-body approximations to the ground state of the SIAM can be found numerically, but in principle, the SIAM ground state is effectively a
FIG. 7. Top panel: Correlation matrix spectrum for the single impurity Anderson model (SIAM) for various ratios of the onsite interaction $U$ to the hybridization $\Gamma$. In all cases $\Gamma = 0.01D$. As in Fig. 1, the right side shows eigenvalues $0 < \lambda_{n\sigma} < 1/2$, while the left side shows $1 - \lambda_{n\sigma}$ for $1/2 < \lambda_{n\sigma} < 1$. Spin degenerate pairs of eigenvalues $\lambda_{n\sigma}$ decay exponentially $\sim \exp(-|n|x)$ to full occupancy or vacancy. Bottom panel: Decay rate $x$ of correlation matrix eigenvalues, versus Kondo temperature $T_K$.

few-body correlated state in terms of SIAM fermions, in the same way that the IRLM ground state is few-body in nature, provided $T_K$ is finite.

VI. CONCLUSIONS

We have calculated the correlation matrix of the IRLM and the SIAM, two quantum impurity models that are equivalent to the single channel Kondo Hamiltonian. Several recent studies have noted that the eigenvalues of the correlation matrix of quantum impurity models often decay exponentially towards full occupation or vacancy[18–20], and our results confirm this observation, provided that the ground state is not quantum critical. We have however identified results in the literature about the Kondo model, namely that the exponential decay rate of correlation matrix eigenvalues become large close to the weak coupling critical point, that are finite size artefacts. We demonstrated that, in fact, the decay rate tends to zero as the critical point is approached for a macroscopically large electronic bath. Finite size systems that are smaller than the Kondo length prevent the full development of correlations. We have also investigated the spatial structure of the most correlated natural orbitals as the critical point is approached and detected clear fingerprints of the Kondo screening cloud.

Our main result presents a general method for determining the effective number of correlated particles (on top of an uncorrelated Fermi sea). This involves using the natural orbital single-particle basis to identify correlated and uncorrelated sectors of Fock space. Owing to the exponential decay of the correlation matrix spectrum to full occupancy or vacancy, the correlated sector can, to a good approximation, be chosen to contain a finite number of particles $M/2$, whereas the uncorrelated sector contains an infinite number of particles within a single Slater determinant in the thermodynamic limit. The full ground state can be reconstructed approximately by solving an effective few-body problem for the particles in the correlated sector. If the reconstructed state has an energy expectation value that differs from the true ground state by an amount that is significantly less than the Kondo temperature, then the reconstructed state is a faithful approximation of the true ground state. By comparing the energy of this reconstructed state to the true ground state energy, as a function of $M$, we can thus determine the effective number of correlated particles. Whereas the number of correlated particles diverge at the weak coupling fixed point ($T_K \rightarrow 0$), for realistic Kondo temperatures of $\sim 10^{-3}$ of the Fermi energy, the ground state only hosts around seven correlated particles in the IRLM representation, and a larger but still finite number in the SIAM. The different models host different numbers of correlated particles at the same Kondo temperature because their microscopic degrees of freedom are nontrivially related. We have investigated how this picture is affected when correlations are frustrated, either by finite size effects, or by symmetry-breaking fields. We showed that, as expected, physical cutoffs acting near the Kondo scale are accompanied by a sharp reduction in the number of correlated particles. However, we anticipate that models tuned to criticality, such as the two-channel and two-impurity Kondo models, remain truly many-body in any single-particle basis. Our results open many interesting avenues for research, such as generalizations to other quantum impurity problems or even to disordered lattice models. It would also be interesting to investigate whether this few-body picture is robust for excited or unitarily time-evolved states, a notoriously challenging problem for strongly interacting fermions.

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Appendix A: Convergence of the spectrum of $\hat{Q}$ to the thermodynamic limit.

The thermodynamic limit of the Wilson chain used in NRG is obtained mathematically by sending the chain length $N$ to infinity and subsequently sending $\Lambda$ to 1. For the IRLM, this limit describes a one-dimensional conduction band with a constant density of states coupled via hybridization and short range Coulomb interactions to a resonant level. In practice, numerical calculations are performed at finite $N$ and $\Lambda > 1$, and also introduce a further regularization parameter, $N_{\text{kept}}$, the maximum dimension to which fixed particle number sectors of Hilbert space are truncated in each renormalization step. In this section we demonstrate that our numerical results are converged to the thermodynamic limit with respect to these three regularization parameters. We first show in Fig. 8 (top panel) that the $\hat{Q}$-matrix spectrum is indeed well converged for sufficiently long chains. Here, we consider an interaction value $U = -1.2D$ very close to the quantum critical point $U_c = -1.3D$, leading to an exponentially small Kondo temperature of order $T_K/D \sim \Lambda^{-75/2} \approx 10^{-13}$, which is estimated from the crossover at $N \approx 75$ seen in the flow of the lowest eigenvalues of the rescaled Hamiltonian (bottom right panel in Fig. 8), using the value $\Lambda = 2.25$ for this NRG computation. The same crossover scale is seen for all eigenvalues $\lambda_n$ (see bottom left panel in Fig. 8), which are well saturated to their $N = \infty$ limit for $N > 75$. Note however, that eigenvalues $\lambda_n$ with $n > N/2$ are not defined since the chain is too short to harbor those modes. Longer chains are thus required to obtain such small eigenvalues.

We then investigate the issue of the convergence to the continuum limit $\Lambda \rightarrow 1$. In the left panel of Fig. 9, we plot the $\hat{Q}$-spectrum for $U = 0.5$, with $N_{\text{kept}} = 110$ many-body states per block, for various $\Lambda$ values. The first 5 eigenvalues are clearly independent of $\Lambda$, showing that the exponential falloff is robust in the thermodynamic limit. For the smaller eigenvalues $\lambda_n$ with $n \geq 6$, some departure of the exponential decay is seen for $\Lambda = 1.5$ and $\Lambda = 1.4$. We show in the middle panel of Fig. 9 that this artefact is purely an effect of the truncation error on the exponentially small magnitude of the eigenvalues, that disappears progressively when increasing $N_{\text{kept}}$. Thus, in practice, calculations with $\Lambda = 2$ and $N_{\text{kept}} \sim 100$ provide good convergence for spinless models, emphasizing that it is not useful to consider $\lambda_n$ eigenvalues below the machine precision $10^{-16}$. We found similar results for other values of the interaction $U$.

In Sec. V we presented results for the spectrum of the correlation matrix of the single impurity Anderson...
model. Given the larger single particle Hilbert space, it is important to make sure that these results are converged with respect to NRG truncation. In the right panel of Fig. 9, we show that this is the case: The evolution of the spectrum of the numerically computed correlation matrix for the SIAM as a function of $N_{\text{kept}}$ closely mirrors that of the IRLM (compare to the middle panel of Fig. 9.) We clearly see that the truncation error is pushed closer and closer to full occupancy or vacancy as $N_{\text{kept}}$ is increased, and that results are consistent with a spectrum that decays exponentially to full occupancy or vacancy.

Appendix B: Few-body diagonalization in the $Q$-eigenbasis

We present here some technical details on how to perform an exact diagonalization of an arbitrary non-local Hamiltonian, using the eigenvectors of the $Q$-matrix as an optimized set of $M$ correlated orbitals $q_{n}^{\dagger}$, with $n = -M/2, \ldots, 1, \ldots, M/2$. The orbitals with $-N/2 \leq n < -M/2$ are fully occupied, while orbitals with $M/2 < n \leq N/2$ are totally empty. As discussed in the main text, we write the full wave function as follows:

$$|\Psi_{\text{few}}\rangle = \sum_{\{N_n=0,1\}} \Psi(N_{-\frac{M}{2}}, \ldots, N_{\frac{M}{2}}) \prod_{n=-\frac{M}{2}}^{\frac{M}{2}} |q_{n}^{\dagger}| N_{n} |\Psi_{0}\rangle,$$

$$|\Psi_{0}\rangle = \prod_{m=-\frac{M}{2}}^{-\frac{M}{2}-1} q_{n}^{\dagger} \; |0\rangle,$$

with $N_n = 0,1$ the occupancy of correlated orbital $q_{n}^{\dagger}$, the summation restricted to occupations such that $\sum_{n=-M/2}^{M/2} N_n = M/2$ at half-filling, and $\Psi(N_{-\frac{M}{2}}, \ldots, N_{\frac{M}{2}})$ the complete wave function in the correlated subspace.

We then split the full Hamiltonian between the correlated and uncorrelated sectors as $H = H_{\text{corr}} + H_{\text{mix}} + H_{\text{uncorr}}$. We label the correlated orbitals with roman indices, such as $q_{n}^{\dagger}$ with $n = -M/2, \ldots, -1, 1, \ldots, M/2$, and uncorrelated orbitals with greek indices, such as $q_{\alpha}^{\dagger}$ with $\alpha = -N/2, \ldots, -M/2 - 1, 1, \ldots, N/2$. The various terms read:

$$H_{\text{corr}} = \sum_{n,m} t_{nm} q_{n}^{\dagger} q_{m} + \sum_{n,m,p,q} U_{nmpq} q_{n}^{\dagger} q_{m} q_{p} q_{q},$$

$$H_{\text{mix}} = \sum_{n,m,\alpha,\beta} \left( U_{n,\alpha,m,\beta} q_{n}^{\dagger} q_{m} q_{\alpha} q_{\beta} + U_{\alpha,n,m,\beta} q_{n}^{\dagger} q_{m} q_{\alpha} q_{\beta} + U_{\alpha,n,\beta,m} q_{n}^{\dagger} q_{\alpha} q_{m} q_{\beta} + U_{\alpha,\beta,n,m} q_{n}^{\dagger} q_{\alpha} q_{\beta} q_{m} \right),$$

$$H_{\text{uncorr}} = \sum_{\alpha,\beta} t_{\alpha,\beta} q_{\alpha}^{\dagger} q_{\beta} + \sum_{\alpha,\beta,\gamma,\delta} U_{\alpha,\beta,\gamma,\delta} q_{\alpha}^{\dagger} q_{\beta} q_{\gamma} q_{\delta},$$

where $H_{\text{odd}}$ contains odd terms in the uncorrelated orbitals, such as the hopping term $q_{n}^{\dagger} q_{n}$ mixing both sectors, or interaction terms of the form $q_{n}^{\dagger} q_{m} q_{n} q_{p}$. The terms in $H_{\text{odd}}$ vanish once we project the Hamiltonian in the family of states of the form (B1). The resulting effective few-body Hamiltonian reads:

$$H_{\text{few}} = \sum_{n,m} t_{nm} q_{n}^{\dagger} q_{m} + \sum_{n,m,p,q} U_{nmpq} q_{n}^{\dagger} q_{m} q_{p} q_{q},$$

$$+ \sum_{n,m,\alpha} q_{n}^{\dagger} q_{m} n_{\alpha} \left( -U_{n,\alpha,m,\alpha} + U_{n,\alpha,\alpha,m} \right) + U_{\alpha,n,\alpha,m} \right) + U_{\alpha,n,\alpha,m} \right)$$

$$+ \sum_{\alpha} t_{\alpha,\alpha} n_{\alpha} + \sum_{\alpha,\beta} \left( U_{\alpha,\beta,\alpha} - U_{\alpha,\beta,\alpha} \right) n_{\alpha} n_{\beta},$$

(B3)
where \( n_\alpha \) is the occupancy of the uncorrelated orbitals in the wavefunction (B1), namely \( n_\alpha = 1 \) for \( \alpha < -M/2 \) and \( n_\alpha = 0 \) for \( \alpha > M/2 \). We note that projecting \( \mathcal{H}_{\text{mix}} \) generates a renormalization of the hopping term \( q_m^d q_m^\dagger \) within the correlated sector (last term under parenthesis in the first line of the equation above). The projection of \( \mathcal{H}_{\text{uncorr}} \) provides only a constant contribution to the Hamiltonian (second line of the equation above). The ground state energy of the initial many-body Hamiltonian \( \mathcal{H} \) is obtained by exact diagonalization of \( \mathcal{H}_{\text{few}} \) in the few-body correlated sector.

Appendix C: Extraction of the Kondo temperature

For the IRLM, we take the following definition for the Kondo temperature:

\[
T_K = \frac{1}{4\chi} \quad (C1)
\]

\[
\chi = \lim_{\epsilon_d \to 0} \frac{d}{d\epsilon_d} \langle d^d \rangle, \quad (C2)
\]

upon adding to the IRLM Hamiltonian a local potential on the \( d \)-level, namely a term \( \epsilon_d d^d \). This is equivalent to the standard definition [31] for the Kondo model in terms of the magnetic susceptibility of the impurity spin. The resulting Kondo \( T_K \) temperature as a function of interaction \( U \) is given in Fig. 10. A fit of the essential singularity at the critical point allows to determine the critical value \( U_c \simeq -1.3 \). We also recover our previous estimate \( T_K/D \simeq 10^{-13} \) at \( U = -1.2 \) shown previously in Fig. 8.

![FIG. 10. Kondo temperature of the IRLM as a function of interaction \( U \) computed by NRG with Wilson discretization parameter \( \Lambda = 2 \) and chains of length up to \( N = 110 \).](image-url)

[1] H. R. Krishna-murthy, J. W. Wilkins, and K. G. Wilson, Renormalization-group approach to the anderson model of dilute magnetic alloys. i. static properties for the symmetric case, Phys. Rev. B 21, 1003 (1980).

[2] S. R. White, Density matrix formulation for quantum renormalization groups, Phys. Rev. Lett. 69, 2863 (1992).

[3] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Continuous-time monte carlo methods for quantum impurity models, Rev. Mod. Phys. 83, 349 (2011).

[4] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions, Rev. Mod. Phys. 68, 13 (1996).

[5] J. Eisert, M. Cramer, and M. B. Plenio, Colloquium: Area laws for the entanglement entropy, Rev. Mod. Phys. 82, 277 (2010).

[6] S. Östlund and S. Rommer, Thermodynamic limit of density matrix renormalization, Phys. Rev. Lett. 75, 3537 (1995).

[7] Dukelsky, J., Martin-Delgado, M. A., Nishino, T., and Sierra, G., Equivalence of the variational matrix product method and the density matrix renormalization group applied to spin chains, Europhys. Lett. 43, 457 (1998).

[8] G. Vidal, Efficient classical simulation of slightly entangled quantum computations, Phys. Rev. Lett. 91, 147902 (2003).

[9] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, Annals of Physics 326, 96 (2011), january 2011 Special Issue.

[10] D. A. Abanin, E. Altman, I. Bloch, and M. Serbyn, Colloquium: Many-body localization, thermalization, and entanglement, Rev. Mod. Phys. 91, 021001 (2019).

[11] A. C. Hewson, The Kondo problem to heavy fermions (Cambridge University Press, Cambridge New York, 1993).

[12] R. Bulla, T. A. Costi, and T. Pruschke, Numerical renormalization group method for quantum impurity systems, Rev. Mod. Phys. 80, 395 (2008).

[13] V. Barzykin and I. Affleck, The kondo screening cloud: What can we learn from perturbation theory?, Phys. Rev. Lett. 76, 4959 (1996).

[14] J. Park, S.-S. B. Lee, Y. Oreg, and H.-S. Sim, How to directly measure a kondo cloud’s length, Phys. Rev. Lett. 110, 246603 (2013).

[15] G. Barcz, K. Bauerbach, F. Eichhoff, F. B. Anders, F. Gebhard, and O. Legeza, Symmetric single-impurity kondo model on a tight-binding chain: Comparison of analytical and numerical ground-state approaches, Phys. Rev. B 101, 075132 (2020).

[16] I. V. Borzenets, J. Shim, J. C. H. Chen, A. Ludwig, A. D. Wieck, S. Tarucha, H. S. Sim, and M. Yamamoto, Observation of the kondo screening cloud, Nature 579, 210 (2020).

[17] C. Yang and A. E. Feiguin, Unveiling the internal entanglement structure of the kondo singlet, Phys. Rev. B 95, 115106 (2017).

[18] R. Zheng, R. He, and Z. Lu, Natural orbitals renormalization group approach to a kondo singlet, Science China Physics, Mechanics & Astronomy 63, 297411 (2020).
[19] R.-Q. He and Z.-Y. Lu, Quantum renormalization groups based on natural orbitals, Phys. Rev. B 89, 085108 (2014).
[20] Y. Lu, M. Höppner, O. Gunnarsson, and M. W. Haverkort, Efficient real-frequency solver for dynamical mean-field theory, Phys. Rev. B 90, 085102 (2014).
[21] M. T. Fishman and S. R. White, Compression of correlation matrices and an efficient method for forming matrix product states of fermionic gaussian states, Phys. Rev. B 92, 075132 (2015).
[22] P. E. M. Siegbahn, J. Almlöf, A. Heiberg, and B. O. Roos, The complete active space scf (casscf) method in a newton–raphson formulation with application to the hno molecule, The Journal of Chemical Physics 74, 2384 (1981), https://doi.org/10.1063/1.441359.
[23] P. B. Vigman and A. M. Finkel’shtein, Resonant-level model in the Kondo problem, Sov. Phys. JETP 48, 102 (1978).
[24] T. Giamarchi, Quantum Physics in One Dimension (Oxford University Press, New York, 2004).
[25] A. O. Gogolin, A. A. Nersesyan, and A. M. Tsvelik, Bosonization and Strongly Correlated Systems (Cambridge University Press, 2004).
[26] U. Weiss, Quantum Dissipative Systems, 4th ed. (WORLD SCIENTIFIC, 2012) https://www.worldscientific.com/doi/pdf/10.1142/8334.
[27] F. Guinea, V. Hakim, and A. Muramatsu, Bosonization of a two-level system with dissipation, Phys. Rev. B 32, 4410 (1985).
[28] G. Zaránd and J. von Delft, Analytical calculation of the finite-size crossover spectrum of the anisotropic two-channel kondo model, Phys. Rev. B 61, 6918 (2000).
[29] H. T. M. Nghiem, D. M. Kennes, C. Klöckner, V. Meden, and T. A. Costi, Ohmic two-state system from the perspective of the interacting resonant level model: Thermodynamics and transient dynamics, Phys. Rev. B 93, 165130 (2016).
[30] Z. Blunden-Codd, S. Bera, B. Bruognolo, N.-O. Linden, A. W. Chin, J. von Delft, A. Nazir, and S. Florens, Anatomy of quantum critical wave functions in dissipative impurity problems, Phys. Rev. B 95, 085104 (2017).
[31] M. Hanl and A. Weichselbaum, Local susceptibility and kondo scaling in the presence of finite bandwidth, Phys. Rev. B 89, 075130 (2014).