Real-time dynamics induced by quenches across the quantum critical points in gapless Fermi systems with a magnetic impurity

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The energy-dependent scattering of fermions from a localized orbital at an energy-dependent rate \( \Gamma(\varepsilon) \propto |\varepsilon|^r \) gives rise to quantum critical points (QCPs) in the pseudo-gap single impurity Anderson model separating a local moment phase with an unscreened spin moment from a strong-coupling phase which slightly deviates from the screened phase of standard Kondo problem. Using the time-dependent numerical renormalization group (TD-NRG) approach we show that local dynamic properties always equilibrate towards a steady-state value even for quenches across the QCP but with systematic deviations from the thermal equilibrium depending on the distance to the critical coupling. Local non-equilibrium properties are presented for interaction quenches and hybridization quenches. We augment our numerical data by an analytical calculation that becomes exact at short times and find excellent agreement between the numerics and the analytical theory. For interaction quenches within the screened phase we find an universal function for the time-dependent local spin moment which decouples from the system in the unscreened phase, the Gutzwiller ansatz only allows the formation of the spin moment on the local impurity orbital.

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I. INTRODUCTION

The investigation of the real-time dynamics in quantum-impurity systems (QIS) is essential for our understanding of dissipation and decoherence in qubits and electronic transport through nanodevices. Such systems consist of a small subsystem comprising of a finite number of degrees of freedom, interacting with an infinitely large environment of non-interacting particles.

Elzerman et al. [1] have reported the usage of gate-voltage pulses for a single-shot read-out of the spin configuration of a single-electron transistor in a finite magnetic field. Such a system can be modeled by an Anderson impurity model [2] coupled to a non-interacting metallic host. While the normal single impurity Anderson model (SIAM) has a well established and rather simple phase diagram [3, 4], it can be viewed as a special case \( (r=0) \) of a more general class of models [5–8] whose coupling function \( \Gamma(\varepsilon) \) to the local impurity contains a pseudo-gap, i.e. \( \Gamma(\varepsilon) \propto |\varepsilon|^r \). Withoff and Fradkin were the first to point out the existence of a critical coupling [9] using a perturbative renormalization group argument. This system exhibits a wide variety of different phases for \( r > 0 \). These phases are characterised by different fixed points whose properties and occurrence depend on the bath exponent \( r \) as well as on particle-hole symmetry or the absence of it. For \( 0 < r < 1/2 \), there exists [5, 6, 10, 11] a critical coupling strength \( \Gamma_c \) governing the transition between a local moment (LM) phase for a weak coupling and a strong-coupling (SC) phase for a large coupling to the metallic host.

In this paper, we analyse the real-time dynamics of different quenches within the LM or the SC phase but also quenches across the quantum critical point (QCP) from one to the other phase for the particle-hole symmetric pseudo-gap Anderson impurity model (pg-SIAM). We employ a recent extension of Wilson’s numerical renormalization group (NRG) [4, 12] to the non-equilibrium quench dynamics, the time-dependent NRG (TD-NRG) [13–15].

While the quench dynamics in the SIAM \( (r=0) \) has been investigated [13] using the TD-NRG, the non-equilibrium dynamics in the pg-SIAM within and across the QCP has only recently been addressed by a time-dependent Gutzwiller ansatz [16]. Using this extension of the well established variational Gutzwiller technique [17, 18] to non-equilibrium [19, 20] it has been demonstrated that the pseudo-gap coupling function can yield nontrivial dynamics as a consequence of the diverse low-energy fixed points of the model [16].

The pg-SIAM has been extensively investigated in the context of Kondo impurities in unconventional superconductors [5–8, 10, 11] or in the context of defects in graphene sheets [21, 22]. Some of the low-energy properties of the fixed points have been worked out in detail [23–25] and it has been shown that the universality class of the fixed point changes with the coupling function exponent \( r \).

One intriguing property of this model is the absence of the Kondo screening at low coupling strength [6, 9–11] while for a large coupling a SC fixed point is found but with an only partially screened moment for particle-hole symmetric models. The question arises how these orthogonal ground states of the different phases influence the real-time dynamics of a system driven out of equilibrium by a quantum quench.

Since an effective spin degree of freedom decouples from the impurity in the LM phase, this fixed point...
(FP) property is expected to have a strong influence on the steady-state formation and the thermalization when quenched into the LM phase. We will show, however, that an oversimplified picture [16] encoded in a specific Gutzwiller wave-function ansatz does not hold and requires some modification.

Indeed, we find thermalization even for quenches across the QCP as long as the distance to the QCP is not too large. This surprising finding is related to the extended nature of the local moment dynamically forming and decoupling from the rest of the system in the LM FP. It has been pointed out already in Ref. 6 that the local properties such as double occupancy as well as the fractional local moment on the impurity are continuous across the QCP. The crossover scale $T^*$ governing the excitations around the LM FP vanishes at the QCP and increase with decreasing coupling to the pseudo-gap metallic host.

The length scale $\xi^* = v_F/T^* - v_F$ being the average Fermi velocity of the host material – can be interpreted as estimate for the spatial extension of the local moment decoupling from the impurity. Only for a very large local Coulomb repulsion $U$, $T^*$ is large, indicating that the local moment is mainly formed closely to or on the impurity.

Bearing in mind these known equilibrium properties [6] of the model it becomes apparent that an ansatz for the ground state restricted to a local moment formation on the impurity site only, as used in the Gutzwiller approach [16, 17, 19, 20], significantly underestimates the critical coupling $\Gamma_c$. Then, the local moment formation can only happen at much lower coupling $\Gamma$ or much larger local Coulomb repulsion $U$ in such an approach compared to the solution provided by the NRG.

This has also a profound consequence for the observed real-time dynamics. Due to the extended nature of the decoupled local moment, the local observable still can explore a larger phase space of itinerant states and, therefore, shows signs of thermalization. Reducing the size of the local moment by increasing $U$ away from the critical $U_c$ will still yield a steady-state whose asymptotic properties start to deviate significantly from the thermal expectation values: due to the increase of the non-decaying fraction of the expectation value [26–28] the difference between the steady-state and the thermal expectation value increases in the LM phase.

A. Plan of the paper

The main objective of this paper is to discuss the real-time dynamics of the pseudo-gap SIAM with respect to interaction and hybridization quenches within a given phase and across the quantum critical point.

To be more specific, we will introduced the model in Sec. II A and briefly the TD-NRG in Sec. II B. We continue with a short overview over the rich phase diagram in Sec. II C – a much more comprehensive review can be found in the Refs. 6 and 8 – in order to define the types of quenches that will be investigated in Sec. III, the main part of the paper.

For completeness and defining the parameter space, we present the known NRG phase diagram for the symmetric pg-SIAM and also discuss the differences between the NRG and the equilibrium Gutzwiller results in Sec. III A. We start with analysing our data for interaction quenches, i.e. the sudden switching on the local Coulomb repulsion. For small $U$ and finite hybridization, the system remains in the SC phase. In section III B 1, we show that universality can be found for this type of quenches with an $U$-independent time-scale. Interaction quenches across the QCP are investigated in Sec. III B 2. We address the difference between equilibration and thermalization.

Section III C is devoted to the two types of hybridization quenches. We augment our TD-NRG results with a perturbative analysis – details can be found in appendix A – and show an excellent agreement between the numerics and the analytics in Sec. III C 2. We also discuss the energy flow from the reservoir to the impurity after the quench in Sec. III C 3. We end the paper with a short conclusion.

II. THEORY

A. The pseudo-gap single impurity Anderson model (pg-SIAM)

We consider a magnetic impurity comprising a spin-degenerated level that is coupled to a single conduction band. The Hamiltonian consists of three parts: $H_c$ accounts for the conduction band of non-interacting electrons

$$H_c = \sum_{k\sigma} \varepsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}$$

(1)

where $c_{\vec{k}\sigma}$ annihilates an electron with energy $\varepsilon_{\vec{k}\sigma}$ and spin $\sigma$, $\vec{H}_{\text{imp}}$ models the magnetic impurity

$$H_{\text{imp}} = \sum_{\sigma} \varepsilon_{d\sigma} d_{\sigma}^\dagger d_{\sigma} + U n_{d\uparrow} n_{d\downarrow},$$

(2)

where $d_{\sigma}^\dagger$ creates an electron in the localised impurity orbital with spin $\sigma$, the energy $\varepsilon_{d\sigma}$, and $U > 0$ denotes the Coulomb repulsion between two localised electrons with opposite spin. Hereby $n_{d\sigma} = d_{\sigma}^\dagger d_{\sigma}$ is the occupation operator of the level with spin $\sigma$. These two subsystems are coupled by the hybridization term

$$H_{\text{hyb}} = \sum_{\vec{k}\sigma} V_{\vec{k}} (c_{\vec{k}\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{\vec{k}\sigma}^-)$$

(3)

so that the full dynamics is given by $H = H_c + H_{\text{imp}} + H_{\text{hyb}}$. 

It has been realized [5–7] that the dynamics of the magnetic impurity is fully determined by the coupling function

$$
\Gamma_\sigma(\epsilon) = \pi \sum_k V^2_k \delta(\epsilon - \epsilon^\gamma_k) \tag{4}
$$

which we will take as spin-independent in the following. In real materials such as d superconductors [8] or graphene sheets [22, 29, 30] \( \Gamma(\epsilon) \) is a complicated function of energy. It turned out, however, that only the low-energy part of the spectrum close to the chemical potential is relevant for the structure of the low-energy fixed points. Ignoring the high-energy details, \( \Gamma(\epsilon) \) is replaced by the particle-hole symmetric power-law form

$$
\Gamma(\epsilon) = (r + 1) \Gamma_0 |\epsilon|^r \Theta(D - |\epsilon|) \tag{5}
$$

where the cutoff \( D \) defines the effective band width [5–11]. The normalization factor \( (r + 1) \) ensures that the integral over the coupling function,

$$
\pi V^2_0 = \int d\epsilon \Gamma(\epsilon) = 2\Gamma_0 D, \tag{6}
$$

remains independent of the bath exponent \( r \geq 0 \). The parameter \( \Gamma_0 \) serves as energy scale of the problem that turns into the standard charge fluctuation scale for a constant density of states \( (r = 0) \). While \( r = 0 \) and \( r = 1 \) are the prototypical experimental realizations, we take \( r \) as an arbitrary parameter of the model.

The particle-hole asymmetry is governed by the deviation of \( \Delta\epsilon = 2\epsilon_d + U \) from zero energy. Unless otherwise stated, we focus only on the particle-hole symmetric case in this paper.

**B. The time-dependent numerical renormalization group (TD-NRG)**

In this work, we exploit the NRG approach [4, 12] for obtaining all thermodynamic properties of the pg-SIAM. The key idea of Wilson was to map the logarithmically discretized coupling function \( \Gamma(\epsilon) \) onto an effective semi-infinity tight-binding chain where the impurity is coupled only to the first chain link. The energy hierarchy is controlled by the discretization parameter \( \Lambda > 1 \), and the problem is solved by iterative diagonalization.

Due to the exponential growth of the Hilbert space, high-energy states are discarded after each iteration. Since the initial basis set is known, the set of all discarded states form a complete basis set [13, 14] and simultaneously serve as an approximate eigenbasis of the Hamiltonian governing the time evolution of the problem.

Then the time-dependent expectation value \( \langle O(t) \rangle \) of a general local operator \( \hat{O} \) can be casted into the form

$$
\langle O(t) \rangle = \sum_{m} \sum_{r,s} e^{it(E^m_r - E^m_s)} O^m_{r,s} \rho^\text{red}_{s,r}(m), \tag{7}
$$

where \( E^m_r \) and \( E^m_s \) are the dimension-full NRG eigen-energies of the Hamiltonian \( \hat{H}_t = H(t > 0) \) at iteration \( m \leq N \), \( O^m_{r,s} \) is the matrix representation of \( \hat{O} \) at that iteration, and \( \rho^\text{red}_{s,r}(m) \) is the reduced density matrix defined as

$$
\rho^\text{red}_{s,r}(m) = \sum_{e,r,s} \langle s,e;m|\hat{\rho}_0|r,e;m \rangle \tag{8}
$$

where \( \hat{\rho}_0 \) being the initial density operator of the problem prior to the quench. The restricted sum over \( r \) and \( s \) in Eq. (7) requires that at least one of these states is discarded at iteration \( m \).

Implementing the TD-NRG requires two NRG runs: one for the initial Hamiltonian \( \hat{H}_t = H(t < 0) \) to construct the initial density operator \( \hat{\rho}_0 \) of the system and one for \( \hat{H}_t \) to obtain the approximate eigenbasis governing the time evolution in Eq. (7). For more details on the TD-NRG see the Refs. 13 and 14. Recently, the TD-NRG has been extended to use the full density matrix including pulsed Hamiltonians [15] and periodic switching [31].

**C. Overview of the phases and the quench types**

The equilibrium phase diagram of the pg-SIAM is very rich and has been carefully explored by Gonzalez-Buxton and Ingersent [6]. Details can also be found in Refs. 8 and 4.

For a particle-hole (ph) symmetric model, an instable intermediate coupling fixed point governs the transition between the local moment (LM) fixed point (FP) and the strong-coupling (SC) FP for \( 0 < r < 1/2 \), where the critical coupling ratio \( U_c/\Gamma_0 \) depends on the band width \( D \) and the exponent \( r \). The intermediate FP is also unstable with respect to ph-symmetry breaking since potential scattering is a marginal relevant perturbation at this FP.

In contrary to the standard SC FP for \( r = 0 \), the SC FP of the ph-symmetric pg-SIAM is characterised by a residual impurity entropy \( S_{\text{imp}} = 2r k_B \ln(2) \) and a residual unscreened effective local moment [6] of \( \mu^2_{\text{eff}}(0) = \lim_{T \to 0} \mu^2_{\text{eff}}(T) = r/8 \).

For \( 1/2 < r \) the low-energy density of states is too small to screen the local spin, and only the LM FP remains stable for all coupling strengths at ph-symmetry. Breaking ph-symmetry, a asymmetric SC (ASC) fixed point is found for all \( r \). Its thermodynamic properties are closely related to the standard \( r = 0 \) SC FP since \( S_{\text{imp}} = 0 \) and \( \mu^2_{\text{eff}}(0) = 0 \).

In addition, a second intermediate coupling fixed point at a finite value of the potential scattering is found for \( r^* \approx 0.375 < r \), where the perturbation \( V - V_c \) with respect to the critical potential scattering \( V_c \) is a marginal irrelevant operator [6].

In this paper, however, we will focus on the non-equilibrium dynamics of the particle-hole symmetric model close and across the quantum-phase transition.
Therefore, we mainly focus on the parameter regime \(0 < r < 1/2\). There are two different ways to drive the ph-symmetric system across the quantum critical point (QCP) for \(0 < r < 1/2\). For a fixed value of \(U\) we can vary the hybridization strength \(\Gamma_0\), which will be called hybridization quench (HQ) in the following, or for a fixed \(\Gamma_0\) we can change \(U\) that defines the interaction quench (IQ). In Tab. I we summarize our notation for the different quench types. The phase refers to the equilibrium low-temperature FP of the final Hamiltonian \(H_f\) after the quench. Note that we neither imply thermalization nor equilibration [32] of local observables by referring to the equilibrium low-temperature FP of the final Hamiltonian \(H_f\).

In equilibrium, the SC FP can be reached in two ways: choosing the charge-fluctuation scale \(\Gamma_0 > \Gamma_c(U)\) for fixed \(U\) or by setting \(U < U_c(\Gamma_0)\) for fixed \(\Gamma_0\). The resulting phase diagram for \(U_c(r)\) and \(\Gamma_c(r)\) for fixed \(\Gamma_0\) and \(U\) respectively is shown in Fig. 1(b). The details of how the phase diagram is obtained from equilibrium NRG calculations is presented in Sec. III A below.

An approximative description of the ground state wave function of the model for a finite hybridization has been proposed using a Gutzwiller wave-function ansatz [16]. For \(r = 0\), the quasi-particle renormalization factor \(Z \propto T_{K}^{D/2} \propto \exp(-\pi U/16\Gamma_0)\) is a smooth function of the Coulomb interaction \(U\) and has been interpreted as effective Kondo temperature within the Gutzwiller approach [17]. Note, however, that (i) the exponent differs by a factor of two from the standard Kondo temperature and, therefore, underestimates the exponential decay [33] and (ii) an incorrect Kondo scale is found for the wide-band limit as it has been pointed out in Ref. 33.

For \(r > 0\), a finite critical \(U_c\) and a QCP is found [16] for all \(r\). The prediction for \(U_c\) by the Gutzwiller approach has been added to Fig. 1(b) as analytical curve for the wide-band limit. That restricts the possible validity of the Gutzwiller approach to \(r < 1/2\) since for \(1/2 < r\) the LM FP is stable for all \(U > 0\). The prediction of a SC phase even for \(1/2 < r\) by the Gutzwiller approach is directly related to the restriction of the wave function to the formation of a decoupled spin moment on the impurity site while the true ground state properly accounts for the formation of an extended spin moment as we will discuss in the next section. The comparison with the correct NRG phase boundary reveals again an underestimation of the renormalization effects and, hence, an overestimation of the critical \(U_c\). We have to bare in mind these limitations of the Gutzwiller approach of the equilibrium when comparing recent results [16] obtained with a time-dependent Gutzwiller approach [19, 20] with our TD-NRG data.

### III. RESULTS

We begin with a short review of the established thermodynamic properties in Sec. III A and discuss the differences between the NRG findings [6] and the predictions of the equilibrium Gutzwiller ansatz. Then we proceed with the results of our TD-NRG calculations for interaction quenches (IQ) in Sec. III B and for hybridization quenches (HQ) in Sec. III C.

#### A. Equilibrium properties

In order to set the stage for the real-time dynamics, we extend the review of the equilibrium properties to the temperature-dependent impurity observables [4, 6, 8].

One important quantity revealing the QCP is the effective magnetic moment for different band widths \(D\) and exponents \(r\) is given in Tab. II. The phase type refers to the low-temperature FP of the final Hamiltonian. The numerical values of the critical parameters for different band widths \(D\) and exponents \(r\) are given in Tab. II.
fective local moment

$$\mu_{\text{eff}}^2(T) = \Delta \left( \langle S_z^2(T) \rangle - \langle S_z(T) \rangle^2 \right)$$

(9)

whereby \(\Delta (X)\) is measuring the observable \(X\) in presence of the impurity and the Wilson chain and subtracts the effect of the quantity \(X\) of the pure Wilson chain without the impurity at temperature \(T\), and \(S_z\) denotes the \(z\)-component of the total spin of the system. By this definition \([6, 12]\) the impurity contribution of the quantity \(X\) is extracted.

Note, however, that \(\mu_{\text{eff}}^2(T)\) does not measure the local impurity spin observable but rather the difference in the total system properties with and without the impurity. Hence, the effective impurity spin momentum \(\mu_{\text{eff}}^2(T)\) is in general related to a degree of freedom (DOF) comprising a linear combination of local and conduction electron spin observables. This will become important for understanding the impurity expectation values in the different phases.

In the LM FP, the effective local moment of the impurity spin, i.e. \(\mu_{\text{eff}}^2(0) = \lim_{T \rightarrow 0} \mu_{\text{eff}}^2(T)\), is given by those of the free spin 1/4 while for the symmetric SC FP a residual moment \(r/8\) has been found \([6]\) revealing the inability of a power-law density of states to completely screen the Kondo spin.

In Fig. 1(a), \(\mu_{\text{eff}}^2(T)\) is shown as function of temperature for different Coulomb interactions \(U\) for the bath exponent \(r = 0.4\) with the band width \(D/T_0 = 100\). If not mentioned otherwise we used the NRG parameter \([12]\) \(\Lambda = 2\) and kept \(\mathcal{N}_3 = 2000\) states after each iteration step.

For \(U/U_c < 1\) the effective local moment \(\mu_{\text{eff}}^2(T)\) declines at low temperatures towards the SC FP value \(r/8\) whereas for \(U/U_c > 1\) it inclines towards 1/4 indicating a free local moment of the LM FP. For \(U/T_0 = 0.34 \approx U_c\), \(\mu_{\text{eff}}^2(T)\) approaches the value of the unstable intermediate coupling FP. We used the clear distinction between \(\mu_{\text{eff}}^2(T)\) of the symmetric SC FP and the LM FP to define the critical Coulomb interaction \(U_c\) at which the value of the intermediate coupling FP is obtained.

In Fig. 1(b) we present the phase diagram of the ph-symmetric pg-SIAM defined by the critical parameter \(U_c\) (or \(\Gamma_c\) respectively) for different band widths \(D\). The numerical values of the critical parameters are given in Tab. II. We observe a strong influence of the band width \(D\) onto the critical \(U_c\), and our \(\Gamma_c\) agrees excellently with Fig. 5 in Ref. 6.

In order to qualitatively understand the phase diagram in Fig. 1(b), we start from \(U = 0\), where we always find a SC FP for \(r < 1/2\). Since we systematically eliminate the high-energy degrees in a RG procedure, a finite \(U\) will matter only once the effective band width \(D \rightarrow D_{\text{eff}}\) has reached the order \(U\). At those energies, the system starts detecting the differences between the local doubly occupied state and the local moment states, and the effective coupling to the remaining conduction band is given by \(\Gamma(U)\). Since \(\Gamma(U)\) decreases with increasing \(r\) and increasing \(D, U_c\) also must decrease.

| \(r\)  | \(U_c/\Gamma_0\) | \(D/\Gamma_0\) | \(\Gamma_c/\Gamma_0\) | \(D/\Gamma_0\) | \(\Gamma_c/\Gamma_0\) |
|-------|----------------|---------------|----------------------|---------------|----------------------|
| 0.05  | 49.84          | 44.87         | 0.02154              | 0.0268        |
| 0.1   | 25.00          | 18.81         | 0.04586              | 0.07094       |
| 0.2   | 12.10          | 5.332         | 0.10637              | 0.2535        |
| 0.3   | 7.331          | 1.6414        | 0.19246              | 0.7060        |
| 0.4   | 4.426          | 0.3392        | 0.3358               | 1.918         |
| 0.45  | 3.0826         | 0.1075        | 0.4724               | 3.423         |

TABLE II. Summary of the critical parameters \(U_c(\Gamma_0)\) and \(\Gamma_c(U)\) as they are presented in Fig. 1.

From the NRG calculation of the local moment as depicted in Fig. 1(a) it is apparent that the approach to the LM FP close to the QCP is governed by a small energy scale \(T^*\) vanishing at \(U_c\) [34]. Consequently all energy scales contribute to the local moment formation in the LM phase close to \(U_c\), similar to estimated dimension of the Kondo cloud by \(\xi_K = \pi v_T/K\) in the SC phase [35–40]. Therefore, we interpret \(\xi^* \propto v_T/T^*\) as an estimate for the spatial extension of the local moment decoupling from a free conduction band.

Additionally we have included the analytical prediction for the critical Coulomb interaction \(U_c/\Gamma_0 = 16(r + 1)/(\pi r)\) derived by a Gutzwiller ansatz [20] for the pg-SIAM [16] into Fig. 1(b). The Gutzwiller approach systematically overestimates \(U_c\) since its wave-function ansatz is trying to strictly enforce a formation of the free local moment on the impurity in the LM phase. Such a picture is only valid for very large \(U\) for that the system is already deeply located in the LM phase. The Gutzwiller ansatz has two shortcomings: (i) it overestimates the critical \(U_c\) and, therefore, the SC regime since it cannot describe an extended local moment formation and (ii) the local impurity decouples completely from the conduction band in the LM phase which will have profound consequences for the real-time dynamics within such an approach.

Since we investigate the real-time dynamics of the double occupancy \(\langle D(t)\rangle\) for different type of quenches, we also provide results for the equilibrium double occupancy \(\langle D \rangle_{\text{eq}}\) vs \(U/\Gamma_0\) at fixed \(D/\Gamma_0 = 100\) in Fig. 2. The NRG data depicted in Fig. 2(a) demonstrates that \(\langle D \rangle_{\text{eq}}\) is continuous across the QCP. This continuity of local observables across the QCP has already been pointed out by Gonzalez-Buxton and Ingersent more the 15 years ago – see Fig. 8 in Ref. 6. We also added Gutzwiller equilibrium data calculated for the same hybridization function \(\Gamma(z)\) as Fig. 2(b) to illustrate the difference to the NRG. Within the Gutzwiller ansatz, \(\langle D(U_c)\rangle)_{\text{eq}} = 0\) and remains zero for \(U > U_c\). Consequently, the physical properties of Gutzwiller wave function deviate significantly from the true ground state as obtained by the NRG. Apparently, the Gutzwiller wave function ansatz cannot be applied in the LM phase close the the QCP since it misses the spatial extension of the local moment that is decoupling from the system.
B. Interaction quenches

In an interaction quench, we switch the Coulomb repulsion from its initial value $U_i$ at times $t < 0$ to the value $U_f$ for $0 \leq t$. In order to maintain ph-symmetry at all times, i.e. $U(t) + 2\epsilon_d(t) = 0$, we enforce also a switching in the d-level energy $-2\epsilon_d(t) = \Theta(-t)U_i + \Theta(t)U_f$. The hybridization strength $\Gamma(t) = \Gamma_1 = \Gamma_r = \Gamma_0$ is kept constant and is used as unit of energy. Short, intermediate, and long times will correspond to $t\Gamma_0 \ll 1$, $t\Gamma_0 \sim 1$ and $t\Gamma_0 \gg 1$.

We prepare the system initially in the uncorrelated state by setting $U_i = \epsilon_i = 0$. Since the impurity is coupled to the conduction band, the system approaches the SC FP for $T \to 0$. Therefore, the initial double occupancy is given by the uncorrelated value $\langle D \rangle_{eq} = 1/4$. In the LM FP, the double and the empty state on the magnetic impurity remain unoccupied, and $\langle D \rangle_{eq} = 0$.

1. Quenches within the SC phase

For switching on the Coulomb repulsion at $t = 0$, we can distinguish two cases: (i) for $U_f < U_c$ the system remains in the SC phase while (ii) for $U_f > U_c$ the equilibrium properties of the quenched system belong to the LM phase. Since we maintain ph-symmetry, the local occupancy always remains at half-filling and is unaffected by the quench. Therefore, we focus on the dynamics of the local double occupancy $\langle D(t) \rangle$. For a clear energy separation of band width $D$ and charge fluctuation scale $\Gamma_0$, we have chosen $D/\Gamma_0 = 10, 100 \gg 1$.

In Fig. 3 we present the time-dependent local double occupancy $\langle D(t) \rangle$ for quenches within the SC phase, $U_f < U_c$, for two different band widths $D$ for $r = 0.4$. All curves start at the non-interacting value $\langle D(t = 0) \rangle = 1/4$ and reduced to smaller values since the Coulomb interaction is suppressing the charge fluctuations and the local double occupancy.

Quenches within the SC phase thermalize at long times to the equilibrium value of the quenched system. The equilibrium values obtained from an independent equilibrium NRG calculation are indicated as arrows on the right side of the graph. The decay is governed by the time scale set by the charge fluctuation scale $\Gamma_0$. In contrary to results [16] obtained by a time-dependent Gutzwiller ansatz – see Fig. 2 in Ref. 16 – we do not find any oscillations in the double occupancy: a damped oscillation and a slow decay towards the equilibrium value seems to be counter-intuitive for the SC regime where the energy dissipation into the bath is strong.

It is interesting to note that we find universality for interaction quenches within the SC phase. In order to eliminate the influence of the different long-time expectation values of $\langle D(t \to \infty) \rangle$ that includes the $U_f$ dependency,
we define the function

\[ f(t) = \frac{\langle D(t) \rangle - \langle D(\infty) \rangle}{\langle D(0) \rangle - \langle D(\infty) \rangle} \]  

(10)
of the time-dependent double occupancy \( \langle D(t) \rangle \). The function \( f \) starts at \( f(0) = 1 \) and approaches \( f = 0 \) at infinitely long times independent of the parameters.

In Fig. 4(a) we demonstrate that all data depicted in Fig. 3 collapse onto one universal curve that is only dependent on the ratio \( D/\Gamma_0 \). To eliminate the \( \Gamma_0 \)-dependency, we define a crossover time \( t_{\text{co}} \) as \( f(t_{\text{co}}) = 0.5 \). Plotting \( f(t) \) versus the dimensionless time scale \( t/t_{\text{co}} \) maps all data for different ratios \( D/\Gamma_0 \) onto one unique curve, depicted in Fig. 4(b). Only the curve for \( D/\Gamma_0 = 10 \) deviates slightly from the others: in this case the separation of energies scales is much less pronounced. The inset of Fig. 4(b) illustrates the dependency of \( t_{\text{co}} \) on \( D/\Gamma_0 \): we find that

\[ t_{\text{co}} \propto \frac{1}{\Gamma_0 \sqrt{\Gamma_0}}. \]  

(11)

This establishes universality in the \( f(t) \) dynamics: the \( U_t \)-dependency enters only via \( \langle D(\infty) \rangle \) while the remaining real-time dynamics is only governed by the time scale \( t_{\text{co}} \) which depends on \( D \) and \( \Gamma_0 \).

Sofar, we only used a fixed bath exponent \( r = 0.4 \).

We extended our investigation to interaction quenches within the SC phase to \( r = 0, 0.1, 0.2, 0.3, 0.4 \). Again, we find universality in \( f(t/t_{\text{co}}) \) for fixed \( r \); the different universal functions for different \( r \) are depicted in Fig. 5(a). With decreasing \( r \) the universal curve shows a dip at short times after that it increases again to the long-time value. This correlates to a small peak structure in the effective local moment \( \mu_{\text{eff}}^2(T) \) for small \( r \) as depicted in the inset of Fig. 5(a).

In order to extract the \( r \)-dependence of the universality time scale, we plot \( \ln(t_{\text{co}} \Gamma_0 \sqrt{\Gamma_0/D}) \) vs \( r \) in Fig. 5(b) where the inset of the panel shows the bare time scale \( t_{\text{co}} \). Scaling \( t_{\text{co}} \) with \( \sqrt{r} \) for \( r \geq 0.1 \), we found an exponential dependency of the time scale \( t_{\text{co}} \) on \( r \),

\[ t_{\text{co}} \propto \frac{e^{m(D) r}}{\sqrt{r}} \sqrt{\frac{D}{\Gamma_0}} \]  

(12)

with a band width dependent exponent \( m(D) \). Note, however, that the phenomenological estimate (12) for the time scale does not interpolate to \( r \to 0 \) and, therefore, is only valid for \( 0.1 \leq r < 1/2 \).

When the charge-fluctuation scale \( \Gamma_0 \) approaches the band width \( D \), the non-equilibrium dynamics is dominated by local high-energy oscillations and, therefore, is non-universal as already indicated above. We present the time evolution of the double occupancy for the case \( D/\Gamma_0 = 1 \) in Fig. 6. We have plotted \( \langle D(t) \rangle \) versus \( \sqrt{U_t D} \) for \( U_t/\Gamma_0 = 0.5, 1, 2, 3, 4 \) to reveal the quadratic decrease \( \langle D(t) \rangle = 0.25(1-\alpha(t/t_{\text{short}})^2) \) where the short-time scale \( 1/t_{\text{short}}^2 \propto U_t \). It steams for a linear contribution of \( \langle n \rangle \) in a perturbative expansion of the time-dependent density operator after the interaction quench.

For \( U_t/\Gamma_0 = 2 \) the local single-particle excitation energies \( E_d \) and \( E_d + U \) approach the band edges, for \( U_t/\Gamma_0 = 3, 4 \) they exceed the band edges. Then, the states are only weakly coupled to the continuum with a finite energy gap preventing thermalization.

### Math Equations

1. \[ f(t) = \frac{\langle D(t) \rangle - \langle D(\infty) \rangle}{\langle D(0) \rangle - \langle D(\infty) \rangle} \]  
2. \[ t_{\text{co}} \propto \frac{1}{\Gamma_0 \sqrt{\Gamma_0}}. \]  
3. \[ t_{\text{co}} \propto \frac{e^{m(D) r}}{\sqrt{r}} \sqrt{\frac{D}{\Gamma_0}} \]
suggests a damped oscillation with a frequency that is only weakly $U_t$ dependent. Asymptotically, the double occupancy only thermalizes to the equilibrium value obtained directly with $H_t$ for smaller values of $U_t$. With increasing $U_t$, $\langle D(\infty) \rangle$ is decreasing and, therefore, the oscillation amplitude must increase.

In order to gain some understanding on the origin of these short-time oscillations we consider the limit of a vanishing band width at a constant hybridization $\pi V_f^2 = \int d\epsilon \Gamma(\epsilon) = \text{const}$. In this case we are left with a purely local problem described by the $r$-independent Hamiltonian $H_0$ of the first Wilson shell [3] whose eigenenergies are analytically known [3]. In this limit, there would be no damping, and we find a perfect oscillatory solution for $\langle D(t) \rangle$ whose frequency is determined by the difference of eigenenergies. A careful analysis of the local dynamics reveals that the oscillation of $\langle D(t) \rangle$ can be traced back to an admixture of two singlet states in the charge sector $Q = 0$ – (the quantum number $Q$ measures the deviation from half-filling [3]) – in the ground state wave function. The difference of the eigenenergies of those states labeled by $r = 1$ and $r = 2$ in Tab. I of the Ref. 3 coincide with the oscillation frequency extracted from $\langle D(t) \rangle$.

When we release the constrain of a vanishing band width, additional DOF of the Wilson chain need to be included in the analysis. Adding a single additional Wilson chain link, i.e. $H_0 \rightarrow H_1$ immediately causes a more complex response due to the splitting of these eigenfrequencies. Since $V_0/D \approx 1$ for $\Gamma_0/D = 1$, the energy splitting of the eigenenergies due to an increasing Wilson chain length must be smaller than $D$ and, therefore, $V_0$ and $U$. Hence the short-time dynamics on time-scales much shorter than $tU_t$ is dominated by energy differences coming from a slightly modified local dynamics. This is the origin of the pronounced minimum observed in $\langle D(t) \rangle$ in Fig. 6.

When the local excitation energies $E_d$ and $E_d + U$ are lying inside the band continuum, i.e. $|E_d|, |E_d + U| \leq D$, we observe thermalization. Once these local energies exceed the band continuum, bound states are formed outside of the band which contribute to the expansion of the initial ground state but cannot provide a relaxation channel. Even though we remain in the SC phase, $\langle D(t) \rangle$ cannot thermalize and remain oscillatory. This is the case for $U_t/\Gamma_0 = 3, 4$.

2. Quenches across the QCP

In this section we investigate interaction quenches across the QCP from the SC into the LM phase. Initially the system is prepared in the SC FP at $t = 0$ by setting $U_t = \epsilon_i = 0$.

For Coulomb repulsions $U_c < U_f$ the equilibrium properties of $H_f$ governing the real-time dynamics belong to the LM phase. The LM FP can be described by an effective local moment comprising a linear combination of the impurity spin and the conduction electron bath spins in addition to a decoupled remaining free effective conduction electron band. Therefore, a finite equilibrium double occupancy $\langle D \rangle_{\text{eq}}$ remains present even in the LM phase.

Similar to the Kondo temperature $T_k$ that determines the low-energy crossover to the SC fixed point, the characteristic temperature $T^*$ governs the crossover to the LM FP for $U > U_c$. We have defined $T^*$ as $\mu_{\text{eq}}^2(T^*) = 0.21$ and plotted $\mu_{\text{eq}}^2(T)$ versus $T/T^*$ to illustrate the universality in Fig. 7(b). We noted that $T^* \propto (U - U_c)^{\nu(r)}$ with $\nu(r) = 4.3$ for $r = 0.4$, and
$T^*$ vanishes at $U = U_c$.

In Fig. 7(a) we present $\langle D(t) \rangle$ for quenches over the QCP with $U_c/\Gamma_0 \approx 0.3392 < U_l/\Gamma_0 = 0.4, 0.6, 1, 4$ for a wide band $D/\Gamma_0 = 100$ and temperature $T/\Gamma_0 \sim 10^{-10}$. The data obtained at a temperature $T/\Gamma_0 \sim 10^{-6}$ remains indistinguishable from the results depicted in Fig. 7(a) and, therefore, $T \to 0$. Even though $T > T^*$ for the lowest $U_l$ value, the real-time dynamics remains temperature independent and is only governed by the overlap of the initial ground state with the eigenstates of the final Hamiltonian.

We have plotted the data as function of the dimensionless time $t U_l$ to reveal the time scale of the short-time dynamics. For quenches within the SC phase, we have demonstrated that the characteristic time scale is independent of $U_l$. For quenches across the QCP into the LM phase, we find that the time scale is proportional to $1/U_l$. The real-time dynamics is dominated by the local dynamics since part of the impurity DOFs decouple from the rest of the conduction band to participate in the local moment formation.

The characteristic energy scale $T^*$ extracted from the universality of $\mu^2_{eq}(T)$ in the LM phase depicted in Fig. 7(b) increases with increasing distance $U_c - U_l$ to the QCP. The length scale $\xi^* = v_F/T^*$ used as an estimate for the spatial extension of the local moment decreases with increasing $U_c$. The decoupled spin DOF become more localized and, consequently, the thermalization is increasingly suppressed with increasing $U_l$.

For $U_l/\Gamma_0 = 4$, we observe a decaying oscillatory behavior driven by a frequency proportional to $U_l$ with a strong deviation between the long-time steady-state and the thermal equilibrium. For the smallest two interactions, $U_l/\Gamma_0 = 0.4, 0.6$, however, we found a steady-state value that is very close to the thermodynamic result and, therefore, be considered as evidence for thermalization.

Although the equilibrium expectation value $\langle D \rangle_{eq}$ is continuously reduced with increasing $U$ even across the QCP $U_c$, Fig. 7(a) demonstrates nicely the qualitative different response for quenches across the QCP versus the previously investigated dynamics within the SC phase in Sec. III B.1. While the characteristic time scale only depends on $\Gamma_0$ for quenches within the SC phase and shows universal behavior as long as all local excitation remain in the bath continuum, the real-time dynamics across the QCP is governed by $1/U_l$.

In order to illustrate the connection between the spatial extension of the local moment and thermalization we calculated the difference between the steady-state value $D_\infty$ defined as

$$D_\infty = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt \langle D(t) \rangle$$  \hspace{1cm} (13)

and the thermal equilibrium value $\langle D \rangle_{eq}$ obtained for $H_0$.

The results are depicted versus $T^*/\Gamma_0$ in Fig. 8 using the data of Fig. 7. Close to the QCP, the deviation is less the 3% given by the typical discretization error of the TD-NRG. For increasing $U_l$ the deviation increases, supporting the picture of an increasingly localised free moment, leading to an increasing non-decaying fraction of the local double occupancy.

We also have supplemented data for fixed $U_l/\Gamma_0 = 1$ but a variation of $D$ as crosses connected with a blue line (color online) in Fig. 8. Interestingly, the deviation $\Delta D = D_\infty - \langle D \rangle_{eq}$ follows the same trend, and agrees within the numerical error with the data for fixed $D/\Gamma_0$ when approaching the QCP.

The deviation $\Delta D$ systematically increases with increasing $T^*$. Once $T^*$ becomes large, the physics changes to an effectively decoupled free moment that is strongly localised and therefore prevents thermalization of the local expectation values.

Our results are in contrast to the results of Fig. 3 in Ref. 16 where this type of quenches were examined by a time-dependent Gutzwiller approach. Therein it was reported that the double occupancy $\langle D(t) \rangle$ strongly oscillates and never reaches a steady-state value at long times.

The reason for this disagreement is the nature of the Gutzwiller state whose dynamics has been traced via a time-dependent Gutzwiller equation [16]. This ansatz wave function is not able to properly represent the LM phase: $\langle D \rangle_{eq}$ vanishes for $U > U_c$ and is taken as indicator for the QPT while an equilibrium NRG calculation [6] has proven the continuity of $\langle D \rangle_{eq}$ across $U_c$ – see also Fig. 2. While the NRG correctly contains the spatially extended nature of the decoupled local moment, the Gutzwiller state restricts the free moment to the local impurity site. Therefore, the time-dependent Gutzwiller approach is restricted to the strong-coupling regime.

In Fig. 9(a) we examine the effect of the bandwidth $D$ onto the real-time dynamics using four different values $D/\Gamma_0 = 100, 125, 175, 200$ for a constant ratio $U_l/\Gamma_0 = 3$.

For this series, $U_c(D/\Gamma_0 = 100)/\Gamma_0 = 0.3358$ has the largest value and decreases further with increasing bandwidth $D$. So $U_l$ exceeds $U_c$ almost by one decade even...
for the largest $U_c$. Therefore, we quench deeper into the LM phase, indicated by a decreasing equilibrium double occupancy $\langle D\rangle_{eq}$ — see arrows at right side of graph. With increasing band width $D$, the amplitude of the damped oscillations are increased while the frequency is only proportional to $U_t$.

In Fig. 9(b) we vary the bath exponent $r$ for a fixed ratio $D/\Gamma_0 = 100$ and choose $U_i$ such that the equilibrium expectation value $\langle D(U_i)\rangle_{eq} \approx 0.02$ remains nearly constant for all $r$ as indicated by the arrows on the right side. $\langle D(t)\rangle$ is plotted vs $tU_t$ to remove the leading order frequency dependency of the oscillations for different Coulomb interactions $U_i$. The remaining small frequency shift with increasing $r$ is related to the different ratios $U_i/\Gamma_i$: the larger $r$, the larger the ratio $\Gamma_i/U_i$ and corrections of the order $\sqrt{1+2\Gamma_i D/(\pi U_i^2)}$ need to be taken into account stemming from the energy difference of eigenstates of the first Wilson shell as previously discussed in the context of Fig. 6.

### 3. Quenches from the LM phase

In a reverse type of quench the initial $U_i$, exceeding the critical $U_c$, is reduced to values $U_t$ that are either larger than $U_c$, such that the systems remains in the LM phase, or $U_t < U_c$, for quenching across the QCP into the symmetric SC phase. The initial value of $\langle D(t=0)\rangle$ depends on the distance $U_i - U_c$ and reaches $\langle D(0)\rangle \to 0$ for $U_i \to \infty$. Since we always maintain ph-symmetry, $2\varepsilon_d(t) + U(t) = 0$ holds at any time.

In order to investigate the dependency of $U_i$, we calculate the real-time dynamics for three different values $U_i \approx U_c$, $U_i/U_c = 10$ and $U_i/U_c = 100$. The results are depicted in Fig. 10(a)-(c). Each graph shows $\langle D(t)\rangle$ for a fixed $U_i$ and a series of four values of $U_i$: For quenches within the LM phase, we use $U_i/U_c = 1.2, 1.5$ while for quenches across the QCP into the SC phase we choose $U_i/U_c = 0.25, 0.5$.

The initial value $\langle D(t=0)\rangle$ decreases with increasing value $U_i$. Starting with $U_i/U_c = 1$, we observe an increase of $D_{\infty}$ for $U_i < U_c$ and a decrease for $U_i > U_c$ as...
expected. Furthermore, \( D_\infty \approx \langle D \rangle_{\text{eq}}(U_i) \) as indicated by the arrows on the right side of Fig. 10(a) which we interpret as indication for thermalization.

For Fig. 10(b), we have prepared the system with \( U_i/U_c = 10 \), and quench to the same four final values of \( U_f \) as in Fig. 10(a). Again, the initial short-time dynamics is \( U_f \) independent, starting from a much smaller initial value. The saturation is almost reached at \( t \Gamma_0 \approx 1 \). However, we observe a slight deviation from the thermal equilibrium. Those deviations remain negligible small for quenches from the LM to the SC phase but become visible for quenches within the LM phase: the deviations are of the order of 7\%. For the last value \( U_i/U_c = 100 \), starting deep in the LM phase with a completely suppressed initial double occupancy, the short-time dynamics is again \( U_f \) independent and the steady-state value is approached very fast, governed by the time scale of \( 1/\Gamma_0 \). However, the deviation from the thermal equilibrium is much more pronounced and reaches about 15\% for \( U_i/U_c = 1.5 \).

### C. Hybridization quenches

Up to now, we have investigated interaction quenches. In this section, we focus on a second type of quenches, the hybridization quenches. They are defined by switching the hybridization strength \( \Gamma_0 \rightarrow \Gamma(t) = \Theta(-t)\Gamma_i + \Theta(t)\Gamma_f \) between the initial value \( \Gamma_i \) and the final value \( \Gamma_f \) at time \( t = 0 \). In contrast to the previous sections, we keep here the Coulomb repulsion \( U_i/D = U_f/D = \text{const} \) and finite at all times and restrict ourselves to particle-hole symmetry. In order to have a well defined, unique reference point, we choose \( \Gamma_i = 0 \) implying that the system is initially prepared in the LM FP whose ground state is \( U \) independent with a double occupancy \( \langle D(t = 0) \rangle = 0 \) for all parameters.

Since we change \( \Gamma_0 \), we use the band width \( D \) as unit of energy in this section. The terms short, intermediate, and long times will correspond to \( tD \ll 1 \), \( tD \sim 1 \) and \( tD \gg 1 \).

As discussed in Sec. II C, \( H_I \) has two different low-energy FP depending on \( \Gamma_f \). For \( \Gamma_f < \Gamma_c \), the LM FP is reached at low temperature in equilibrium, while for \( \Gamma_f > \Gamma_c \), the system is described by the symmetric SC FP. We have checked that the equilibrium FP has been reached for all parameters such that the real-time dynamics results correspond to \( T \rightarrow 0 \).

#### 1. Quenches within the LM phase

We start with quenches within the LM phase, i.e. \( \Gamma_f < \Gamma_c \), and present data in the wide-band limit by setting \( D/U = 100 = \text{const} \). The results for the time-dependent double occupancy \( \langle D(t) \rangle \) are depicted for the short-time dynamics in Fig. 11(a) and the long-time asymptotic in Fig. 11(b) for \( \Gamma_f/D = 0.002, 0.004, 0.008, 0.012, 0.016 < \Gamma_c/D \approx 0.019 \).

The double occupancy \( \langle D(t) \rangle \) rises quickly from its initial value and exhibits a peak at intermediate times before it falls off towards a steady-state value. With increasing hybridization \( \Gamma_f \) the peak height raises and is more pronounced. Plotting all data versus the dimensionless time \( \tau = t\sqrt{\Gamma_f/D} \) reveals that the short-time dynamics is \( U \)-independent and only driven by the final hybridization strength \( \Gamma_f \).

Although a steady-state is reached, the difference to the thermodynamic equilibrium value – indicated by the arrows in Fig. 11(b) – is significant and increases with increasing \( \Gamma_f \). This indicates that the real-time dynamics is not governed by the FP properties but from the overlap of the initial wave function with the excited states of \( H_I \).

Deviations from the thermodynamic equilibrium could originate in limitations of the method due to the discretization of the conduction band continuum [14, 15, 31, 41]. The low-energy FP of \( H_I \), however, is still given by the LM FP with a two-fold generate ground state so that the increase of the deviation with increasing \( \Gamma_f \) is explained. Varying \( \Gamma_f \) within the LM phase has a profound impact on the physics. With increasing \( \Gamma_f \) the system approaches \( \Gamma_c \) and, therefore, the characteristic energy scale \( T^* \) decreases. This implies that the effective
spin moment decoupling from the rest of the system becomes more extend with increasing \( \Gamma_f \) and a larger fraction of the impurity DOF hybridize with the conduction band leading to an continuous increase of \( \langle D \rangle \). There are two states of finite range that form the effective moment decoupling from the rest of the chain. An admixture of those states to the initial ground state cannot relax further due to the decoupling of these states in the LM regime. Consequently, we observe a state-state differing significantly from the thermal state.

2. Analytic result for the short-time dynamics

In order to shed some more light into the dynamics for hybridization quenches when \( \Gamma_f < \Gamma_c \), we analytically calculate \( \langle D(t) \rangle \) for the short-time dynamics. Knowing all eigenstates and eigenenergies for \( \Gamma_0 = 0 \), we expand the time-dependent density operator in powers of the hybridization, and evaluate \( \langle D(t) \rangle \) exactly up to second-order – see appendix A for more details.

The short-time dynamics of the double occupancy is given by the analytic expression

\[
\langle D(t) \rangle = \frac{\Gamma_f D^2}{\pi t^2} + \frac{2\Gamma_f (1 + r)}{\pi} \sum_{n=2}^{\infty} \frac{(-1)^{2n}}{(2n)!} \int_{-D}^{0} \left( \frac{\epsilon}{D} \right)^{n-1} (\epsilon - \epsilon_d - U) t^{2n} \, d\epsilon \; .
\]

which is asymptotically exact for \( t \to 0 \). In leading order in \( t \), \( \langle D(t) \rangle \) increases quadratically in time with an \( U \) independent prefactor \( \Gamma_f D/\pi \) defining the squared characteristic time scale for the short-time dynamics. Our analytical result confirms the dimensionless time scale \( \tau = t \sqrt{\Gamma_f D} \) used previously in Fig. 11 to reveal the universality in the short-time TD-NRG response. The \( U \)-dependent corrections enter the higher terms in \( t \) and account for a weak oscillation.

In order to illustrate the leading \( t^2 \)-behavior in the short-time dynamics of the full TD-NRG calculations and their excellent agreement with the analytical result for the full continuum, we present the numerical results of Fig. 11(a)+(b) in a log-log plot as Fig. 11(c). We added the analytical results of Eq. (14) for selected times as crosses in the same color. Numerics and analytics coincide perfectly for short and intermediate times even up to \( t \sqrt{\Gamma_f D} \approx 1 \). The analytical result does not only describe the leading order \( O(t^2) \) term correctly but also accounts for the deviation from the parabola starting at \( t \sqrt{\Gamma_f D} \approx 10^{-3} \) and the long-time steady-state. Of course the deviation between the analytic steady-state value and the TD-NRG results is stronger with increasing \( \Gamma_f \) as expected from the perturbative nature of the analytical approach.

3. Energy flow in the LM phase

It has been conjectured that the choice of a Wilson chain might be unsuitable for describing hybridization quenches [42] because the chain might not be able to serve as a heat reservoir for larger changes in the hybridization energy. However, Wilson’s NRG targets only the local dynamics and corresponding bath expectation values do not have any physical meaning: a discretized finite bath, as used in any NRG calculation has always only finite energy content while the thermodynamic bath provides a reservoir with infinitely large energy. Since a quantum state by itself can never thermalize when subject to the energy conserving dynamics defined by the Schrödinger equation, one needs to restrict such an investigation to quantum impurity expectation values. The deviation from a corresponding equilibrium NRG calculation using identical discretisation parameters serves as a criterion how well the quantum impurity subsystem is able to thermalize.

We have investigated the local energy flow for quenches within the LM phase for the quench parameters presented in Fig. 11. For those parameters we have demonstrated already that thermalization of the double occupancy \( \langle D(t) \rangle \) is absent, and switching on the hybridization results in an overestimation of the double occupancy compared to the thermal equilibrium that increases with \( \Gamma_f \). For particle-hole symmetry, \( E_{d\bar{n}_d} \) is discontinuous at \( t = 0 \), since work has been performed on the system, but afterwards \( E_{d\bar{n}_d} \) remains constant for \( t > 0 \). In addition,
the contribution of $U \langle D(t) \rangle$ to the impurity energy is very small compared to $E_{\text{hyb}}(t) = \langle H_{\text{hyb}}(t) \rangle$. Therefore, the main energy flow of the impurity is governed by the hybridization energy $E_{\text{hyb}}(t)$ which is initially zero for $t \leq 0$.

The results of $E_{\text{hyb}}(t)$ are depicted in Fig. 12: the arrows on the right side in Fig. 12(a) indicate the thermal expectation value of the hybridization energy indicating clearly that $E_{\text{hyb}}(t)$ is approaching its thermal equilibrium in the long-time limit, even though the system remains in the LM regime and $\langle D(t) \rangle$ does not equilibrate. $E_{\text{hyb}}(t)$ has been measured in units of the constant $U$ and plotted versus $r = t\sqrt{\Gamma f D}$. Clearly the dynamics is not governed by the characteristic time scale of the double occupancy.

Since the hybridization energy is proportional to $\Gamma_f$, 

$$\sum_{k\sigma} V_k \langle d^\dagger_{k\sigma} c_{\sigma} \rangle \propto \Gamma_f,$$  

we have divided out the leading order prefactor of $E_{\text{hyb}}$, $\Gamma_f$, and have plotted $E_{\text{hyb}}/\Gamma_f$ vs $tD$ in Fig. 12(b). Surprisingly, the short-time dynamics of $E_{\text{hyb}}/\Gamma_f$ appears to be universal and is governed by the band width $D$ while the overall magnitude of $E_{\text{hyb}}$ is determined by $\Gamma_f$ for a finite $r = 0.4$. While for $r = 0$ $E_{\text{hyb}}/\Gamma_f \propto \ln(D/\Gamma_f)$ in equilibrium as can be shown by a simple analytic calculation, this is not the case for $r > 0$: the larger $r$ the less $E_{\text{hyb}}/\Gamma_f$ depends on the ratio $D/\Gamma_f$ for the wide-band limit. Since the hybridization energy approaches its steady-state value very fast, apparently this expectation value is not influenced by the build-up of low energy correlations characterising the LM FP.

4. Quenches across the QCP

Now, we proceed with hybridization quenches across the QCP, from the initial LM FP with $\Gamma_1 = 0$ into the symmetric SC phase with $\Gamma_c < \Gamma_f$. The time-dependent double occupancy $\langle D(t) \rangle$ is depicted in Fig. 13 for $\Gamma_c/D < \Gamma_f/D = 0.06, 0.08, 0.1$. As shown in Fig. 13, the contribution of $U \langle D(t) \rangle$ to the impurity energy is very small compared to $E_{\text{hyb}}(t) = \langle H_{\text{hyb}}(t) \rangle$. Therefore, the main energy flow of the impurity is governed by the hybridization energy $E_{\text{hyb}}(t)$ which is initially zero for $t \leq 0$.

The results of $E_{\text{hyb}}(t)$ are depicted in Fig. 12: the arrows on the right side in Fig. 12(a) indicate the thermal expectation value of the hybridization energy indicating clearly that $E_{\text{hyb}}(t)$ is approaching its thermal equilibrium in the long-time limit, even though the system remains in the LM regime and $\langle D(t) \rangle$ does not equilibrate. $E_{\text{hyb}}(t)$ has been measured in units of the constant $U$ and plotted versus $r = t\sqrt{\Gamma f D}$. Clearly the dynamics is not governed by the characteristic time scale of the double occupancy.

Since the hybridization energy is proportional to $\Gamma_f$, 

$$\sum_{k\sigma} V_k \langle d^\dagger_{k\sigma} c_{\sigma} \rangle \propto \Gamma_f,$$  

we have divided out the leading order prefactor of $E_{\text{hyb}}$, $\Gamma_f$, and have plotted $E_{\text{hyb}}/\Gamma_f$ vs $tD$ in Fig. 12(b). Surprisingly, the short-time dynamics of $E_{\text{hyb}}/\Gamma_f$ appears to be universal and is governed by the band width $D$ while the overall magnitude of $E_{\text{hyb}}$ is determined by $\Gamma_f$ for a finite $r = 0.4$. While for $r = 0$ $E_{\text{hyb}}/\Gamma_f \propto \ln(D/\Gamma_f)$ in equilibrium as can be shown by a simple analytic calculation, this is not the case for $r > 0$: the larger $r$ the less $E_{\text{hyb}}/\Gamma_f$ depends on the ratio $D/\Gamma_f$ for the wide-band limit. Since the hybridization energy approaches its steady-state value very fast, apparently this expectation value is not influenced by the build-up of low energy correlations characterising the LM FP.

5. Comparison with Gutzwiller results

In Sec. III A we have pointed out that the local equilibrium properties obtained by the accurate NRG approach deviate significantly from the approximate Gutzwiller approach. This discrepancy can be traced back to the physical content of the Gutzwiller ansatz wave function that focuses only on the local spin moment formation on the impurity site while the NRG ground state correctly accounts for the extended nature of the decoupling moment. Consequently, the local nature of Gutzwiller ansatz largely overestimates the critical $U_c$ as already shown in Fig. 2.
A choice of identical model parameters always yield different local properties in the two different methods. In order to make a useful comparison between the approaches, we have chosen the NRG parameters such that the equilibrium double occupancies approximately agree between both approaches, i.e. $D_{\infty}^{\text{TD-NRG}} \approx D_{\infty}^{\text{Gutzwiller}}$ as well as both approaches describe the same type of quench.

The Gutzwiller data is taken from Fig. 2 in Ref. 16 calculated for a hybridization quench in the wide-band limit with $U/\Gamma_t = 9$, and $r = 0.4$, where a hybridization quench from the initial LM phase into the SC phase across the QCP has been investigated.

While the equilibrium Gutzwiller approach predicts a screened local moment and hence describes the SC phase, these parameter would be located deeply in the LM phase in a NRG calculation. Therefore, we had to reduce $U$ to $U/\Gamma_0 = 1.6 < U_\infty/D$, cf. the NRG parameters of the TD-NRG calculation to also maintain the NRG dynamics in the SC regime.

We compare the double occupancy $\langle D(t) \rangle$ from the TD-NRG and the Gutzwiller approach in Fig. 14(a). The Gutzwiller approach predicts a very long silent phase for $0 < t < 1/\Gamma_t$ after the quench, before $\langle D(t) \rangle$ steeply rises for $1 < t \Gamma_t$ and then approaches oscillatory the equilibrium value at long times. In contrary to these approximate results, the TD-NRG data perfectly agrees with the analytical prediction of Eq. (14) for the short-time dynamics, predicting a fast quadratic raising of $\langle D(t) \rangle \approx 2\bar{\Gamma}_t D/\pi$ for short times before higher order terms cause a convergence to a finite value.

The origin of the long silence phase in the Gutzwiller approach is directly related to the slow increase of $|E_{\text{hyp}}|$ caused by the strong analytic restriction of the parameter space in the ansatz as can be seen from the equation of motions stated in the supplement of Ref. 16. In the accurate TD-NRG, however, the energy flow away from the impurity is very fast and occurs on the time scale of the inverse band width.

6. Quenches for exponents $r > 1/2$

So far we restricted ourselves to exponents $0 < r < 1/2$ since a QCP can be found only for those values if $U > 0$. For $1/2 < r$ and $U > 0$, the system always approaches the LM FP for $T \to 0$ in equilibrium [6].

Let us briefly review the equilibrium properties of these regimes for varying the bath exponent $r$ and a fixed $D/\Gamma_0 = 100$ depicted in Fig. 15. The effective local moment $\mu_{\text{eff}}^2(T)$ is plotted versus $T$ in the strongly correlated regime $\Gamma_0/U = 0.1$ in Fig. 15(a) and in the weakly correlated regime $\Gamma_0/U = 10$ in Fig. 15(b) for $r = 0, 0.2, \cdots, 1.2$. For $r = 0$ the system always approaches the SC FP with $\mu_{\text{eff}}^2(0) = \lim_{T \to 0} \mu_{\text{eff}}^2(T) = 0$ while for $0.2 \leq r < 1/2$, the symmetric SC FP with $\mu_{\text{eff}}^2(0) = r/8$ for $\Gamma_0/U = 10$, and the LM FP $\mu_{\text{eff}}^2(0) = 1/4$ for $\Gamma_0/U = 0.1$. For $1/2 < r$, the system always flows to the LM FP, and the crossover scale $T^*$ is increasing with increasing $r$.

The corresponding equilibrium double occupancy $\langle D_{\text{eq}} \rangle$ versus $r$ is shown in Fig. 15(c) for $T \to 0$. In the weakly correlated regime $\Gamma_0/U = 10$ the double occupancy $\langle D_{\text{eq}} \rangle$ remains close to the uncorrelated value of 0.25 and only weakly dependent on $r$ for $0 < r < 1/2$. The slow decrease of $\langle D_{\text{eq}} \rangle$ is related to a reduced screening of the impurity with increasing $r$ and fixed $\Gamma_0/U = 10$. For $1/2 < r$ the double occupancy $\langle D_{\text{eq}} \rangle$ declines much faster with increasing $r$ since the system approaches the LM FP for $T \to 0$. For the strongly correlated regime $\Gamma_0/U = 0.1$, the double occupancy $\langle D_{\text{eq}} \rangle$ is already strongly suppressed for small $r$.

Now we present our results for hybridization quenches as function of $r$ for $D/\Gamma_1 = D/\Gamma_1 = 100$ and fixed $\epsilon_d = -U/2$. The TD-NRG results for the double occupancy $\langle D(t) \rangle$ are depicted for two values for $\Gamma_1/U = 0.1$, 10 and $r = 0, 0.2, 0.4, 0.6, 0.8, 1.0, 1.2$ in Fig. 16.

With the exception of $r = 0$, Fig. 16(a) shows quenches within the LM phase. The double occupancy $\langle D(t) \rangle$ rises from its initial value towards its steady-state value which differs significantly from its thermal equilibrium.
the order of magnitude of $\langle D \rangle_{\text{eq}}$ is depicted in Fig. 15(c) we have divided out its steady-state value $D_\infty$ and also indicated the ratio $\langle D \rangle_{\text{eq}} / D_\infty$ as arrows on the right side with the same color to illuminate the short-time oscillatory behavior independently of the absolute value of $\langle D(t) \rangle$. Due to the rescaling, the time scale $\tau = 1/\sqrt{\Gamma_f D}$ governing the overall response is not directly discernible as in Fig. 16 (b).

On an intermediate time scale, we observe a damped oscillatory behavior for small $r$. This oscillations are stronger pronounced with increasing $r$ due to a stronger concentrated local moment formation around the impurity, and therefore the local dynamics between the impurity an the first Wilson shell is more emphasized. The deviation of the equilibrated steady-state value and the thermodynamic equilibrium, indicated by the arrows on the right of the graph, is increasing with increasing $r$ which is also correlated with the increasing localization of the effective moment.

For the weakly correlated regime, depicted in Fig. 16(b), we find thermalization only for quenches into the SC phase. For $1/2 < r$, the steady-state value of $\langle D(t) \rangle$ is reduced with increasing $r$, and the difference to the thermal equilibrium is also continuously increasing due to quenching into the LM phase. Plotting the data versus $t \sqrt{\Gamma_f D}$ clearly reveals the universal $r$-independent time scale governing the short-time dynamics, as predicted by our perturbation theory. For quenches remaining in the LM phase, we observe short-time oscillations whose damping decreases with increasing $r$. This oscillations have the same frequency dependency as in Fig. 16(a) proportional to the Coulomb repulsion $U$.

IV. CONCLUSION

We have analysed in detail the impurity dynamics of the pg-SIAM after local quenches.

In Sec. IIIA we have summarized the known equilibrium properties of the pseudo-gap model. There we have discussed the limitations of a Gutzwiller ansatz [16, 17, 19, 20] which only allows a decoupling spin moment forming on the impurity site in the LM phase whereas the NRG is able to generate the correct ground state describing a spatially extended spin-moment formation.

We have distinguished two quench types: the interaction quench in Sec. III B and the hybridization quench in Sec. III C.

For the former we have found an universal curve for interaction quenches within the SC phase: All dependencies of the Coulomb repulsion $U_f$, the band width $D$ and the bath exponent $r$ are included in the scaling function $f(t)$ defined by Eq. (10) and the crossover time scale $t_{\text{crossover}}$ approximated by Eq. (12).

From the temperature-dependent effective moment $\mu_{\text{eq}}^2(T)$ in the LM regime we have defined the crossover scale $T^*$ that depends on the distance $U - U_c$ and vanishes for $U_c$. Since $T^*$ is directly related to the NRG iteration $N^*$ beyond which the LM FP is approached, $1/T^*$ can be interpreted as a characteristic length scale of the local-moment formation: the larger $T^*$ will be, the more localized the effective spin moment decoupling from the rest of system will be. Moreover, we have demonstrated that the difference between the steady-state value $D_\infty$ and thermodynamic expectation value $D_{\text{eq}}$ only depends on $T^*$ independent of varying $U_f$ at fixed $D$ or varying $D$ for fixed $U_f$. This spatial dependency of the decoupled moment encoded in the NRG ground state cannot be accounted for in the Gutzwiller approach [16] since the wave-function ansatz restricts the moment formation onto the impurity site.

In the presented hybridization quenches we always start from a decoupled impurity at $t = 0$ and switch on $H_{\text{hyp}}$ with different coupling strength. For a small hybridization, the system remains in the LM phase while a large hybridization drives the system across the QCP into the SC phase. We have gauged the quality of our numerical results by our analytic second-order perturbation theory, which becomes exact for times $t \rightarrow 0$, and found excellent agreement between the analytics and the numerics in the applicability range of the perturbation theory. We could show that the short-time dynamics is governed by the time scale $1/\sqrt{\Gamma_f D}$ which is independent of the Coulomb interaction.

By comparison of our data with the recent Gutzwiller results [16] we could demonstrate the shortcomings of this variational ansatz that already strongly deviates from the
asymptotically exact perturbative result for short-time scales. After illustrating the major difference of the physical content in the ground state wave function between the approximate Gutzwiller approach and the exact NRG ground state, the differences between the equilibrium as well as the non-equilibrium results of both methods become transparent.

Thermalization was observed within the errors of the TD-NRG [31, 41] for quenches within or into the SC phase. Due to the extended nature of the decoupling effective spin in the LM phase, we still found a steady-state value for $\langle D(t) \rangle$ that, however, increasingly deviates from the thermodynamic expectation value. Interestingly, we found a thermalization of the hybridization energy $E_{\text{hyb}}$ which accounts for the major local energy change after the quench. We also provide a short overview for hybridization quenches for exponents $1/2 < r$ where only a LM FP is found for $U > 0$.

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Appendix A: Perturbation theory for hybridization quenches

In general, we assume that the system is in equilibrium for $t < 0$ and that its dynamics is governed by the initial Hamiltonian $H_0$ which is switched to $H_1 = H_0 + H_p$ by the additional perturbation $H_p$.

The real-time dynamics of any operator $\hat{O}$ can be calculated using a time-dependent density operator $\hat{\rho}(t)$

$$\langle O(t) \rangle = \text{Tr} \left\{ \hat{\rho}(t) \hat{O} \right\} = \text{Tr} \left\{ \hat{\rho}^I(t) \hat{O}^I(t) \right\} \quad (A1)$$

where we have transformed all the operators into the interaction picture $\hat{O}^I(t) = \exp(iH_0 t) \hat{O} \exp(-iH_0 t)$ in the last step.

The time evolution of the density operator is calculated by integrating the von Neumann equation

$$\frac{\partial \hat{\rho}^I}{\partial t} = i [\hat{\rho}^I(t), H_p^I(t)] \quad (A2)$$

to

$$\hat{\rho}^I(t) = \hat{\rho}_0 + i \int_0^t dt_1 [\hat{\rho}^I(t_1), H_p^I(t_1)] \quad (A3)$$

where we have used the boundary condition $\hat{\rho}^I(0) = \hat{\rho}_0 = \exp(-\beta H_0)/Z_0$ and $Z_0 = \text{Tr} \{\exp(-\beta H_0)\}$.

Iterating Eq. (A3) once more and substituting the expression into (A1) the time evolution of an expectation value up to second order of the perturbation is given by the general expression

$$\langle O(t) \rangle \approx \text{Tr} \left\{ \hat{\rho}_0 \hat{O} \right\} + i \int_0^t dt_1 \text{Tr} \left\{ \hat{\rho}_0 [H_p^I(\tau_1), \hat{O}^I(t)] \right\}$$

$$- \int_0^t dt_1 \int_0^{\tau_1} dt_2 \text{Tr} \left\{ \hat{\rho}_0 [H_p^I(\tau_2), [H_p^I(\tau_1), \hat{O}^I(t)]] \right\} \quad (A4)$$

For a hybridization quench, we start with a decoupled impurity and switch on the hybridization $H_p = H_{\text{hyb}}$ at $t = 0$. Although the Hamiltonian

$$H_0 = \sum_{\sigma k} \epsilon_k c_{\sigma k}^{\dagger} c_{\sigma k} + \sum_{\sigma} \epsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U d_{\sigma}^{\dagger} d_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} \quad (A5)$$

is not bilinear, it can be diagonalized exactly and all expectation values with respect to $\hat{\rho}_0$ are known. The transformation of $H_{\text{hyb}}$ into the interaction picture only requires

$$c_{\sigma k}(t) = c_{\sigma k} e^{-i\epsilon_k t} \quad , \quad c_{\sigma k}^{\dagger}(t) = c_{\sigma k}^{\dagger} e^{i\epsilon_k t} \quad (A6)$$

and

$$d_{\sigma}(t) = |\sigma\rangle \langle \sigma| e^{-i\epsilon_d t} \quad , \quad d_{\sigma}^{\dagger}(t) = |\sigma\rangle \langle \sigma| e^{i\epsilon_d t} \quad (A7)$$

Now we specialize to a particle-hole symmetric model, $\epsilon_d = -U/2$ and $n_\sigma = 1/2$. For $T \to 0$, the initial double occupancy $\text{Tr} \left\{ \hat{\rho}_0 \hat{D} \right\} = 0$; likewise also the first-order contribution in Eq. (A4) vanishes since $\text{Tr} \left\{ \hat{\rho}_0 [H_{\text{hyb}}^I(t), \hat{D}] \right\} = 0$.

After evaluating the commutators and the traces of the second-order contribution for $T \to 0$, we are left with

$$\langle D(t) \rangle = \sum_k V_k^2 f(\epsilon_k) (I^+(\epsilon_k) + I^-(\epsilon_k)) \quad (A9)$$

where the two integrals

$$I^\pm(\epsilon_k) = \int_0^t dt_1 \int_0^{t_1} dt_2 \ e^{i(\epsilon_k - \epsilon_d - U)t_2} \times e^{\mp i(\epsilon_k - \epsilon_d - U)t_1} \quad (A10)$$

can be evaluated analytically.

Using the pseudo-gap density of states we rewrite the sum over $k$ as an integral over $\epsilon$

$$\langle D(t) \rangle = \int_{-D}^{D} \frac{\Gamma(\epsilon)}{\epsilon} \left[ 1 - \cos((\epsilon - \epsilon_d - U)t) \right] d\epsilon \quad (A11)$$

which requires numerical evaluation.

For $T \to 0$, we can perform the integration analytically in a series expansion and obtain the final result

$$\langle D(t) \rangle = \frac{\Gamma_0 D}{\pi} t^2 + 2\frac{\Gamma_0 (1 + r)}{\pi} \sum_{n=2}^{\infty} \frac{(-1)^{2n}}{(2n)!} t^{2n} \quad (A12)$$

$$\times \int_{-D}^{D} \left| \frac{\epsilon}{D} \right| \left[ (\epsilon - \epsilon_d - U \right)^t d\epsilon.$$
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