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Optimized auxiliary representation of non-Markovian impurity problems by a Lindblad equation

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# Abstract

We present a general scheme to address correlated nonequilibrium quantum impurity problems based on a mapping onto an auxiliary open quantum system of small size. The infinite fermionic reservoirs of the original system are thereby replaced by a small number  $N_{\rm B}$  of noninteracting auxiliary bath sites whose dynamics are described by a Lindblad equation, which can then be exactly solved by numerical methods such as Lanczos or matrix-product states. The mapping becomes exponentially exact with increasing  $N_{\rm B}$ , and is already quite accurate for small  $N_{\rm B}$ . Due to the presence of the intermediate bath sites, the overall dynamics acting on the impurity site is non-Markovian. While in previous work we put the focus on the manybody solution of the associated Lindblad problem, here we discuss the mapping scheme itself, which is an essential part of the overall approach. On the one hand, we provide technical details together with an in-depth discussion of the employed algorithms, and on the other hand, we present a detailed convergence study. The latter clearly demonstrates the above-mentioned exponential convergence of the procedure with increasing N<sub>B</sub>. Furthermore, the influence of temperature and an external bias voltage on the reservoirs is investigated. The knowledge of the particular convergence behavior is of great value to assess the applicability of the scheme to certain physical situations. Moreover, we study different geometries for the auxiliary system. On the one hand, this is of importance for advanced manybody solution techniques such as matrix product states which work well for short-ranged couplings, and on the other hand, it allows us to gain more insights into the underlying mechanisms when mapping non-Markovian reservoirs onto Lindbladtype impurity problems. Finally, we present results for the spectral function of the Anderson impurity model in and out of equilibrium and discuss the accuracy obtained with the different geometries of the auxiliary system. In particular, we show that allowing for complex Lindblad couplings produces a drastic improvement in the description of the Kondo resonance.

# 1. Introduction

Strongly correlated systems out of equilibrium have recently attracted considerable interest due to progress in several experimental fields, such as ultrafast pump-probe spectroscopy [1–5], ultracold quantum gases [6–10], and solid-state nanotechnology [11–13]. These advances have also prompted interest in related theoretical questions concerning thermalization [14–16], dissipation and decoherence [17], and nonequilibrium quantum phase transitions [18–20]. An interesting aspect is the interplay between correlation and dissipation in systems where the latter is not included phenomenologically but is part of the microscopic model. The challenge lies in the fact that one has to treat inhomogenous correlated systems of truly *infinite* size since any finite system would not feature dissipation. When considering purely fermionic correlated systems, dissipation is usually modeled by infinite reservoirs of noninteracting fermions. These reservoirs are in contact with a correlated central region of interest. A paradigmatic example of such a system is the single-site Kondo or Anderson impurity model [21–25]. If there is

just one reservoir with a single chemical potential  $\mu$  and temperature *T*, then the whole system (typically) reaches thermodynamic equilibrium, a problem which is nowadays well understood [25–32]. Alternatively, one can consider a nonequilibrium situation [33–55] in which several reservoirs with different  $\mu$  and *T* are in contact with the central region. Since the reservoirs are infinite, they act as dissipators and the system in most cases reaches a nonequilibrium steady state in which a particle and/or heat current flows across the central region<sup>2</sup>.

There are several approaches to treat such systems numerically [35-51]. Some of them start out from the situation in which the central region and the reservoirs are decoupled, which allows the individual systems to be treated exactly [56-61]. There are different schemes to include the missing coupling between the reservoirs and the central region. First of all, one could carry out a perturbative expansion in terms of the reservoir–central region coupling [56-59]. Low-energy properties are better addressed within a renormalization–group treatment of the perturbation (see, e.g. [62]). Alternatively, one can try and compute the self-energy (most nonequilibrium quantities of interest follow from Dyson's equation) for the correlated sites based on finite clusters consisting of the central region plus a small number  $N_r$  of reservoir sites. This is done in nonequilibrium cluster perturbation theory [56, 61], whose accuracy increases with increasing  $N_r$ . A generalization of this idea is the nonequilibrium variational cluster approach, [57-60], where single-particle parameters of the model are optimized self-consistently, which allows for the adjustment of the self-energy to the nonequilibrium situation.

## 1.1. Markovian approximations and beyond

In a different class of approaches, one tries to 'eliminate' the degrees of freedom of the reservoir and take into account its effects on the dynamics of the interacting central region [63-67]. One way to do this is by treating the coupling to the reservoir within a Lindblad equation [63-65]. In this way, the effect of the reservoir is to introduce nonunitary dynamics in the time dependence of the reduced density operator  $\rho_f$  of the central region leading to the Lindblad equation, which is a linear, time-local equation for  $\rho_f$  preserving its hermiticity, trace, and positivity. One important precondition for the validity of this mapping, however, is the Markovian assumption that the decay of correlations in the reservoir is much faster than typical time scales of the central region. As pointed out, e.g. in [63, 66], the approximations leading to the Markovian Lindblad master equation are justified provided the typical energy scale  $\Omega$  of the reservoir is much larger than the reservoir–central region coupling. However, for a fermionic system,  $\Omega$  can be estimated as min $(W, \max(|\mu - \varepsilon|, T))$ , where W is the reservoir's bandwidth, and  $\varepsilon$  is a typical single-particle energy of the central region. Therefore, even in the wideband limit  $W \to \infty$ , the validity of the Markov approximation is limited either to high temperatures or to chemical potentials far away from the characteristic energies of the central region. As a matter of fact, the effect of a noninteracting reservoir with W,  $|\mu| \to \infty$  (or  $T \to \infty$  with finite  $\mu/T$ ) can be exactly written in terms of a Lindblad equation. This can be easily deduced from the 'singular coupling' derivation of the Lindblad equation [63]. This is valid independently of the strength of the coupling between central region and reservoir. A nontrivial situation is obtained by introducing different reservoirs with different particle densities. The pleasant aspect of this limit is that the Lindblad parameters depend on the properties of the reservoir and of its coupling with the central region only, but not on the ones of the central region.

This is in contrast to the more standard weak-coupling Born–Markov version in which the Lindblad couplings (see, e.g. [63–65]) depend on the central region's properties. To illustrate this, consider a central region consisting of a single site with energy  $\varepsilon_f$ , i.e. with Hamiltonian

$$H_f = \varepsilon_f f^{\dagger} f \tag{1}$$

(omitting spin) and reduced density matrix  $\rho_f$ . The part of the Lindblad operator  $\mathcal{L}_b$  describing the coupling to a noninteracting reservoir is given by

$$\mathcal{L}_b \ \rho_f = \Gamma_1(2f\rho_f f^\dagger - \{f^\dagger f, \ \rho_f\}) + \Gamma_2(2f^\dagger \rho_f f - \{ff^\dagger, \ \rho_f\}) \tag{2}$$

with

$$\Gamma_1 = \Gamma(1 - f_F(\varepsilon_f)) \qquad \Gamma_2 = \Gamma f_F(\varepsilon_f). \tag{3}$$

Here,  $\Gamma$  is proportional to the reservoir's density of states at the energy  $\varepsilon_f$ , and  $f_F$  is the Fermi function which obviously contains the information on the chemical potential and temperature of the reservoir but also on the onsite energy  $\varepsilon_f$  in the central region. This could be unsatisfactory since one would like to describe the effect of the reservoir in a form which is independent of the properties of the central region, especially when the latter consists of many coupled sites.

One possible way to eliminate the dependence of the Lindblad couplings on the parameters of the central region is to use an intermediate auxiliary buffer zone (mesoreservoir) between the Lindblad couplings and the

<sup>&</sup>lt;sup>2</sup> A notable exception is when a bound state is present, i.e. a state with energy outside of the continuum of the reservoir. In this case, there is no unique steady state.



**Figure 1.** Sketch of the five geometries (setups) for the auxiliary system equation (15). An explicit form of the corresponding matrices for  $N_{\rm B} = 4$  is given in appendix B. The impurity is represented by a red circle while the bath sites are filled green ones. The hoppings described by the matrix E are represented by thick black lines. The couplings to the Markovian environments given by  $\Gamma^{(1/2)}$  are expressed by gray lines connected to empty ( $\Gamma^{(1)}$ ) or full ( $\Gamma^{(2)}$ ) reservoirs. On-site terms in the  $\Gamma^{(1/2)}$  matrices are illustrated as a double gray line. The setup 'full' represents the most general case with dense  $\Gamma^{(1)}$  and  $\Gamma^{(2)}$  matrices, which couple each bath site with every other one via the  $\Gamma^{(1/2)}_{i,j}$ . For simplicity, we don't depict all terms for this 'full' case. For the other (sparse) cases all couplings are drawn, and n.n. denotes nearest neighbor terms in  $\Gamma^{(1/2)}$ .

central region (see, e.g. [68–71]). The buffer zone consists of isolated discrete sites (levels), each one coupled to a Markovian environment described by Lindblad operators with the same T and  $\mu$  as given in equations (2) and (3). If the buffer zone is sufficiently large, i.e. if its levels are dense enough, then one can show that the buffer zone including Lindblad operators yields an accurate representation of the reservoir, which becomes exact in the limit of an infinite number of levels. Importantly, the parameters of this buffer zone do not depend on the central region's properties. The disadvantage of this approach is, however, that one needs a quite large number of buffer levels, especially at low temperatures where the Fermi function is sharp. Consequently, the many-body Hilbert space becomes very large, resulting in a challenging problem for the treatment of the correlated situation.

A very effective technique to solve low-dimensional correlated systems are matrix product states (MPS), and great progress has been made in recent years to apply MPS techniques to interacting Lindblad equations [72–85]. With this, rather large systems are within reach even though the numerical effort for Hubbard-type problems is rather high due to an extensive entanglement growth with system size [77, 85].

#### 1.2. This work

In this paper, rather than focusing on solution techniques for the interacting Lindblad equation, we investigate different strategies for the mapping of a general physical ('ph') reservoir onto an auxiliary ('aux') one, consisting of a small number  $N_{\rm B}$  of noninteracting fermionic sites (auxiliary levels) and arbitrary Lindblad terms. This is important since the accuracy of the buffer-zone idea discussed above can be significantly improved by allowing for more general Lindblad couplings, which are determined through an optimization procedure. In this way, the associated interacting impurity solver becomes exponentially accurate with increasing  $N_{\rm B}$ . Moreover, if the appropriate geometry is chosen (figure 1), already a modest value of  $N_{\rm B}$  produces an accurate representation of the physical reservoir. An interesting aspect is that, as in the buffer-zone approach, the combination of intermediate bath levels and couplings to Markovian environments via Lindblad terms allows one to describe a *non-Markovian* bath seen on the impurity site.

We have used these ideas in previous works [85–88] to address nonequilibrium impurity physics in the Kondo regime, with manybody solution techniques based on exact diagonalization (ED) and MPS. Especially in the latter case, we achieved very accurate results for the splitting of the Kondo peak with applied bias. Furthermore, in the equilibrium limit, we found a close agreement with numerical renormalization group (NRG) temperatures well below  $T_{\rm K}$ . The sizes of the auxiliary systems were rather small,  $N_{\rm B} = 16$  for MPS and  $N_{\rm B} = 6$  for ED only,<sup>3</sup> which demonstrates the significant improvement provided by using a Lindblad coupling in the appropriate geometry.

<sup>&</sup>lt;sup>3</sup> Consider that within the many-body Lindblad equation, we have to deal with the space of density matrices not of state vectors, so that the Hilbert space size is that of an  $2(N_B + 1)$  sites Hubbard Hamiltonian.

Here, we want to elaborate in much more detail the advantages of considering long-ranged Lindblad couplings in combination with the optimization strategy. In particular, we investigate five different geometries for the auxiliary Lindblad system, see figure 1. These setups, described in detail in section 2.6, feature different connections between the Markovian bath and the auxiliary levels. The important point is that the accuracy of our approach for fixed  $N_{\rm B}$  crucially depends on the choice of the appropriate geometry. A systematic analysis of the performance of these geometries is, therefore, the main content of this paper. Besides determining the scaling of the accuracy as a function of the number of bath sites  $N_{\rm B}$ , we discuss the importance of the different couplings and relate our results to the commonly used buffer-zone idea. With the applicability of manybody solution techniques in mind, we consider also the case of sparse geometries. This highlights the huge potential for improvement and furthermore yields important insights into the underlying mechanisms. For ED approaches, any of the discussed geometries can be applied and one is generally interested in finding the best possible mapping for a fixed and low value of  $N_{\rm B}$ . In this case the geometry with long-ranged and complex Lindblad terms outperforms the other choices, as shown below.

Finally, we also discuss results for the interacting spectral function of the Anderson impurity model in and out of equilibrium, obtained with the different geometries. In particular, we show here for the first time to our knowledge that allowing for complex Lindblad couplings produces a drastic improvement in the description of the Kondo resonance.

This paper is organized as follows: in section 2.1, we introduce the models under study and define the basic notation. In section 2.2, we illustrate the most important aspect of this work, namely the mapping of the physical Hamiltonian problem onto an auxiliary open quantum system described by a Lindblad equation. In section 2.3, we present the expressions for the non-interacting Green's function of the auxiliary system, and in section 2.4 we illustrate the fit procedure. In section 2.5, we briefly discuss the relation with the interacting case. In section 3, we present in detail the convergence of the fit as a function of  $N_{\rm B}$  for the different geometries presented in section 2.6 and for different temperatures, as well as a discussion on the advantages and disadvantages of these setups. As an example, we present results for the spectral function of the Anderson impurity model. Finally, in section 4 we summarize our results and discuss possible improvements and open issues. In three appendices we present technical details of the minimization procedure (appendix A), show the explicit form of the matrices for the different geometries (appendix B), and discuss certain redundancies of the auxiliary system (appendix C).

# 2. Model and method

## 2.1. Model

We begin with a general discussion, which we eventually apply to the single-site Anderson impurity model. In the general case the central region may represent a small cluster or molecule. The Hamiltonian of the physical system at study is written as

$$H = \sum_{\alpha} (H_{\alpha} + H_{\alpha f}) + H_f \tag{4}$$

where  $H_f$  is the Hamiltonian of the central region describing a small cluster of interacting fermions,  $H_{\alpha}$  is the Hamiltonian of the reservoir  $\alpha$  describing an infinite lattice of noninteracting particles, and  $H_{\alpha f}$  is the coupling between central region and reservoirs.

$$H_f = H_{0f} + H_U \tag{5}$$

consists of a noninteracting part

$$H_{0f} = \sum_{ij} h_{ij} f_i^{\dagger} f_j \tag{6}$$

and an interaction term  $H_U$ . The fermions in the reservoirs can be described by

$$H_{\alpha} = \sum_{p,p'} \varepsilon_{\alpha p,p'} d^{\dagger}_{\alpha p} d_{\alpha p'}$$
<sup>(7)</sup>

in usual notation. For simplicity, spin indices are not explicitly mentioned here. Quite generally, a suitable single particle basis can be chosen such that  $\varepsilon_{\alpha p,p'} \sim \delta_{p,p'}$ . In the context of impurity problems, such a basis is often referred to as 'star representation', see also figure 1.  $H_{\alpha f}$  is taken to be quadratic in the fermion operators:

$$H_{\alpha f} = \sum_{p,i} v_{\alpha p i} d^{\dagger}_{\alpha p} f_i + h.c.,$$
(8)

and  $d_i(f_i)$  are the fermionic destruction operators on the reservoir's (central region's) sites *i*.

We are interested in a steady-state situation, although the present approach can be easily extended to include time dependence, especially if this comes from a change of the central region's parameters only. In the steady state, the Green's functions depend only on the time difference and we can Fourier transform so that the Green's functions depend on a real frequency  $\omega$  only, which here is kept implicit. We assume that initially the hybridization  $H_{\alpha f}$  is zero and the reservoirs are separately in equilibrium with chemical potentials  $\mu_{\alpha}$  and temperatures  $T_{\alpha}$ . Then the  $H_{\alpha f}$  are switched on and after a certain time a steady state is reached. We use the nonequilibrium (Keldysh) formalism [89–94] whereby the Green's function can be represented as a 2 × 2 block matrix

$$\underline{G} = \begin{pmatrix} G^{\mathrm{R}} & G^{\mathrm{K}} \\ 0 & G^{\mathrm{A}} \end{pmatrix},\tag{9}$$

where the retarded  $G^{R}$ , advanced  $G^{A}$ , and Keldysh  $G^{K}$  components are matrices in the site indices (i, j) of the central region. We will adopt this underline notation in order to denote this  $2 \times 2$  structure. We use lowercase  $\underline{g}(\underline{g}_{\alpha})$  to denote Green's function of the decoupled central region (reservoir  $\alpha$ ), while uppercase  $\underline{G}$  represent the full noninteracting Green's function of the central region. For simplicity we omit the subscript  $_{0}$ , since in this paper we deal mainly with noninteracting Green's functions anyway. We use the subscript  $_{\text{int}}$  for interacting ones.  $\underline{G}$  is easily obtained from the Dyson equation as

$$\underline{G} = (\underline{g}^{-1} - \underline{\Delta})^{-1},\tag{10}$$

where

$$\underline{\Delta}_{ij} = \sum_{\alpha, p, p'} v_{\alpha p i} \; v^*_{\alpha p' j} \; \underline{g}_{\alpha p, p'} \tag{11}$$

is the reservoir hybridization function (commonly called bath hybridization function) in the Keldysh representation. The retarded Green's functions  $g_{\alpha}^{R}$  for reservoirs with non-interacting fermions in equilibrium can be determined easily by standard tools, and the Keldysh components  $g_{\alpha}^{K}$  can be obtained from the retarded ones by exploiting the fluctuation-dissipation theorem:

$$g_{\alpha}^{\rm K}(\omega) = (g_{\alpha}^{\rm R}(\omega) - g_{\alpha}^{\rm R}(\omega)^{\dagger}) \, s_{\alpha}(\omega), \tag{12}$$

which is valid since the uncoupled reservoirs are in equilibrium. Here,

$$s_{\alpha}(\omega) = 1 - 2 f_{\rm F}(\omega, \,\mu_{\alpha}, \,T_{\alpha}) \tag{13}$$

and  $f_{\rm F}(\omega, \mu_{\alpha}, T_{\alpha})$  is the Fermi function at chemical potential  $\mu_{\alpha}$  and temperature  $T_{\alpha}$ .

From now on, for simplicity of presentation, we restrict to the Anderson impurity model (SIAM) in which the central region, described by equation (5), consists of a single site, i.e. there is only one value for the index *i*, which we drop, and

$$H_U = U n_{f\uparrow} n_{f\downarrow} \qquad n_{f\sigma} = f_{\sigma}^{\dagger} f_{\sigma}. \tag{14}$$

The idea we are going to present in section 2.2 can be immediately extended to the case of a central region consisting of many sites in which each site is connected to separate reservoirs. In the most direct fashion, this can be done with exactly the same approach as formulated here for the SIAM by just mapping each reservoir independently onto auxiliary Lindblad bath sites. An interesting application is, for example, the case of an interacting chain coupled on both sides to reservoirs with different chemical potentials [95]. Also, the extension to the case of arbitrary (quadratic) couplings with the reservoirs that intermix the central region sites relevant, e.g., for cluster dynamical mean-field theory, is conceptually straightforward although more involved.

### 2.2. Mapping onto an auxiliary master equation

A crucial point in the following considerations is the fact that, even in the interacting case, the influence of the reservoirs upon the central region is completely determined by the bath hybridization function  $\underline{\Delta}(\omega)$  only. In other words, any interacting correlation function of the central region solely depends on the central region Hamiltonian  $H_f$  and on  $\underline{\Delta}$ . This result is well known at least in equilibrium, and can be easily proven; for example, diagrammatically (see footnote<sup>4</sup>). The argument holds independently on whether one works with equilibrium or nonequilibrium Green's functions. Moreover, it crucially depends on the fact that the reservoir is noninteracting.

<sup>4</sup> Since there are no interactions in the reservoir, external indices of any bare interaction vertex belong to the central region only. Moreover, an interacting correlation function of the central region consists, by definition, of diagrams whose external lines belong to the central region. Consequently, all diagrams consist only of vertices (determined by  $H_U$ ) and of propagator lines whose endpoints belong to the central region only, i.e. they correspond to noninteracting Green's functions  $\underline{G}$  of the central region equation (10). Therefore, all relevant diagrams only depend on  $H_U$  and the noninteracting  $\underline{G} = (g^{-1} - \underline{\Delta})^{-1}$ .

This can be exploited to choose different representations for the reservoir. A convenient discretization in *equilibrium* is to represent the reservoir by a finite number of bath sites, as commonly used in the context of NRG [25, 27] or exact-diagonalization-based dynamical-mean-field theory (ED-DMFT) [96–98]. Here, the desired physical hybridization function  $\Delta_{ph}$  is approximated by an *auxiliary* one  $\Delta_{aux}$ ,<sup>5</sup> corresponding to a bath with a finite number of sites. In ED-DMFT, the parameters of these  $N_B$  bath sites are obtained through fitting the hybridization function in Matsubara space. As can be readily shown, only  $2N_B$  bath parameters are of relevance per spin degree of freedom, and it is common to choose a 'star' or 'chain' representation.

Clearly, the same fit strategy is inconvenient *out of equilibrium* for several reasons. First of all, the auxiliary system cannot dissipate since it is finite, and a steady state cannot be reached. In [86, 99] we have suggested an auxiliary master equation approach (AMEA), which adopts an auxiliary reservoir consisting of a certain number  $N_{\rm B}$  of bath sites which are additionally coupled to Markovian environments described by a Lindblad equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathcal{L}\ \rho = (\mathcal{L}_H + \mathcal{L}_D)\rho.$$
(15)

Here, the Hamiltonian for the auxiliary system is given by (we reintroduce spin)

$$H_{\rm aux} = \sum_{ij\sigma} E_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U n_{f\uparrow} n_{f\downarrow}, \qquad (16)$$

and enters the unitary part of the Lindblad operator

$$\mathcal{L}_H \rho = -i[H_{\text{aux}}, \rho]. \tag{17}$$

The dissipator  $\mathcal{L}_D$  describes the coupling of the auxiliary sites to the Markovian environment and is given by

$$\mathcal{L}_{D}\rho = 2\sum_{ij\sigma}\Gamma^{(1)}_{ij} \left( c_{j\sigma}\rho c_{i\sigma}^{\dagger} - \frac{1}{2} \{\rho, c_{i\sigma}^{\dagger}c_{j\sigma}\} \right) + 2\sum_{ij\sigma}\Gamma^{(2)}_{ij} \left( c_{i\sigma}^{\dagger}\rho c_{j\sigma} - \frac{1}{2} \{\rho, c_{j\sigma}c_{i\sigma}^{\dagger}\} \right).$$
(18)

in terms of matrices  $\Gamma^{(1/2)}$  with matrix elements  $\Gamma^{(1/2)}_{ij}$  to be determined by an optimization procedure, as discussed below. The indices *i*, *j* in equations (17) and (18) run over the impurity i = f (we identify  $c_{f\sigma} = f_{\sigma}$ ) and over the  $N_{\rm B}$  bath sites<sup>6</sup>. Similar to the case of the ED-DMFT impurity solver previously mentioned, the idea is to optimize the parameters of the auxiliary reservoir in order to achieve a best fit to the physical bath hybridization function equation (11), i.e., for a given  $N_{\rm B}$ ,  $\Delta_{\rm aux}(\omega)$  should be as close as possible to  $\Delta_{\rm ph}(\omega)$ :

$$\underline{\Delta}_{aux}(\omega) \approx \underline{\Delta}_{ph}(\omega). \tag{19}$$

As for the ED-DMFT case, one can choose a single-particle basis for the auxiliary bath such that the matrix E is sparse, <sup>7</sup>, i.e. it has a 'star' or a 'chain' form and is real valued. However, there is no reason why the matrices  $\Gamma^{(1)}$  and  $\Gamma^{(2)}$  should be sparse and real in the same basis as well, and, in fact, as discussed below, for an ED treatment of the Lindblad problem it is convenient to allow for a general form in order to optimize the fit. This larger number of parameters allows one to fulfill equation (19) to a very good approximation. The introduction of dissipators equation (18) additionally allows us to carry out the fit directly for real  $\omega$  (see section 2.4) since  $\Delta_{aux}(\omega)$  is a continuous function. This makes this approach competitive with ED-DMFT for the equilibrium case as well.

Notice that equation (18) is not the most general form of the dissipator, and one could think of including Lindblad terms that contain four or more fermionic operators or also anomalous and spin-flip terms. This would increase the number of parameters available for the fit. However, the latter would violate conserved quantities and the former would describe an *interacting bath*, so that the argument of section 2.2 (see footnote 3) does not apply. As a matter of fact, the exact equivalence to a *noninteracting bath* (see footnote 6) only holds for a quadratic form of the Lindblad operator as in equation (18).

Once the optimal values of the matrices E,  $\Gamma^{(1)}$  and  $\Gamma^{(2)}$  for a given physical model are determined for the non-interacting system, one could solve for the dynamics of the correlated auxiliary system defined by equation (15), which amounts to a linear equation for the reduced many-body density matrix. If the number of sites of this system is small, one can solve exactly for the steady state and the dynamics of this interacting system by methods such as Lanczos exact diagonalization or matrix product states (MPS) [81–83, 85].

 $<sup>^{5}</sup>$  We shall use suffixes  $_{ph}$  and  $_{aux}$  to distinguish between the physical bath hybridization function equation (11) and the ones produced by the auxiliary reservoir . Whenever necessary to avoid ambiguities, these suffixes will be used also for other quantities.

<sup>&</sup>lt;sup>6</sup> It can be easily shown that the dissipative form (equation (18)) exactly corresponds to the coupling of the auxiliary baths to a small number of noninteracting reservoirs with constant density of states and infinite chemical potentials and/or temperatures. This can be easily deduced from the 'singular coupling' derivation of the Lindblad equation [63], see also [115].

<sup>&</sup>lt;sup>7</sup> We use boldface to denote matrices in the indices *i*, *j* of the auxiliary system. This should not be confused with  $\dots$ , which denotes matrices in Keldysh space.

## 2.3. Computation of the auxiliary bath hybridization function

In order to carry out the fit equation (19), we need to compute the auxiliary reservoir hybridization function  $\underline{\Delta}_{aux}(\omega)$  for many values of the bath and Lindblad parameters. This can be done in an efficient manner since only noninteracting Green's functions are needed, see also equation (10) and the preceding discussion. Computing the single-particle Green's function matrix  $\underline{Z}$ , obtained from the steady-state solution of equation (15), amounts to solving a noninteracting fermion problem, which scales polynomially with respect to the single-particle Hilbert space . A method to deal with quadratic fermions with linear dissipation based on a so-called 'third quantization' has been introduced in [100]. We adopt the approach of [69] in which the authors recast an open quantum problem like equation (15) into a standard operator problem in an augmented fermion Fock space with twice as many sites and with a non-Hermitian Hamiltonian [69, 101, 102]. This so-called super-fermionic representation is convenient for our purposes, not only to solve for the noninteracting Green's functions but also to treat the many-body problem in an analogous framework to Hermitian problems. An analytic expression for the noninteracting steady-state retarded and Keldysh auxiliary Green's functions was derived in [86]. An alternative derivation, which does not rely on super-fermions, is given in [71]. For the retarded component, we get (see footnote 7)

$$\mathbf{Z}^{\mathbf{R}}(\omega) = (\omega - \mathbf{E} + i(\mathbf{\Gamma}^{(2)} + \mathbf{\Gamma}^{(1)}))^{-1},$$
(20)

and the Keldysh component of the inverse Green's function reads

$$(\underline{Z}^{-1})^{K} = -2i(\Gamma^{(2)} - \Gamma^{(1)}),$$
(21)

yielding the Keldysh Green's function

$$\mathbf{Z}^{\mathrm{K}} = -\mathbf{Z}^{\mathrm{R}} (\underline{\mathbf{Z}}^{-1})^{\mathrm{K}} \mathbf{Z}^{\mathrm{A}}$$
$$= 2i \mathbf{Z}^{\mathrm{R}} (\mathbf{\Gamma}^{(2)} - \mathbf{\Gamma}^{(1)}) \mathbf{Z}^{\mathrm{A}}.$$
(22)

The ff component of Z is the auxiliary impurity Green's function

$$\underline{G}_{aux} = (\underline{Z})_{ff}.$$
(23)

From this, one can determine the retarded component of  $\underline{\Delta}_{aux}(\omega)$ 

$$\Delta_{\text{aux}}^{\text{R}}(\omega) = 1/g^{\text{R}} - 1/G_{\text{aux}}^{\text{R}}.$$
(24)

For the Keldysh component, one has to carry out two inversions of Keldysh matrices (see, e.g. [92]), yielding

$$\Delta_{\text{aux}}^{\text{K}}(\omega) = -(\underline{G}_{\text{aux}}^{-1})^{\text{K}} = 1/|G_{\text{aux}}^{\text{R}}|^2 \ G_{\text{aux}}^{\text{K}},\tag{25}$$

where the contribution from  $g^{K}$  is infinitesimal.

#### 2.4. Fit procedure

From the preceding equations, we can efficiently compute  $\Delta_{aux}(\omega)$  for a given set of parameters of the auxiliary reservoir. The numerical effort for a single evaluation is low and scales only at most as  $\mathcal{O}(N_B^3)$ . We introduce a vector of parameters  $\mathbf{x}$  which yields a unique set of matrices  $\mathbf{E}$ ,  $\Gamma^{(1)}$  and  $\Gamma^{(2)}$  within a chosen subset (see, e.g. figure 1 and appendix B) and quantify the deviation from equation (19) through a cost function

$$\chi(\mathbf{x})^{2} = \frac{1}{\chi_{0}^{2}} \int_{-\omega_{c}}^{\omega_{c}} |\underline{\Delta}_{ph} - \underline{\Delta}_{aux}| W(\omega) d\omega,$$
$$|\underline{\Delta}_{ph} - \underline{\Delta}_{aux}| = \sum_{\xi \in \{\mathbf{R}, \mathbf{K}\}} \Im m \{ \Delta_{ph}^{\xi}(\omega) - \Delta_{aux}^{\xi}(\omega; \mathbf{x}) \}^{2},$$
(26)

and minimize  $\chi(\mathbf{x})$  with respect to  $\mathbf{x}$ . The normalization  $\chi_0$  is hereby chosen such that  $\chi(\mathbf{x}) = 1$  when  $\underline{\Delta}_{aux}(\omega) \equiv 0$ . It is important to note that both the retarded and the Keldysh component must be fitted. Due to Kramers–Kronig relations, the real part of  $\Delta_{ph}^{R}(\omega)$  is fully determined by its imaginary part, provided the asymptotic behavior is fixed. Therefore, we can restrict to fit its imaginary part, while  $\Delta_{ph}^{K}(\omega)$  is purely imaginary. Furthermore, in equation (26) we introduced a cut-off frequency  $\omega_c$  and a weighting function  $W(\omega)$ . In this work, we take  $W(\omega) = 1$  and  $\omega_c = 1.5 D$ , with D the half-bandwidth of  $\underline{\Delta}_{ph}(\omega)$ . Different forms of  $W(\omega)$  can be used, for instance in order to increase the accuracy of the fit near the chemical potentials. In general, other definitions for equation (26) are possible such as a piecewise definition with varying interval lengths. By this, one may combine the present approach with NRG ideas such as the logarithmic discretization, and work along these lines is in progress (see also [71]). On the whole, the minimization of equation (26) constitutes a multi-dimensional optimization problem and appropriate numerical methods for it are discussed in appendix A.

As asymptotic limit, we require here  $\underline{\Delta}_{aux}(\omega) \to 0$  for  $\omega \to \pm \infty$ , which is obtained when setting  $\Gamma_{ff}^{(1/2)} = 0$ . Semipositivity further requires  $\Gamma_{if}^{(1/2)} = \Gamma_{fi}^{(1/2)} = 0$ . For simplicity, we restrict here to the particle-hole symmetric case. This reduces the number of free parameters in  $\boldsymbol{E}, \boldsymbol{\Gamma}^{(1)}$  and  $\boldsymbol{\Gamma}^{(2)}$ . For the case in which the

impurity site f is located in the center and that one has an even number of bath sites N<sub>B</sub>, particle-hole symmetry in the auxiliary system is obtained when

$$E_{ij} = (-1)^{i+j+1} E_{N_{\rm B}+2-j,N_{\rm B}+2-i},$$
  

$$\Gamma_{ij}^{(1)} = (-1)^{i+j} \Gamma_{N_{\rm B}+2-j,N_{\rm B}+2-i}^{(2)},$$
(27)

for  $i, j \in \{1, ..., N_B + 1\}$ . More details for the particular form of  $E, \Gamma^{(1)}$ , and  $\Gamma^{(2)}$  are given in appendix B.

#### 2.5. Interacting case

We now briefly discuss here some relevant issues in connection with the evaluation of particular observables of the physical system from results of the auxiliary system. More details can be found in [85, 86].

As already discussed, by mapping onto an auxiliary interacting open quantum system of finite size described by the Lindblad equation (equation (15)), we obtain a manybody problem which can be solved exactly or at least with high numerical precision, provided  $N_{\rm B}$  is not too large. In [86], we presented a solution strategy based on exact diagonalization (ED) with Krylov space methods, and in [85] one based on MPS. In the end, both techniques allow us to determine the interacting impurity Green's function  $\underline{G}_{aux,int}(\omega)$  of the auxiliary system. As discussed previously, in the limit  $\underline{\Delta}_{aux}(\omega) \rightarrow \underline{\Delta}_{ph}(\omega)$  (i.e. for large  $N_B$ ) this becomes equivalent to the physical one  $\underline{G}_{ph,int}(\omega)$ . However, this equivalence only holds for impurity correlation functions, and, for example, it does not apply for the current flowing from a left ( $\alpha = l$ ) to a right ( $\alpha = r$ ) reservoir across the impurity. Therefore, the current evaluated within the auxiliary Lindblad system does not necessarily correspond to the physical current even for large  $N_{\rm B}$ , <sup>8</sup> unless one fits the bath hybridization functions  $\Delta_{\rm ph,\alpha}(\omega)$  for the left and right reservoirs separately. Such a separate fit, however, is not necessary and would simply worsen the overall accuracy for a given  $N_{\rm B}$ . Once the approximate  $\underline{G}_{\rm ph,int}(\omega) \approx \underline{G}_{\rm aux,int}(\omega)$  is known, the current of the *physical* system can be evaluated by means of the well-known Meir–Wingreen expression [92, 103, 104], albeit by using the Fermi functions and density of states (hybridization functions) of the two physical reservoirs separately.

Therefore, the knowledge of  $\underline{G}_{aux,int}(\omega)$  enables one to compute most quantities of interest.

An additional step consists in extracting just the self-energy from the solution of the auxiliary impurity system

$$\underline{\Sigma}_{aux}(\omega) = \underline{G}_{aux}^{-1}(\omega) - \underline{G}_{aux,int}^{-1}(\omega).$$

and inserting it into the Dyson equation for the physical system with the exact physical noninteracting Green's function

$$\underline{G}_{\text{ph,int}}(\omega) \approx (\underline{G}_{\text{ph}}(\omega)^{-1} - \underline{\Sigma}_{\text{aux}}(\omega))^{-1}.$$
(28)

Clearly, this step is only useful when the relation equation (19) is approximate, since for  $\underline{\Delta}_{aux}(\omega) \rightarrow \underline{\Delta}_{ph}(\omega)$ also the noninteracting Green's functions  $\underline{G}_{ph}(\omega)$  and  $\underline{G}_{aux}(\omega)$  would coincide, i.e. in the hypothetical  $N_{\rm B} \rightarrow \infty$  case, and one could just set  $\underline{G}_{\rm ph,int}(\omega) \rightarrow \underline{G}_{\rm aux,int}(\omega)$ . For finite  $N_{\rm B}$ , this substitution has the advantage that in equation (28) the noninteracting part  $\underline{G}_{ph}(\omega)$  is exact, and the approximation equation (19) only affects the self energy.

## 2.6. Different geometries for the auxiliary system

With the goal in mind of providing the best approximation to the full interacting impurity problem described by the Hamiltonian equation (4), we would like to approximate  $\underline{\Delta}_{ph}(\omega)$  by  $\underline{\Delta}_{aux}(\omega)$  as accurately as possible for a given number of bath sites  $N_{\rm B}$ . In principle, one has the freedom to choose different geometries for the auxiliary system, and a generic set of five different setups is depicted in figure 1. (An explicit form of the corresponding matrices for  $N_{\rm B} = 4$  is given in appendix B.) For large  $N_{\rm B}$  all geometries converge to the exact solution  $\underline{\Delta}_{aux}(\omega) \rightarrow \underline{\Delta}_{ph}(\omega)$ , and the question is how fast. In section 3, we want to elaborate on this point in detail and present results obtained with those geometries, which we briefly discuss and motivate here.

In all cases one can restrict the geometries to a sparse (e.g. tridiagonal) and real-valued matrix E. As is commonly true for impurity problems, the physics on the impurity site is invariant under unitary transformations among bath sites only. For an arbitrary unitary transformation U with  $U_{if} = U_{fi} = \delta_{if}$  to new fermionic operators, one obtains an analogous auxiliary system with modified bath parameters  $E' = U^{\dagger}EU$ ,  $\Gamma^{(1)'} = U^{\dagger}\Gamma^{(1)}U$  and  $\Gamma^{(2)'} = U^{\dagger}\Gamma^{(2)}U$ . It is easy to check that the *ff*-component of the Green's functions equations (20) and (22) is not affected by this transformation. Therefore, we choose without loss of generality Eto be sparse as well as real, and for  $\Gamma^{(1/2)}$  in the most general case dense matrices with  $\mathcal{O}(N_{\rm B}^2)$  parameters. The

 $<sup>^8</sup>$  This situation is particularly interesting in equilibrium: with large enough  $N_{
m B}$  and an appropriate choice of the parameters of the nonequilibrium Lindblad system, one can still produce an auxiliary  $\Delta_{aux}(\omega)$  so that the fluctuation dissipation theorem equation (12) is fulfilled to high precision at the impurity, representing an equilibrium physical  $\Delta_{ph}(\omega)$ . While a finite current may flow in the auxiliary system, the equilibrium properties at the impurity are correctly reproduced.

particular form of E is irrelevant, i.e. whether it is diagonal for bath sites (star) or tridiagonal (chain), as long as the  $\Gamma^{(1/2)}$  matrices are transformed accordingly.

Such a general geometry with sparse E and dense  $\Gamma^{(1/2)}$  is referred to as 'full' setup in the following. Here, we will further distinguish between the case in which the  $\Gamma^{(1/2)}$  are real or they have complex elements ('full complex'). In addition, we consider the four sparse cases '2 chains n.n.', '2 chains onsite', 'star', and '1 chain n. n.', in which also the  $\Gamma^{(1/2)}$  are sparse. The meaning of these abbreviations is given in figure 1, see also appendix B. These sparse geometries are, however, not linked to each other by unitary transformations and represent nonequivalent subsets of the 'full' setup. Which one of these is advantageous in practice is not obvious *a priori*, and is discussed in the next section<sup>9</sup>.

The 'full' geometry comprises all other ones and thus, obviously, gives the best possible fit for a given  $N_{\rm B}$ . In addition, one can allow for the off-diagonal matrix elements of the  $\Gamma^{(1/2)}$  to be complex, thus extending the set of fit parameters. Nevertheless, the sparse setups may be of great value for sophisticated manybody solution strategies for the interacting Lindblad equation, such as MPS. We made use of the 'full' setup (with real parameters) in the ED treatment [86], which is applicable to dense  $\Gamma^{(1)}$  and  $\Gamma^{(2)}$  matrices and could consider up to  $N_{\rm B} = 6$ . Larger systems are prohibitive due to the exponentially increasing Hilbert space (see footnote [2]). On the other hand, within MPS, we can currently consider up to  $N_{\rm B} = 20$  bath sites. However, in favor of the applicability of MPS methods, one should avoid long-ranged hoppings and we thus employed the '2 chains n.n.' geometry. As becomes evident also from the results below, the gain in  $N_{\rm B}$  hereby outweighs the restriction of the fit setup, so that the MPS approach is clearly more accurate. Also, the other sparse setups investigated below are possible candidates for MPS, see also [105]. Besides this, approaches such as the previously mentioned buffer zone scheme and variations of it [68–70], which are often applied concepts in Lindblad-type representation of noninteracting environments, are related to the 'star' geometry; see also our later discussion.

## 3. Results

As just discussed, while the 'full' geometry is the most efficient one, for the purpose of employing efficient manybody eigenvalue solvers such as MPS, it is of great relevance to consider setups which feature only sparse E,  $\Gamma^{(1)}$ , and  $\Gamma^{(2)}$  matrices. Furthermore, it is also of general interest to investigate the importance of long-range terms in the  $\Gamma^{(1/2)}$  matrices and why they are crucial to improving the fit. These are the questions that are addressed in this section. Moreover, we will analyze the rate of convergence as a function of  $N_{\rm B}$  for the different setups shown in figure 1, and for different temperatures of the physical system. The detailed knowledge of the convergence properties is important in order to be able to estimate whether or not certain systems can be accurately treated.

We consider a 'physical' SIAM consisting of an impurity site coupled to two reservoirs (leads) at different chemical potentials, corresponding to a bias voltage  $\phi$  across the impurity, and with a flat density of states as plotted in figures (2–4). Typical results for a given  $\phi$  and temperature T are shown in figures (2–4). For the different setups, the quality of the fit is measured by the minimum of the cost function equation (26). As discussed previously, the 'full' setups give the best results. Already for a rather small number of bath sites  $N_{\rm B}\gtrsim$  4, a good agreement between  $\Delta_{\rm aux}$  and  $\Delta_{\rm ph}$  is achieved, and the convergence is exponential as a function of  $N_{\rm B}$ . Allowing for complex matrix elements produces a drastic improvement. The accuracy obtained with  $N_{\rm B} = 8$  for the real case is essentially achieved already with  $N_{\rm B} = 6$  in the complex case (see also figure 5). In particular, figure 8 shows that this improvement produces a much better description of the Kondo resonance. This is crucial, since  $N_{\rm B} = 6$  is the maximum size that we can currently address by Krylov-space methods. Here, an excellent agreement is evident with minor differences in the Keldysh component. In the retarded component, the largest differences occur at the positions of the jumps in the Keldysh component, i.e. at the chemical potentials. This is a consequence of the simultaneous fit of the retarded and Keldysh components in equation (26), which produces oscillations in the retarded one. These oscillations are strongly reduced in the complex case. By increasing the number of bath sites, the amplitude and the extension of these oscillations in the retarded component decay rapidly.

We now consider the sparse geometries. In contrast to the 'full' setups, no improvement is obtained by allowing the matrix elements to be complex in this case. Among the sparse geometries, the ones with two chains are the most accurate. Both setups perform quite well. Again, a good agreement for small  $N_{\rm B}$  is obtained and a quick improvement shows up with increasing  $N_{\rm B}$ . '2 chains n.n.' has off-diagonal  $\Gamma^{(1/2)}$  terms in contrast to '2 chains onsite', which leads to a faster convergence as seen, e.g., for  $N_{\rm B} = 12$ . The 'star' and most notably the '1 chain n.n.' geometry are clearly worse. Both exhibit a rather poor convergence as a function of  $N_{\rm B}$ . For the 'star' setup, this is due to the fact that the fitted auxiliary hybridization function consists of a sum of Lorentzian peaks.

<sup>&</sup>lt;sup>9</sup> The number  $C(N_{\rm B})$  of fit parameters for each geometry for the particle-hole symmetric case, which we consider here, is presented in appendix B.



**Figure 2.** Fit to the bath hybridization functions for the 'full' setups (real and complex) (see figure 1). The physical  $\Delta_{ph}(\omega)$  (black lines) describes a reservoir with a flat density of states with hybridization strength  $\Gamma$  and a half bandwidth of  $D = 10 \Gamma$  which is smeared at the edges. An applied bias voltage  $\phi = 3 \Gamma$  shifts the chemical potentials of the two reservoirs (leads) anti-symmetrically and a temperature of  $T = 0.1 \Gamma$  is considered here.



These enter in the Keldysh component with either positive or negative weights and can thus cancel each other. However, the rather broad Lorentzians with  $\log 1/\omega^2$  tails make it apparently difficult to resolve the Fermi edges properly. The problem with slow convergence is most severe for the '1 chain n.n.' geometry. Here, the single chain is clearly inadequate to represent at the same time the desired density of states and the sudden changes in the occupation number, see also the subsequent discussion. While the Keldysh component is roughly reproduced, this comes at the price of large oscillations in the retarded component. In addition, the improvements with increasing  $N_{\rm B}$  are minor and the results for  $N_{\rm B} = 4$  and  $N_{\rm B} = 12$  are very close to each other.

The behavior just discussed is even more visible in the convergence study presented in figures 5 and 6. In figure 5, the minimal values of the cost function  $\chi$ , equation (26), for various values of  $N_{\rm B}$  and the different setups are shown. Four different temperatures, each of them with  $\phi = 0$  and  $\phi = 3 \Gamma$ , are considered. As expected, the 'full complex' setup gives the lowest values of  $\chi$  in all cases, and, moreover, the fastest rate of convergence as a function of  $N_{\rm B}$ . The 'full' setup without complex terms also performs quite well. The sparse geometries '2 chains n.n.' and '2 chains onsite' perform not as well, although still achieving a rather high rate of







convergence. In most cases studied here, the off-diagonal  $\Gamma^{(1/2)}$  terms in '2 chains n.n.' result in a significant improvement compared to '2 chains onsite', which is the reason why we favored the former in our MPS manybody calculations performed in [85]. In that work, we found that an accuracy of at least  $\chi \approx 10^{-2}$  was necessary in order to properly account for Kondo physics. This could be reached already for  $N_B \approx 12$ .

We now discuss the 'star' setup. One should note that in standard buffer zone approaches [68–70], an equidistant energy spacing  $\Delta \epsilon_i \approx 2D/N_{\rm B}$  with equal onsite  $\Gamma^{(1/2)}$  terms is often assumed for the bath sites. Clearly, such a discretization approach cannot converge exponentially and it is only first-order accurate in the spacing  $\Delta \epsilon_i$ . On the other hand, in our scheme, we optimize all parameters within a fitting procedure, so the value of the cost function presented here for the 'star' setup can be seen as a lower bound for an improved buffer zone approach. Despite the exponential convergence of the 'star' geometry, it becomes apparent from figure 5 that a very slow rate of convergence is achieved. To reach an accuracy  $\chi \approx 10^{-2}$  for the case  $T = 0.05\Gamma$  and



**Figure 6.** Same as figure 5 but plotted versus the number of fit parameters  $C(N_B)$ . In order to resolve the scaling with temperature more reliably, we exclude the two data points with the smallest  $N_B$  from each of the linear fits, which have not enough structures to resolve low-energy scales. Dotted lines represent results of linear fits in these semi-logarithmic plots. The temperature dependence of the convergence rates (as a function of  $N_B$ ) obtained in this way are illustrated in figure 7.

 $\phi = 0$  for instance, much larger auxiliary systems with  $N_{\rm B} \approx 40$  would be needed. For the MPS-solver used in [85], such large auxiliary systems are out of reach.

Let us now turn to the results for the 'l chain n.n.' setup in figure 5. Despite the poor performance and the strongly limited practical use, the observed behavior is interesting from a fundamental point of view. As becomes evident from the results, a single chain with local dissipators is a particularly bad choice to represent a partially filled bath. The convergence is very slow and an extremely long chain would be needed in order to achieve results comparable to the other geometries. As just shown, a drastic improvement is obtained when using two chains instead. This would be more or less intuitive for the nonequilibrium case in which the physical system also consists of two baths. However, the advantage of the '2 chains' geometry over the '1 chain' case is even more pronounced in the equilibrium case (see  $\Phi = 0$ ). Another important observation to better understand this is the following: in [85], we found nearly identical accuracies when considering the '2 chains' geometry as used here, or a filled/empty restriction of it. In the latter case, one chain has the purpose of representing the filled spectrum and the other chain the empty spectrum of the physical hybridization function<sup>10</sup>, and not necessarily the two physical reservoirs. This shows that a single chain of small size is very well suited to reproduce a certain density of states but not simultaneously a Fermi edge or other sharp changes in the occupation number. Furthermore, a '2 chains' filled/empty setup seems to be a rather natural representation where the resolution of sharp features in  $\Delta_{
m ph}(\omega)$ , which either correspond to band edges or sudden occupation changes at the Fermi edges, are resolved by appropriate Hermitian couplings E and corresponding broadenings/couplings stemming from  $\Gamma^{(1/2)}$ . In this way, the filled and empty chain together can well reproduce sharp features in  $\Delta_{ph}^{R}(\omega)$  and  $\Delta_{ph}^{K}(\omega)^{11}$ .

Additionally to the convergence as a function of  $N_{\rm B}$ , we depict in figure 6 the cost function versus the number of available fit parameters  $C(N_{\rm B})$ . As can be seen, the trends in the semi-logarithmic plot are well described by straight lines in all cases, which clearly shows the achieved exponential convergence with respect to  $C(N_{\rm B})$ . For the sparse setups this means that  $\chi \propto \exp[-\mathcal{O}(N_{\rm B})]$  whereas, for the 'full' setups, even  $\chi \propto \exp[-\mathcal{O}(N_{\rm B}^2)]$ . Due to this, the 'full' geometries converge much quicker, as observed in the results just given. With respect to the number of fit parameters, however, the '2 chains' setups perform best. This just means that these setups contain the most relevant subset of all possible fit parameters.

Another important aspect is the dependence of the convergence rate r(T) on temperature. The estimated rates r(T) for each setup are depicted in figure 7. Of course, the superior scaling of the 'full' and the '2 chains' setups is also apparent in the magnitude of r(T). Furthermore, in all cases, one observes the trend that the higher

<sup>&</sup>lt;sup>10</sup> The filled (empty) spectrum corresponds to the lesser (greater) hybridization function  $\Delta$ , and furthermore:  $\Delta = \Delta^{K}/2 \mp i \Im m \{\Delta^{R}\}$ . <sup>11</sup> From this point of view, the additional improvement in the 'full' setups can be interpreted in such a way that one achieves an optimal linear combination of filled/empty states with the long-ranged couplings in  $\Gamma^{(1/2)}$ .





the temperature the faster the convergence. This can be understood from the fact that, at high *T*, the Keldysh component  $\Delta_{ph}^{K}(\omega)$  is weakly  $\omega$ -dependent so that less bath sites are necessary for a reliable fit. Eventually, in the  $T \to \infty$  and wide-band limit, the Markov approximation even becomes exact. In the other extreme  $T \to 0$  limit, discontinuous functions are present in  $\Delta_{ph}^{K}(\omega)$ , produced by the abrupt Fermi edges. However, each of the frequency-dependent functions in the effective set given by equations (20)–(25) is continuous. Therefore,  $T \to 0$  can only be reproduced in the limit  $N_{\rm B} \to \infty$ . This explains the observed trend that, for a given  $N_{\rm B}$ , the high-temperature regime is generally better represented than the low-temperature one. Furthermore, a nonzero  $\phi$  tends to result in larger values for the cost function, see also figure 5<sup>12</sup>.

In conclusion, the present analysis clearly demonstrates the huge advantage of optimizing the bath parameters of the auxiliary system, and furthermore, of choosing an appropriate geometry when considering only a restricted subset of the 'full' setup.

#### 3.1. Spectral function of the interacting SIAM

We now present and discuss results for the interacting spectral function of the SIAM,

$$A(\omega) = -\frac{1}{\pi} \Im m \ G_{\text{ph,int}}^{R}(\omega)$$
<sup>(29)</sup>

(see equation (28)) in and out of equilibrium and in particular investigate the accuracy obtained by each of the geometries of figure 1 for a fixed  $N_{\rm B}$ . We also discuss the relation with the fidelity in reproducing the physical hybridization function, i.e. the fit just discussed. In figures 8 and 9, we confront the results of the fit on the left with the interacting spectral function on the right. Results for  $N_{\rm B} = 6$  are presented for two values of the bias voltage,  $\phi = 0$  (equilibrium case) and  $\phi = 3\Gamma$ . In particular, we focus on the region around the Kondo peak, which gets split at finite  $\phi$ , since this is the more sensitive to approximations.

Starting with the equilibrium case, we see that all but the two worse geometries are able to resolve the Hubbard side bands. Further improvements of the fit show that, the better an auxiliary system reproduces the Fermi jump in the Keldysh and the plateau in the retarded hybridization function, the sharper is the corresponding Kondo resonance. Only the '2 chains n.n.' setup seems to break this trend as, for  $\phi = 0$ , its peak is clearly sharper than for the 'full' geometry although the fit is less accurate. However, this peculiarity can be readily explained by looking at the corresponding fit and in particular at the oscillations in the retarded component at low energies. Here, the 'full' geometry shows a substantial dip which in turn leads to a suppression

<sup>&</sup>lt;sup>12</sup> Note that the difficulty of the fit, i.e. the magnitude of  $\chi$ , is determined by the degree of variations in  $\Delta_{\text{ph}}$  and the length scale of these variations wrt the half bandwidth *D*. The coupling strength  $\Gamma$  of the leads enters only trivially. Therefore,  $\phi/D$  and T/D determine  $\chi$ .



**Figure 8.** Fits (left) and spectral function (right) in the equilibrium case ( $\phi = 0\Gamma$ ) for the lowest considered temperature  $T = 0.05\Gamma$  and with  $N_B = 6$ . The value of the Hubbard interaction is  $U = 6\Gamma$  and, as a reference solution (black curve), we take results for  $N_B = 16$  in the '2-chains n.n.' geometry which deviate by at most 1% (at the tip  $\omega = 0$ ) from the numerically exact NRG 85. Geometries in the key are sorted from worst (top) to best fit (bottom).



of the Kondo peak. A way to improve this is to introduce a weight  $W(\omega)$  (cf equation (26)) to the fit that emphasizes regions around the chemical potentials. One can also notice the drastic improvement in the description of the Kondo resonance obtained by allowing for complex values of the parameters  $\Gamma_{ij}^{(1/2)}$ . The same accuracy is expected to be obtained for the real 'full' case for  $N_{\rm B} = 8$ , but this is currently beyond the reach of a Krylov-space solution method.

Turning to the nonequilibrium case, we first note that the 'star' and '1 chain' setup are not able to follow the double Fermi step in the Keldysh hybridization function but rather produce a single jump at an elevated

temperature. Thus, assuming for the moment a flat retarded component, one would expect only a single temperature-broadened Kondo resonance. The fact that the spectral function instead shows a two-peak structure is not a genuine effect but rather is connected to corresponding oscillations in the retarded component of the hybridization function. Notice that the two-peak structures occur here at the wrong frequency. In fact, all but the 'full complex' and 'full' setups fail to correctly reproduce the positions of the peaks, despite resolving the double Fermi step, as oscillations in the retarded component interfere with the physical effect. In general, this example shows that one has to be careful with interpretations of structures in the interacting spectral function when the fit does not resolve important features and/or displays unphysical oscillations. On the other hand, if deviations from the physical hybridization function are small, one can be confident that the results are correct. Results suggest this to be the case already with 6 bath sites for the 'full' setups and about 12 bath sites for the '2 chains' geometries.

## 4. Summary and conclusions

In this work, we presented and developed a general scheme for mapping nonequilibrium correlated quantum impurity problems with infinite non-Markovian fermionic reservoirs onto auxiliary finite open quantum systems. The approach as outlined here can be used to study transport through interacting impurities, Hubbard chains, or small clusters and molecules. For simplicity and clarity we presented results for the single impurity Anderson model (SIAM). The key aspect is to replace the infinite fermionic reservoirs of the original 'physical' problem by an 'auxiliary' one consisting of a combination of a small number  $N_{\rm B}$  of bath levels plus Markovian terms. The auxiliary problem is described by an open quantum system whose dynamics are controlled by a Lindblad equation. Being finite, its manybody problem can be solved with high accuracy by numerical techniques. Despite the fact that the bath levels are directly coupled to a Markovian environment, the dynamics at the impurity site in the auxiliary system correctly describe the *non-Markovian* properties of the physical reservoir.

It is important to note that the overall accuracy can be evaluated by the difference between the bath hybridization functions of the physical and auxiliary system, i.e. the cost function equation (26). While this idea is not new, the key point of our work is the formulation of an optimization procedure in order to determine the parameters of the auxiliary bath levels. This allows us to achieve an exponential convergence of the accuracy of the mapping with increasing *N*<sub>B</sub>. This exponential improvement is probably the reason why a few number of bath sites, such that exact diagonalization can be employed, is sufficient to (at least partially) resolve the exponentially small Kondo scale.

The main scope of this paper was to analyze the mapping procedure itself in detail. One has a certain freedom in the geometry of the auxiliary system. Here, we investigated an exemplary set of possible choices. The most general 'full' geometries achieve the best mapping for a fixed  $N_{\rm B}$  value. In [86] we employed such a real-valued 'full' setup with  $N_{\rm B} = 6$  to analyze the splitting of the Kondo resonance in nonequilibrium. In the present work, we additionally investigated the performance of a complex-valued ('full-complex') geometry and found a drastic improvement for the same  $N_{\rm B}$ . For example, the Kondo resonance turns out to be twice as high and sharp than for the real 'full' case and very close to the one obtained by NRG for  $U/\Gamma = 6$ , see figure 8.

Depending on the requirements and on the algorithm applied to address the manybody problem, one could prefer one setup or the other. For example, if one uses MPS-like approaches, a chain-like or, more generally, a sparse setup is preferable. In this way, one can address interacting auxiliary systems with larger  $N_{\rm B}$  and improve the accuracy. If long-range hoppings are not a problem, like for Lanczos exact diagonalization, one should use the most general 'full complex' geometry. Krylov-space methods are considerably less time-consuming than MPS. Therefore, they could be more convenient when applying the present AMEA approach in the context of nonequilibrium DMFT where repeated solutions of the impurity problem are required for the DMFT selfconsistency. Finally, when combining the approach with NRG, it may be convenient to adopt 'star-like' geometries (see, e.g. [71]).

Concerning sparse setups, we compared the performance of the common 'star' geometry with a '1 chain' and two '2 chains' setups. The results demonstrated clearly that the performance of these individual sparse setups may differ by orders of magnitude. In particular, the widely used 'star' geometry exhibits a very slow rate of convergence with increasing  $N_{\rm B}$ , and a geometry with '1 chain' and local Lindblad drivings performed much worse than the other cases. In contrast, setups with '2 chains' and local Lindblad drivings produced very good results, with an accuracy orders of magnitude better than the other two sparse cases. Together with the results obtained in [85], we can conclude that a so-called filled/empty geometry with '2 chains' is essentially a natural representation of a non-Markovian reservoir by auxiliary Lindblad levels. In this geometry, one chain has the purpose of reproducing the filled spectrum of the original reservoir whereas the other chain reproduces the empty spectrum. This is achieved in each chain separately by an optimal combination of hoppings between the

bath levels and couplings to *one* Markovian environment, which is then either completely filled or empty. By this separation it is possible to resolve sharp features in the original hybridization function in great detail, which may correspond to sharp occupation changes at the Fermi jumps or band edges. A single chain coupled to filled and empty Markovian environments, on the contrary, cannot simultaneously represent a particular density of states and a partially filled spectrum appropriately, as is evident from the '1 chain' setup.

Besides comparing different auxiliary setups, we also analyzed the general convergence properties in detail. As just mentioned, we found an exponential convergence as a function of  $N_{\rm B}$  in all cases, which can be accounted to the optimization strategy for the bath parameters. Furthermore, we analyzed systematically the convergence properties as a function of temperature both in equilibrium as well as in nonequilibrium. This showed the common trend that the high-temperature regime is better represented by the auxiliary system than the low-temperature one, i.e. the rate of convergence of the mapping increases with temperature. Therefore, to achieve a given accuracy it is more challenging to resolve low temperatures, which thus requires larger auxiliary systems. The plain exponential convergence shown here yields a simple tool to extrapolate results for low  $N_{\rm B}$  to higher values, and by this to judge the feasibility of treating certain physical situations.

As a concrete application, we presented results for the spectral function of the interacting SIAM in and out of equilibrium as produced within the different auxiliary setups, and analyzed its relation to a given fit. We found that one has to be careful with interpretations when the fit does not resolve important features and shows sizable oscillations. On the other hand, if deviations from the physical hybridization function are small, one can be confident that the results are correct, which is usually the case already with 6 bath sites for the 'full' setups and about 12 bath sites for the '2 chains' sparse geometries. We also showed that drastic improvements are obtained by allowing for complex-valued parameters.

Besides the technical aspects, the current study contains relevant information to the general question of the representability of *non-Markovian* fermionic reservoirs by open quantum systems, and in particular by Lindblad-type equations. We expect that the insights gained in this work may contribute also to other closely related fields on Markovian and non-Markovian quantum master equations.

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# Appendix A. Multi-dimensional minimization

In this section, we provide detailed information for readers interested in an actual implementation. Furthermore, a working code is available on request; to obtain it, simply contact us via e-mail. Much of the information below is contained in standard textbooks and reviews. However, for completeness we outline here the standard algorithm in detail and point out choices we made which turned out to be convenient for the specific problem.

As stated previously, a single evaluation of equations (20)-(25) is numerically cheap since it involves only one matrix inversion and matrix-vector multiplications of size  $(N_{\rm B} + 1)$ . Thus, the increase in computation time with  $N_{\rm B}$  is rather moderate. However, the multi-dimensional optimization problem itself is demanding and it strongly depends on the particular behavior of  $\chi(\mathbf{x})$  when varying the set of parameters  $\mathbf{x}$ . In the worst case scenario, when  $\chi(\mathbf{x})$  is a rough potential landscape with many local minima and short-scaled variations, one could imagine that it becomes necessary to nearly explore the whole parameter space. However, x is a continuous vector and even when assuming a fixed number of discrete values for each component in x, one faces a number of points in parameter space that grows exponentially with  $\dim(x)$ . In the other extreme, for the case in which  $\chi(\mathbf{x})$  is quadratic in  $\mathbf{x}$ , it is well-known that a conjugate gradient scheme leads to the exact minimum in dim(x) iterations. What we found in practice, when performing the minimization within AMEA [85, 86], is that we have an intermediate situation which exhibits local minima but gradient-based methods still work fine, especially for smaller values of N<sub>B</sub>. In the first work on the ED-solver [86], we employed a quasi-Newton line search with many random starting points. This is particularly useful for  $N_{\rm B} < 6$ . However, the necessary number of starting points increases rapidly with  $N_{\rm B}$ . Therefore, in the course of the work on the MPS-solver, [85], we looked for more efficient solution strategies. In the end, we implemented a parallel tempering (PT) approach with feedback optimization, which is a Monte Carlo scheme that is able to overcome local minima. We describe it in more detail in the following section. In this way, the minimization problem for the ED-solver with  $N_{\rm B} = 6$  and for the MPS-solver with up to  $N_{\rm B} = 16$  can be solved in reasonable time. This amounts to minimizing

in a space of  $\approx$  30 - 60 parameters in both geometries, depending on whether or not one has particle-hole symmetry.<sup>13</sup>

## A.1. Markov chain Monte Carlo

The PT algorithm is outlined in detail in the following. For completeness, let us first briefly recap the basic ideas of the underlying Markov chain Monte Carlo (MCMC), and of the related simulated annealing algorithm.

MCMC techniques were originally developed to evaluate thermodynamic properties of classical systems which exhibit a very large phase space where simple sampling strategies fail. For our purposes here, we are interested in minimizing the cost function  $\chi(\mathbf{x})$  as defined in equation (26) with respect to the parameter vector x. For such high-dimensional minimization problems, one can adapt MCMC schemes by viewing  $\chi(x)$  as an artificial energy and by introducing an artificial inverse temperature  $\beta$ . In the so-called simulated annealing, one samples from the Boltzmann distribution  $p(\mathbf{x}) = 1/Z \exp(-\chi(\mathbf{x})\beta)$  at a certain  $\beta$ , and then successively cools down the artificial temperature. Motivated by the behavior of true physical systems, one expects to end up in the low-energy state when letting the system equilibrate and when cooling sufficiently slowly. Analogous to thermodynamics, one can calculate the specific heat  $C_{\rm H} = \beta^2 \langle \Delta \chi(\mathbf{x})^2 \rangle$  and by this locate regions with large changes, i.e. phase transitions, where a slow cooling is critical. However, in practice it may be time consuming to realize the equilibration and sufficiently slow cooling, and for tests within AMEA we often ended up in local minima. In order to obtain a robust algorithm which can also start from previous solutions as needed, for instance, within DMFT, we sought a method which is able to efficiently overcome local minima and still systematically target the low-energy states. For this, a multicanonical and PT algorithm were tested and the latter turned out to be more convenient. In the following, we briefly outline the PT scheme used within AMEA and refer to [106–110] for a thorough introduction to MCMC, simulated annealing, multicanonical sampling, and PT.

As just stated, in a MCMC scheme, one typically samples from the Boltzmann distribution  $p(\mathbf{x}) = 1/Z \exp(-\chi(\mathbf{x})\beta)$  at some chosen inverse temperature  $\beta$ . This is done through an iteratively created chain of states  $\{\mathbf{x}_l\}$ , whereby one avoids the explicit calculation of the partition function *Z*. An effective and well-known scheme for this is the Metropolis–Hastings algorithm [106, 107]. One starts out with some state  $\mathbf{x}_l$  and proposes a new configuration  $\mathbf{x}_k$ , whereby it has to be ensured that every state of the system can be reached in order to achieve ergodicity. The proposed state  $\mathbf{x}_k$  is accepted with probability [106, 107]<sup>14</sup>

$$p_{\text{pacc.}}^{l,k} = \min\left\{1, \frac{p(\mathbf{x}_k)}{p(\mathbf{x}_l)}\right\} = \min\{1, e^{-(\chi(\mathbf{x}_k) - \chi(\mathbf{x}_l))\beta}\}.$$
(A.1)

If the proposed configuration is accepted, then the next element  $\mathbf{x}_{l+1}$  in the chain is  $\mathbf{x}_k$ , otherwise  $\mathbf{x}_l$  again. From equation (A.1) it is obvious that  $p_{\text{pacc.}}^{l,k} = 1$  when  $p(\mathbf{x}_k) > p(\mathbf{x}_l)$ , so that an importance of sampling towards regions where  $p(\mathbf{x})$  is large is achieved. One can show that the algorithm fulfills detailed balance and draws a set of samples { $\mathbf{x}_l$ } that follow the desired distribution  $p(\mathbf{x})$ . However, stemming from the iterative construction, correlations in the chain are present which require a careful analysis for the purpose of statistical physics [106, 107]. For optimization problems, on the other hand, the situation is much simpler and one is just interested in the element in { $\mathbf{x}_l$ } which minimizes  $\chi(\mathbf{x})$ . Since a proposed step with  $\chi(\mathbf{x}_k) < \chi(\mathbf{x}_l)$  is always accepted, the algorithm targets minima; however, uphill moves in configuration space are also allowed with a probability depending exponentially on the barrier height  $\Delta \chi_{k,l} = \chi(\mathbf{x}_k) - \chi(\mathbf{x}_l)$  and  $\beta$ . Effectively, uphill moves only take place when  $\Delta \chi_{k,l}\beta \lesssim \mathcal{O}(1)$ . For small values of  $\beta$ , large moves in configuration space with large  $\Delta \chi_{k,l}$  are likely to be accepted, whereas for large  $\beta$  the distribution  $p(\mathbf{x})$  is peaked at minima in  $\chi(\mathbf{x})$  so that those regions are especially sampled. For the latter case, configurations in the chain { $\mathbf{x}_l$ } are generally more correlated and once a  $\mathbf{x}_l$  corresponds to a local minimum, the algorithm may stay there for a very long time.

One has great freedom in defining a proposal distribution from which the new state  $x_k$  is drawn given the current configuration  $x_l^{15}$ . Common choices are, for instance, a Gaussian or a Lorentzian distribution with the vector difference  $x_k - x_l$  as argument. We favored the former and updated each component *i* with a probability according to [106]

<sup>&</sup>lt;sup>13</sup> In order to perform the mapping for even larger systems efficiently, it may be of interest to combine the PT approach with, for instance, gradient-based methods.

<sup>&</sup>lt;sup>14</sup> In principle, one has to take the proposal probabilities  $q_{k,l}$  and  $q_{l,k}$  into account. However, since we only consider the case  $q_{k,l} = q_{l,k}$  here, the terms drop out of the equations and are neglected everywhere.

<sup>&</sup>lt;sup>15</sup> Note that, for minimization purposes only, one has in general flexibility in designing the algorithm and the Boltzmann distribution or detailed balance are not compulsory.

$$q_{l,k}^{i} = \frac{1}{\sqrt{2\pi}\sigma_{i}} e^{-\frac{(x_{k}-x_{l})_{i}^{2}}{2\sigma_{i}^{2}}}.$$
(A.2)

Hereby, a different step size  $\sigma_i$  for each component is expedient since the potential landscape  $\chi(\mathbf{x})$  around  $\mathbf{x}_l$  is typically highly anisotropic. Ideally, one should make use of the covariance matrix  $\Sigma_l$  of  $\chi(\mathbf{x}_l)$  and consider as argument for the Gaussian instead  $(\mathbf{x}_k - \mathbf{x}_l)^T \Sigma_l^{-1} (\mathbf{x}_k - \mathbf{x}_l) [106]$ . However, we encountered a problem in that the estimation of the covariance matrix at run time was strongly affected by noise and thus not feasible. The adjustment of the step sizes  $\sigma_i$ , on the contrary, can be done after a short number of updates by demanding that a value of  $p_{\text{pacc.}}^{l,k} \approx 0.5$  is reached on average when modifying the component *i*. For this, we implemented a check at every single proposal that increases  $\sigma_i \rightarrow 1.1\sigma_i$  when  $p_{\text{pacc.}}^{l,k} > 0.6$  and decreases  $\sigma_i \rightarrow 0.9 \sigma_i$  when  $p_{\text{pacc.}}^{l,k} < 0.4$ . Analogous to the treatment of spin systems, we define one sweep as a single update of all the components of  $\mathbf{x}^{16}$ .

## A.2. Parallel tempering

In a PT algorithm one considers, instead of sampling at one certain temperature, a set of different temperatures  $\beta_m^{-1}$  and corresponding replicas  $\mathbf{x}_l^m$ , each of which is evolved through a Markov chain. The largest  $\beta_m$  thereby target local minima whereas low  $\beta_m$  values allow for large moves in configuration space. The key idea of the PT approach is to let the individual replicas evolve dynamically in the set of  $\beta_m$ . By this, one achieves a situation whereby a replica at high  $\beta_m$  values systematically targets local minima but can overcome potential barriers again when its inverse temperature is changed to lower values. As a result, the time scales to reach an absolute minimum are drastically reduced and an efficient sampling of the low-energy states is achieved. For the purpose of calculating thermodynamic properties, one usually chooses a Metropolis–Hastings probability to swap two replicas with adjacent temperatures [109, 110]

$$p_{\text{swap},l}^{m,m+1} = \min\left\{1, \frac{p^m(\mathbf{x}_l^{m+1})p^{m+1}(\mathbf{x}_l^m)}{p^{m+1}(\mathbf{x}_l^{m+1})p^m(\mathbf{x}_l^m)}\right\} = \min\left\{1, e^{(\beta_{m+1}-\beta_m)(\chi(\mathbf{x}_l^{m+1})-\chi(\mathbf{x}_l^m))}\right\},\tag{A.3}$$

with the Boltzmann distribution for each  $\beta_m$  given by  $p^m(\mathbf{x}) = 1/Z_m \exp(-\chi(\mathbf{x})\beta_m)$ . Such swap moves are conveniently proposed after a certain number of sweeps, which satisfies the sufficient condition of balance for thermodynamics [110]. In practice, we chose 10 sweeps before swapping replicas. For the exchange to effectively take place, the underlying requirement is that the adjacent  $\beta_m$  and  $\beta_{m+1}$  values be close enough to each other, so that the two energy distributions  $\Omega[\chi(\mathbf{x})]p^m(\mathbf{x})$  and  $\Omega[\chi(\mathbf{x})]p^{m+1}(\mathbf{x})$  overlap, with  $\Omega[\chi_0] = \int d\mathbf{x} \, \delta(\chi_0 - \chi(\mathbf{x}))$  being the density of states of the cost function. This means that a replica at one temperature must represent a likely configuration for the neighboring temperature [110, 111]. In order to achieve this, a crucial point in the PT algorithm is to adjust the distribution of the inverse temperatures properly to the considered situation. Various criteria for this have been devised, see e.g. [110]. A common choice is to demand that the swapping probability equation (A.3) become constant as a function of temperature [112, 113], and in [114] a feedback strategy was presented which optimizes the round trip times of replicas. We tested the latter within AMEA but favored the simpler former criterion in the end, since it allows for a rapid feedback and quick adjustment to large changes in  $\chi(\mathbf{x}_l^m)$ . In the simple situation of a constant specific heat  $C_{\rm H}$  with respect to energy  $\chi$  for instance, an optimal strategy is known since a geometric progression  $\beta_m/\beta_{m+1} = \text{const. of temperatures yields a constant swapping probability [110, 111]. For interesting$ cases, in practice, this is rarely fulfilled, but within AMEA it served as a good starting point. The set of inverse temperatures is then optimized by averaging  $p_{swap,l}^{m,m+1}$  over a couple of swappings to obtain the mean probability  $\bar{p}_{swap}^{m,m+1}$  and adjusting the  $\beta_m$  thereafter. For this we chose a fixed lowest and highest  $\beta_m$  value and changed the spacings in between according to

$$\Delta\beta'_m = c \frac{\Delta\beta_m}{\log(\bar{p}^{m,m+1}_{\text{swap}})},\tag{A.4}$$

with  $\Delta\beta_m = \beta_{m+1} - \beta_m$  and *c* adjusted properly so that  $\max(\beta'_m) - \min(\beta'_m) = \max(\beta_m) - \min(\beta_m)$ . In [112, 113], it was shown that a constant swapping probability of 20%–23% seems to be optimal. We determined the highest and lowest  $\beta_m$  values by the changes in  $\chi(\mathbf{x})$  we want to resolve or allow for, and the number of inverse temperatures  $\beta_m$  was then set accordingly in order to roughly obtain  $\bar{p}_{swap}^{m,m+1} \approx 0.25$ . Fixing the smallest and largest  $\beta_m$  is, for our purposes, the most convenient choice among the many possibilities.

However, despite the feedback optimization of temperatures as just described, we encountered unwanted behavior in practice, whereby the set of parallel replicas effectively decoupled into several clusters. In suppressing this, we found it advantageous to introduce the following simple modification to equation (A.3)<sup>17</sup>:

 $<sup>^{16}</sup>$  Again, different choices are possible. For instance, in cases where dim(x) is very large, random updates of the most relevant components could be more appropriate.

 $<sup>^{17}</sup>$  One should note that the modification violates balance conditions and therefore the applicability in statistical physics. However, it is perfectly valid for the purpose of minimization problems.

$$p_{\text{swap},l}^{m,m+1} = \max\{p_{\text{swap},l}^{m,m+1}, p_{\text{swap}}^{\text{th.}}\},\tag{A.5}$$

with a certain threshold probability  $p_{swap}^{th.}$ , e.g.  $p_{swap}^{th.} = 0.1$  or 0.05. In this way, one avoids the  $\beta_m$  shifting unnecessarily close to each other and prevents very long time scales in which replicas oscillate only between two neighboring inverse temperatures.

## Appendix B. Matrix form and number of independent parameters for the different setups

For the sake of clarity, we present here for the different setups of figure 1 the form of the (Hermitian) matrices Eand  $\Gamma^{(1)}$  for the case  $N_{\rm B} = 4$  in the particle-hole symmetric case, i.e. under the constraint equation (27) which also fixes  $\Gamma^{(2)}$ . In addition, we quote the number of available fit parameters  $C(N_{\rm B})$  for each setup. The fit parameters are denoted below as  $x_i$  for i = 1,  $C(N_{\rm B})$ , with the only constraint being that  $\Gamma^{(i)}$  should be semipositive definite. This, together with the requirement that  $\Delta_{\rm aux}$  vanish for  $\omega \to \infty$ , further requires  $\Gamma_{ff}^{(1/2)} = \Gamma_{ff}^{(1/2)} = 0$ . In the first four setups, the impurity is in the center (i = 3). In the '1 chain n.n.', it is on the first site (i = 1).

#### B.1. 'Full' geometry

$$\boldsymbol{E} = \boldsymbol{E}_{t} \equiv \begin{pmatrix} x_{1} & x_{3} & 0 & 0 & 0 \\ x_{3} & x_{2} & x_{4} & 0 & 0 \\ 0 & x_{4} & 0 & x_{4} & 0 \\ 0 & 0 & x_{4} & -x_{2} & x_{3} \\ 0 & 0 & 0 & x_{3} & -x_{1} \end{pmatrix}$$
(B.1)  
$$\boldsymbol{\Gamma}^{(1)} = \begin{pmatrix} x_{5} & x_{9} & 0 & x_{11} & x_{12} \\ x_{9}^{*} & x_{6} & 0 & x_{13} & x_{14} \\ 0 & 0 & 0 & 0 & 0 \\ x_{11}^{*} & x_{13}^{*} & 0 & x_{7} & x_{10} \\ x_{12}^{*} & x_{14}^{*} & 0 & x_{10}^{*} & x_{8} \end{pmatrix}$$

The parameters  $x_9$  to  $x_{14}$  can be complex. Therefore, it is straightforward to see that, for general  $N_B$  the number of independent (real) parameters is  $C(N_B) = \frac{N_B}{2}(N_B + 3)$  for the real case and  $C(N_B) = N_B(N_B + 1)$  for the complex case.

#### B.3. '2-chain n.n.' geometry equation (B.1)

so in general  $C(N_{\rm B}) = 3N_{\rm B} - 2$ .

B.4. '2-chain onsite' geometry equation (B.1)

Here,  $C(N_{\rm B}) = 2N_{\rm B}$ .

#### B.5. 'Star' geometry

$$\boldsymbol{E} = \begin{pmatrix} x_1 & 0 & x_3 & 0 & 0 \\ 0 & x_2 & x_4 & 0 & 0 \\ x_3 & x_4 & 0 & x_4 & x_3 \\ 0 & 0 & x_4 & -x_2 & 0 \\ 0 & 0 & x_3 & 0 & -x_1 \end{pmatrix}$$

Also here  $C(N_{\rm B}) = 2N_{\rm B}$ .

# B.6. '1 chain n.n.' geometry

Remember, here the impurity is on i = 1.

$$\boldsymbol{E} = \begin{pmatrix} 0 & x_1 & 0 & 0 & 0 \\ x_1 & 0 & x_2 & 0 & 0 \\ 0 & x_2 & 0 & x_3 & 0 \\ 0 & 0 & x_3 & 0 & x_4 \\ 0 & 0 & 0 & x_4 & 0 \end{pmatrix}$$
$$\boldsymbol{\Gamma}^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & x_5 & x_9 & 0 & 0 \\ 0 & x_9 & x_6 & x_{10} & 0 \\ 0 & 0 & x_{10} & x_7 & x_{11} \\ 0 & 0 & 0 & x_{11} & x_8 \end{pmatrix}$$

In this case,  $C(N_{\rm B}) = 3N_{\rm B} - 1$ .

# Appendix C. Reduction of bath to a 'star' form

In principle, one can represent a noninteracting dissipative bath consisting of  $N_{\rm B}$  sites  $i = 1, ..., N_{\rm B}$ ) coupled to an impurity (i = f, we take f = 0) by specifying the single-particle parameters  $E_{ij}$ ,  $\Gamma_{ij}^{(1)}$ , and  $\Gamma_{ij}^{(2)}$  ( $i, j = 0, ..., N_{\rm B}$ ), with corresponding Hermitian, and in the case of  $\Gamma^{(1)}$ ,  $\Gamma^{(2)}$ , semipositive definite matrices. We show here that, for the sake of fitting the *retarded* component of a given bath spectral function  $\Delta_{aux}^{\rm R}$ , these parameters are redundant.

We rewrite equation (20) in block form

$$\mathbf{Z}^{\mathsf{R}} = \begin{pmatrix} \omega - F_0 & -\widehat{\mathbf{T}} \\ -\mathbf{T} & \omega - \mathbf{F} \end{pmatrix}^{-1}$$
(C.1)

where the first  $1 \times 1$  block contains<sup>18</sup>  $F_0 \equiv E_{00} - i\Gamma_{00}^{(+)}$ , the  $N_{\rm B} \times N_{\rm B}$  complex matrix F is given by  $F_{ij} \equiv E_{ij} - i\Gamma_{ij}^{(+)}$  for  $i, j = 1, ..., N_{\rm B}$ , the column vectors  $T_i \equiv E_{i0} - i\Gamma_{i0}^{(+)}$ ,  $\hat{T}_i \equiv E_{0i} - i\Gamma_{0i}^{(+)}$ , and we have introduced  $\Gamma^{(\pm)} \equiv \Gamma^{(1)} \pm \Gamma^{(2)}$ .

We are interested in  $G_{aux}^{R}$ , which is the  $_{00}$  component of  $\mathbb{Z}^{R}$ . By a well known result of matrix inversion, this is given by

$$1/G_{\text{aux}}^{\text{R}} = (\omega - F_0 - \widehat{T}(\omega - F)^{-1}T), \qquad (C.2)$$

which identifies  $\Delta_{aux}^{R} = T^{T}(\omega - F)^{-1}T + \delta F_{0}$ , where  $\delta F_{0} \equiv F_{0} - \varepsilon_{f}$ , which, for simplicity, we set to zero. The first term can be rewritten by introducing the matrix V which diagonalizes F,<sup>19</sup> i.e.

$$V^{-1}FV = F_{\text{diag}}.$$
 (C.3)

This gives

$$\Delta_{\text{aux}}^{\text{R}} = \widehat{T} V V^{-1} (\omega - F)^{-1} V V^{-1} T$$
$$= \overline{\widehat{T}} (\omega - F_{\text{diag}})^{-1} \overline{T}$$
$$\overline{T} \equiv V^{-1} T \qquad \overline{\widehat{T}} \equiv \widehat{T} V.$$

We can thus replace in equation (C.1) F with a diagonal, complex matrix  $F_{\text{diag}}$  and  $T(\widehat{T})$  with  $\overline{T}(\widehat{T})$ , and we get

$$Z'^{R} = (\omega - F')^{-1}$$

$$F' \equiv \begin{pmatrix} F_{0} & \overline{T} \\ \overline{T} & F_{\text{diag}} \end{pmatrix}^{-1}.$$
(C.4)

<sup>19</sup> Note that diagonalization of F is not always guaranteed.

 $<sup>^{18}</sup>$  In order to be more general, we allow for nonzero elements of the  $\Gamma$  matrices on the impurity site as well.

Here,  $\mathbf{Z}^{\prime R}$  has the same  $_{00}$  element as  $\mathbf{Z}^{R}$  from equation (C.1), i.e. the same  $G_{aux}^{R}$  and  $\Delta_{aux}^{R}$ . In this way, by the requirement that E and  $\Gamma^{(+)}$  must be Hermitian, we can construct new  $E' = (F' + F'^{\dagger})/2$  and  $\Gamma'^{(+)} = (F' - F'^{\dagger})/(2i)$ , i.e. a new auxiliary system which *yield the same*  $\Delta_{aux}^{R}$  and have the 'star' geometry (figure 1)<sup>20</sup>. This means that, concerning the *retarded part*, one can restrict to the case of diagonal bath energies and  $\Gamma^{(+)}$ , i.e., as in the non-dissipative case,  $\Delta_{aux}^{R}$  is fixed by only  $\mathcal{O}(N_{B})$  independent bath parameters, the rest being redundant. This is also the case when the bath hybridization function is represented by a completely empty and a completely full chain, as discussed in section 3, since in that case one simply fits the *retarded* components of the two chains separately. On the other hand, for the most generic case,  $\Gamma^{(1)}$  and  $\Gamma^{(2)}$  will not commute and cannot be simultaneously diagonalized, so that the Keldysh component  $\Delta_{aux}^{K}(\omega)$  appears to still depend on  $\mathcal{O}(N_{B}^{2})$  bath parameters (figure 5). Further investigations should be carried out in order to clarify this issue.

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 $^{20}$  Interestingly, in many cases the new  ${\Gamma'}^{(+)}$  is no longer positive definite.

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