

## Functional interpolation expansion for nonequilibrium correlated impurities

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We present a functional interpolation approach within the auxiliary master equation framework to efficiently and accurately solve correlated impurity problems in nonequilibrium dynamical mean-field theory (DMFT). By leveraging a near-exact auxiliary bath representation, the method estimates corrections via interpolation over a few bath realizations, significantly reducing computational cost and increasing accuracy. We illustrate the approach on the Anderson impurity model and on the Hubbard model within DMFT, capturing equilibrium and long-lived photodoped states.

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**Introduction.** Advances in controlling quantum materials, ranging from ultrafast laser spectroscopy [1–4], solid-state nanoscience [5,6], to ultracold quantum gases [7–10], have sparked growing interest in nonequilibrium strongly correlated systems. These developments drive theoretical challenges, including understanding nonequilibrium quantum phase transitions, [11] thermalization, and decoherence [12–15]. In this context, the theoretical description of strongly correlated quantum systems out of equilibrium remains an exciting challenge in modern theoretical physics.

The extension of dynamical mean-field theory (DMFT) [16,17] to nonequilibrium [18–24] provides a key framework for addressing these systems. DMFT in the time domain has been applied to simulate a variety of phenomena and systems ranging from highly excited states in photoexcited materials to ultracold atoms or Mott insulators under strong DC fields (see, e.g., Ref. [24]). The main bottleneck of DMFT, the solution of a many-body quantum impurity, is a long-standing problem for nonequilibrium systems. Exact quantum Monte Carlo (QMC) [25,26] or matrix-product state [27,28] calculations are limited to short time, so that mostly low-order hybridization expansions, such as the noncrossing approximation, are adopted in practice. When restricting to the steady state, advances have been achieved, among others, via the QMC inchworm [29], scattering-states approaches [30,31], or the auxiliary master equation (AMEA) [32,33] algorithms.

Steady-state algorithms provide a complement to real-time simulations, as they can be used to address the slowly time-evolving regime occurring, for instance, in photoexcited Mott insulators after an initial prethermalization phase

[34–38]. While this regime cannot be reliably addressed by numerically exact real-time approaches, one can adopt a time-local ansatz for the fermionic distribution function of a reference steady-state system [39], which then evolves in time following a generalized quantum Boltzmann scheme [40].

It is therefore crucial to develop nonperturbative, accurate methods that remain computationally efficient enough to be used as quantum impurity solvers in DMFT self-consistent calculations.

The approach presented in this Letter exploits the freedom to replace the “physical” fermionic bath of the impurity problem that needs to be solved, e.g., at each DMFT step, with a so-called “auxiliary” one consisting of a small number  $N_b$  (typically 6–8) of bath sites connected to a Markovian environment which then can be solved exactly by numerical methods. Since the “residual” distance (termed  $\underline{\varepsilon}$  below) between the hybridization functions of the two baths is exponentially small in  $N_b$  [41], a substantial improvement by including perturbative corrections in  $\underline{\varepsilon}$  can be obtained; see Ref. [42] for a similar idea. However, for values of  $N_b \gtrsim 6$  for which  $\underline{\varepsilon}$  is small enough, this expansion becomes prohibitive and computationally quite expensive. The main idea presented here consists in adopting a functional interpolation (FI) approach, which amounts to estimating the  $\underline{\varepsilon}$  linear corrections by a solution of the impurity problem for a few (typically 2–4) different suitably chosen sets of bath parameters.

After testing the approach for the Anderson impurity model in and out of equilibrium, we address, within DMFT, the Hubbard model on both sides of the equilibrium Mott phase, as well as the long-lived nonequilibrium photodoped state.

**Model and method.** A fermionic single-impurity problem is fully characterized by its impurity Hamiltonian  $H_{\text{imp}}$  typically describing electrons on a single orbital with an onsite interaction  $U$ . The coupling of this orbital to a noninteracting fermionic bath is completely characterized by its hybridization function  $\underline{\Delta}_{\text{phys}}(\omega)$ , which in a nonequilibrium steady state consists of a  $2 \times 2$  matrix in Keldysh space [43–48].

Within AMEA [32,33] this “physical” hybridization function  $\underline{\Delta}_{\text{phys}}(\omega)$  is approximated by the hybridization

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function

$$\Delta_{\text{aux}}(\omega) = \Delta_{\text{phys}}(\omega) + \underline{\varepsilon}(\omega) \quad (1)$$

of an “auxiliary” bath consisting of a finite number  $N_b$  of bath sites connected to a Markovian environment, whose dynamics is described by the Lindblad equation, see [32,33]. For a sufficiently small  $N_b$ , the impurity problem connected to the auxiliary bath can be solved exactly, for example, by Lanczos/Arnoldi-like methods [33,49], by matrix-product states (MPSs) [50], or by stochastic wave function approaches [51]. In principle, in the  $\underline{\varepsilon} \rightarrow 0$  limit the computed *interacting* impurity Green’s function of this auxiliary system approaches the physical one for any value of  $U$ . A clever choice of the (Lindblad) parameters [41] of the auxiliary bath obtained, e.g., by fitting  $\Delta_{\text{aux}}$  to  $\Delta_{\text{phys}}$  makes  $|\underline{\varepsilon}|$  vanish exponentially in terms of  $N_b$  [41]. Here  $|\underline{\varepsilon}|$  is some measure of the norm of the deviation  $\underline{\varepsilon}$  integrated over frequencies possibly with some weight factor  $W(\omega)$  to emphasize some physical relevant frequency regions.

Unfortunately, since one must consider the full space of many-body density matrices, the maximum  $N_b$  that can be achieved by Lanczos-like methods [52] is restricted to  $N_b \approx 8 - 10$ . While MPS approaches can address larger systems, the geometry restriction makes the fit less efficient [41]. We, therefore, propose to improve the accuracy by including corrections of  $O(\underline{\varepsilon}^1)$ . In principle, this is in the spirit of hybridization expansion methods, for example, the noncrossing approximation (NCA) [53–55], which corresponds, formally, to taking  $\underline{\varepsilon} = \Delta_{\text{phys}}$  in (1). However, since  $\underline{\varepsilon}$  is not small in this case, only higher orders provide reliable results. For these one has to resort to, e.g., quantum Monte Carlo [26,29,56] or, as shown recently, to tensor trains [57,58].

In Ref. [42] it was suggested to carry out a dual-fermion expansion around a “better” solution, with a  $\Delta_{\text{aux}}$  closer to the physical one obtained with an auxiliary bath with  $N_b = 2$ . While the results of the expansion display a significant improvement with respect to the one of the plain auxiliary system [59], an extension to larger  $N_b$  is quite prohibitive. This is due to the fact that one needs to evaluate a three-point vertex, which is numerically complicated in Lanczos/Arnoldi. On the other hand, only values of  $N_b \gtrsim 6$  guarantee that  $\underline{\varepsilon}$  is sufficiently small so that a first-order expansion is justified. Here, we follow a different path and estimate the  $O(\underline{\varepsilon}^1)$  term numerically by solving the nonequilibrium impurity problem for a batch of  $\underline{\varepsilon}$ . We exploit the fact that, for fixed  $H_{\text{imp}}$ , the steady-state self-energy  $\underline{\Sigma}$  is a functional of  $\underline{\Delta}$  only. Therefore, to first order in  $\underline{\varepsilon}$  we can write

$$\underline{\Sigma}[\Delta_{\text{phys}} + \underline{\varepsilon}] = \underline{\Sigma}[\Delta_{\text{phys}}] + \frac{\delta \underline{\Sigma}[\Delta_{\text{phys}}]}{\delta \Delta_{\text{phys}}} \odot \underline{\varepsilon} + O(\underline{\varepsilon}^2). \quad (2)$$

Strictly speaking, the independent functions in the argument of  $\underline{\Sigma}$  are just  $\text{Im}\Delta^R(\omega)$  and  $\text{Im}\Delta^K(\omega)$ , as  $\text{Re}\Delta^R$  is fixed by Kramers-Kronig and  $\text{Re}\Delta^K = 0$ . Therefore, we will understand the functional dependence, and its corresponding derivative, with respect to these functions only. Similarly,  $\odot$  indicates a convolution, i.e., a sum over these two components and an integral over  $\omega$ . An equation like (2) is obviously valid for the Green’s function as well. Here, we will limit the discussion to the self-energy.

To start with, let us first hypothetically assume that, in addition to (1), one could compute the self-energy for a different “desired” hybridization,

$$\Delta_{\text{des}} = \Delta_{\text{phys}} + k \underline{\varepsilon}, \quad (3)$$

with some real number  $k$  away from 1. Then, by applying (2) for  $\underline{\varepsilon}$  replaced with  $k \cdot \underline{\varepsilon}$ , one can cancel the first-order  $\Delta_{\text{des}} = \Delta_{\text{phys}} + k \underline{\varepsilon}$ , errors exactly yielding

$$\begin{aligned} \underline{\Sigma}[\Delta_{\text{phys}}] &= \frac{1}{1-k} (\underline{\Sigma}[\Delta_{\text{phys}} + k \underline{\varepsilon}] - k \underline{\Sigma}[\Delta_{\text{phys}} + \underline{\varepsilon}]) \\ &\quad + O(\underline{\varepsilon}^2). \end{aligned} \quad (4)$$

For example, for  $k = -1$  this is the average between the two self-energies at  $\Delta_{\text{phys}} \pm \underline{\varepsilon}$ .

The problem is that, in general,  $\Delta_{\text{des}}$  will not be representable within an auxiliary bath with finite  $N_b$  in the sense that there is no set of Lindblad parameters producing it.

An alternative “bottom-up” approach consists in generalizing (4) to a set of  $n_{\text{max}}$  different suitably chosen auxiliary baths with the same  $N_b$  but with different parameters. The deviations  $\underline{\varepsilon}_n$  of their hybridization functions from the physical one,

$$\underline{\varepsilon}_n = \Delta_{\text{phys}} - \Delta_{\text{aux},n} \quad n = 1, \dots, n_{\text{max}}, \quad (5)$$

must remain small, i.e., of the same order of magnitude.

One can then determine coefficients  $\alpha_n$  such that the quantity

$$\underline{\mu} \equiv \sum_{n=1}^{n_{\text{max}}} \alpha_n \underline{\varepsilon}_n \quad \text{with} \quad \sum_{n=1}^{n_{\text{max}}} \alpha_n = 1 \quad (6)$$

is much smaller than the  $\underline{\varepsilon}_n$ . Here,  $\underline{\mu}(\omega)$  controls the “residual” first-order error in an improved approximation for the self-energy of the physical system,

$$\underline{\Sigma}[\Delta_{\text{phys}}] = \sum_{n=1}^{n_{\text{max}}} \alpha_n \underline{\Sigma}[\Delta_{\text{phys}} + \underline{\varepsilon}_n] + O(\underline{\mu}) + O(\underline{\varepsilon}^2). \quad (7)$$

The optimal coefficients  $\alpha_n$  should be, thus, chosen such that

$$|\underline{\mu}|^2 = \sum_{m,n=1}^{n_{\text{max}}} \alpha_n \alpha_m A_{mn} \quad A_{mn} \equiv \underline{\varepsilon}_n \odot \underline{\varepsilon}_m \quad (8)$$

is minimal. The constraint in (6) can be addressed via a Lagrange multiplier  $\lambda$  leading to the optimal values

$$\underline{\alpha} = \lambda \mathbf{A}^{-1} \cdot \mathbf{u} \quad \lambda = (\mathbf{u}^T \cdot \mathbf{A}^{-1} \mathbf{u})^{-1} \quad (9)$$

with  $\mathbf{u}^T = (1, 1, 1, \dots)$ .

We have tried two different procedures to select the set of  $\Delta_{\text{aux},n}$  in (5), or equivalently,  $\underline{\varepsilon}_n$  [60]. The first procedure we will present is *deterministic* and consists of the following steps: We start by finding the (Lindblad) parameters of the auxiliary bath that give the best fit to  $\Delta_{\text{phys}}$ . The corresponding hybridization function is assigned to  $\Delta_{\text{aux},m}$  with  $m = 1$ .

(i) For a given  $\Delta_{\text{aux},m}$  we extract the corresponding  $\underline{\varepsilon}_m$  from (5) and construct the corresponding  $\underline{\mu}$  from (6) and (9) with  $n_{\text{max}} = m$ .

(ii) We use this  $\underline{\mu}$ , which we name  $\underline{\mu}_m$ , to determine a new  $\Delta_{\text{aux},m+1}$  by fitting the Lindblad parameters to a “desired”  $\Delta_{\text{des},m+1} = \Delta_{\text{phys}} + k \underline{\mu}_m$  [cf. (3)]. Here,  $k$  is some number [61] sufficiently away from 1. This choice is motivated by

the fact that if one could fit  $\Delta_{\text{des}}$  exactly, the first-order error would be canceled, similarly to (4). With the new  $\Delta_{\text{aux},m+1}$  we go back to step (i).

Steps (i) to (ii) should be repeated up to a maximum value  $N_T$  for  $m$  or until the condition number [62] of the matrix  $A$  exceeds a given value. Finally, the improved self-energy is obtained via (7).

A modification of this procedure consists in starting with two (or more) different initial  $\Delta_{\text{aux},m=1}$  obtained by different fits, i.e., using different weight functions  $W(\omega)$ . These weight functions are chosen in order to emphasize, for example, low-energy frequency regions, similarly to equilibrium exact-diagonalization-based approaches. Then the corresponding  $\varepsilon_m$  are combined together in (7).

Alternatively, starting with the same  $\Delta_{\text{aux},m=1}$  as for the previous algorithm, one can adopt a random procedure for determining the  $\varepsilon_m$  for  $m > 1$ . This is achieved by replacing the  $N_T$  “desired” hybridization functions of step (ii) in the previous procedure by random functions  $\Delta_{\text{des},m}$  sufficiently close to  $\Delta_{\text{phys}}$  [63]. For each  $m$ , the  $\Delta_{\text{aux},m}$  is obtained, as usual, via a fit. If the condition number of the resulting matrix  $A$  remains reasonably low, we keep that function, otherwise we discard it. After typically around ten accepted random functions the following ones almost always have to be discarded. Therefore, we set  $N_T$  to ten here. Since this is a random procedure, it is convenient to repeat it a certain number of times  $N_{\text{av}}$  and average the corresponding results for the self-energy. After typically  $N_{\text{av}} \approx 10$ , the self-energy  $\Sigma$  is statistically converged [64] so we fix  $N_{\text{av}} = 10$ .

**Results.** Since we have a certain freedom in choosing the details of the procedure, such as the value of  $k$  and  $N_T$  or whether to use the deterministic or the random version, it is convenient to first test different options in order to find out the most efficient and accurate one. We do this by applying the approach for numerically “cheap” auxiliary baths with  $N_b = 4$  and compare the self-energy obtained in this way with a reference evaluated with the plain [65]  $N_b = 8$  one, which is expected to be more accurate than the  $N_b = 4$  case. The benchmark reported in the Supplemental Material [66] suggests that the best accuracy is obtained with the deterministic algorithm with  $k = 2$  and  $N_T = 2$ . This is interesting, as it shows that we can substantially increase the accuracy of the impurity solver by just carrying out two Lindblad many-body calculations. In particular, as we will see below, a many-body calculation with  $N_b = 6$  using the present FI approach yields an accuracy comparable to or better than a plain  $N_b = 8$  one, which is approximately 6 times as costly. In addition, the two many-body calculations required by the FI approach can be done in parallel. This is particularly convenient when using it as an impurity solver for DMFT.

We start by computing the spectral function for an Anderson impurity in and out of equilibrium. Unless otherwise specified, we consider a bath with a flat density of states (DOS) of width  $10\Gamma$  [67] with the following parameters:  $U/\Gamma = 6$ ,  $-\text{Im}\Delta^R(\omega = 0)/\Gamma = 1$ ,  $\varepsilon_{\text{imp}} = -U/2$ . In Fig. 1 we display the spectral function of the impurity coupled to (a) a bath in equilibrium at temperature  $T/\Gamma = 0.02$  and (b) to two baths with a bias voltage  $V/\Gamma = 1.5$ . As one can see, the results with  $N_b = 6$  augmented with the FI approach is in some cases even more accurate than the plain  $N_b = 8$ ,

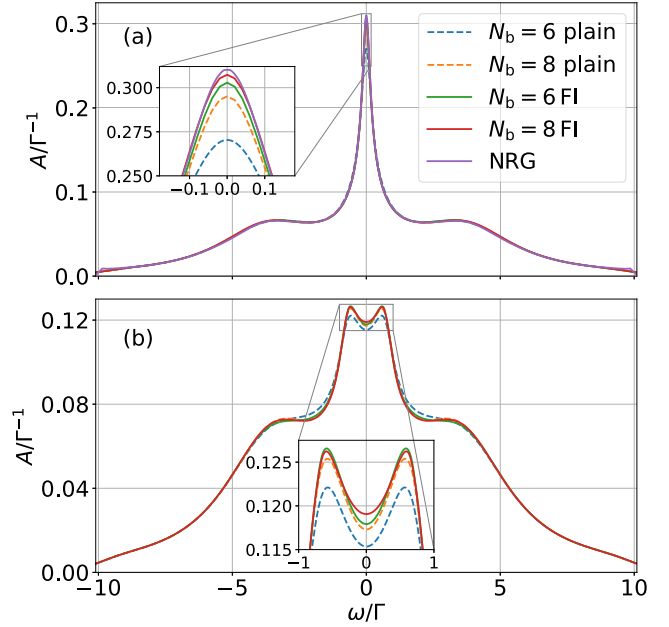


FIG. 1. Spectral function of the equilibrium (a) Anderson impurity model for  $U/\Gamma = 6$ ,  $-\text{Im}\Delta^R(\omega = 0)/\Gamma = 1$ ,  $\varepsilon_{\text{imp}} = -U/2$ , and  $T/\Gamma = 0.02$ , obtained by plain AMEA with  $N_b = 6$  and  $N_b = 8$  and improved results obtained by the FI approach with  $k = 2$  and  $N_T = 2$  for the two cases. The difference ( $\chi[\underline{G}_{\text{NRG}} - \underline{G}_{\text{AMEA}}]$ , cf. Eq. (11) in the Supplemental Material [66]) between the AMEA results with  $N_b = 6$  plain,  $N_b = 8$  plain,  $N_b = 6$  FI,  $N_b = 8$  FI, and the NRG benchmark are  $9.4 \times 10^{-4}$ ,  $1.7 \times 10^{-4}$ ,  $9.2 \times 10^{-5}$  and  $3.5 \times 10^{-5}$  respectively. (b) The same results for the case of a finite bias voltage  $V/\Gamma = 1.5$ . The equilibrium ( $V/\Gamma = 0$ ) results are compared with NRG.

as the comparison with Numerical Renormalization Group (NRG) shows. FI combined with  $N_b = 8$  provides an even better accuracy. Of course, in equilibrium the method cannot compete with NRG, but it has the advantage that it can be straightforwardly extended to nonequilibrium steady states.

As mentioned above, the greatest advantage of the approach consists in its application as an efficient impurity solver for steady-state nonequilibrium DMFT. The method is also quite convenient as a real-frequency impurity solver in the equilibrium case. To illustrate this, we apply it to the infinite-dimensional Hubbard model with the Bethe lattice DOS. We start by addressing the most challenging regime in the equilibrium case, i.e., the vicinity of the metal-insulator transition. We take a point in the metallic phase at  $T/\Gamma = 0.05$  and  $U/\Gamma = 4.4$  and one nearby for  $U/\Gamma = 5.0$  and the same temperature in the insulating phase. The corresponding spectral functions are plotted in Fig. 2. In both cases the results obtained for  $N_b = 6$  FI lead to a significant improvement, i.e., they give a solution closer to  $N_b = 8$  than the plain  $N_b = 6$ . At the same time, the  $N_b = 8$  FI result shows a more pronounced quasiparticle peak in the metallic and a clearer gap in the insulating phase [68].

As a benchmark for a steady-state nonequilibrium situation, we address cold photodoped states in a Mott insulator [34–37]. In Ref. [39] it has been shown that these long-lived states can be reliably described by a time-local quasi-steady

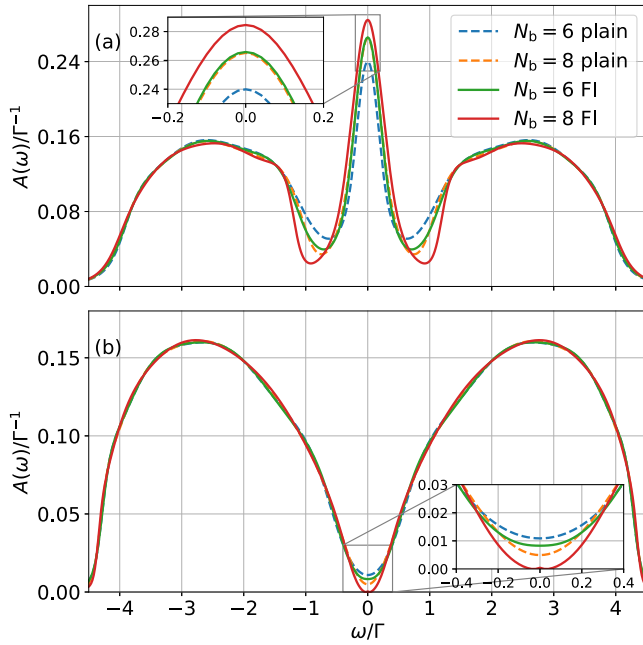


FIG. 2. Spectral function for the infinite-dimensional Bethe lattice at  $T/\Gamma = 0.05$ ,  $\varepsilon_{\text{imp}} = -U/2$ ,  $t/\Gamma = 1$ , and (a)  $U/\Gamma = 4.4$ , i.e., in the metallic phase, or (b) for a point in the insulating phase at  $U/\Gamma = 5$ .

-state ansatz for which numerically exact inchworm Monte Carlo data have been produced. In Fig. 3 we compare the self-energy obtained by AMEA with  $N_b = 6$  and 8 along with the corresponding FI corrections with the inchworm data from Ref. [39]. As one can see, the FI  $N_b = 8$  calculation produces a peak which is very close to the inchworm one. On the other hand, the vanishing of the self-energy at the quasiparticle chemical potential around  $\omega/\Gamma \approx \pm 1.82$  is harder to reproduce. This is probably due to the fact that since the self-energy vanishes quadratically there, some kind of quadratic [instead of linear, as in (2)] extrapolation should be carried out.

**Conclusion.** We have introduced an approach for solving many-body impurity problems, particularly suited for strongly correlated systems out of equilibrium within dynamical mean-field theory. The method involves exactly solving the impurity embedded in a small auxiliary bath coupled to a Markovian environment, then applying a linear correction for the difference between the auxiliary and physical baths. This correction is well justified when the difference between the two baths is small, as achieved with  $N_b = 6-8$ . Our approach significantly improves results over a plain AMEA DMFT impurity solver in and out of equilibrium.

One key advantage of the present FI approach is that good accuracy is achieved with as few as  $N_b = 6$  bath sites,

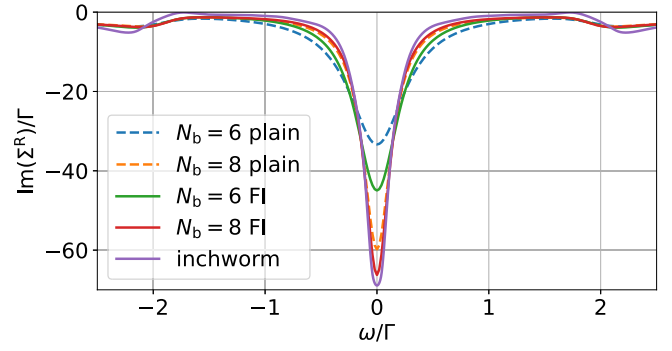


FIG. 3. Imaginary part of the self-energy of a cold photodoped quasisteady state obtained by the FI approach and plain AMEA compared with inchworm QMC data (extracted from Ref. [39]). The deviation between the inchworm reference and the  $N_b = 6$  plain,  $N_b = 8$  plain,  $N_b = 6$  FI, and  $N_b = 8$  FI AMEA self-energies ( $\chi[\Sigma_{\text{inchworm}} - \Sigma_{\text{AMEA}}]$ , just the retarded contribution, cf. Eq. (11) in the Supplemental Material [66]) are 7.4, 3.3, 0.78, and 0.31, respectively [69]. Parameters are as Fig. 2(b) of Ref. [39].

significantly speeding up impurity computations, which is crucial for DMFT self-consistency. Moreover, the ability to use fewer bath sites makes the method extendable to multi-orbital systems, which is essential for first-principles studies of correlated materials.

While the “FI” expression (7) is straightforward, in practice the achieved accuracy sometimes depends on the choice of the batch of  $N_T$  auxiliary hybridization functions. Our extensive analysis for  $N_b = 4$  suggests that a substantial improvement is obtained already with  $N_T = 2$ . The question is whether this conclusion is valid (a) also for larger  $N_b$  and (b) for more structured hybridization functions. Increasing  $N_T$  improves the accuracy of the self-energy in (7) because it reduces  $|\mu|$ . However, when  $|\mu|$  becomes smaller or of the order of  $|\varepsilon|^2$ , the error gets dominated by the latter and there is no point of further reducing  $|\mu|$ . This may suggest that larger  $N_T$  could be necessary when using  $N_b \gtrsim 6$  for which  $|\varepsilon|$  is smaller. In the case of a structured (physical) hybridization function, the FI approach could provide a receipt to cleverly combine the result of auxiliary hybridization functions adapted to one or to the other region. In this case, increasing  $N_T$  should also improve the results. These issues should be addressed in future studies.

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**Data availability.** The data that support the findings of this article are openly available [70].

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- [48] Here and in the following, we use underscore  $\underline{X}$  to denote this Keldysh structure containing the retarded  $X^R$ , Keldysh  $X^K$ , and advanced  $X^A$  components [43,47].  $X$  can be any two-point function, such as  $\Delta$ ,  $G$ , or  $\Sigma$ , or their differences, such as the quantities  $\varepsilon$  or  $\mu$  below. In addition, we shall omit the argument  $\omega$  unless necessary.
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- [59] In Ref. [42] the auxiliary system is referred to as a reference system.
- [60] The linear correction can rarely produce nonphysical self-energies. This means that one of the two “physicality” requirements, namely,  $\text{Im}\Sigma^R < 0$  or the distribution function between 0 and 1, is not fulfilled. In the first case, the causality requirement is included as an additional constraint when minimizing  $|\underline{\mu}|^2$ . If the distribution function becomes unphysical, it is reset to 1 or 0 wherever it exceeds those bounds, and the Keldysh part of the self-energy function is then recalculated from this updated physical distribution function.
- [61]  $k$  can, in principle, change as a function of  $n$ .
- [62] The condition number is a measure of how ill-conditioned the matrix inversion is; see, e.g., <https://numpy.org/doc/2.1/reference/generated/numpy.linalg.cond.html>.
- [63] We do that by adding a random function ( $f_{\text{rand}}(\omega)$ ) to the physical hybridization function,
- $$\text{Im}\Delta_{\text{des } m}^{R/K} = \text{Im}\Delta_{\text{phys}}^{R/K} + f_{\text{rand}}^{R/K}(\omega) \quad \forall m > 1,$$
- where  $f$  is generated by choosing random values for the vertical axis between  $-0.3$  and  $0.3$ , at five equidistant points, between  $-\omega_{\text{max}}$  and  $+\omega_{\text{max}}$ , and interpolating between them. Notice that  $\Delta_{\text{des } m}$  may become unphysical, for example, noncausal. This is, however, not an issue, as the fit ensures that  $\Delta_{\text{aux } m}$  remains physical.
- [64] In the sense that  $\sigma_{\text{typ}, \Sigma}$ , i.e., the maximum over  $\omega$  of the standard deviation of  $\Sigma$ , is less than 0.1 times the average over  $\omega$  of  $\Sigma$ .
- [65] By “plain” we mean without the FI improvement, corresponding to  $N_T = 1$ .
- [66] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevResearch.7.L022044> for details about our benchmark to determine the optimal values of the hyperparameters  $k$  and  $N_T$ .
- [67] The edges of the DOS are smoothed with a “fictitious” temperature  $0.5\Gamma$ .
- [68] The slight increases around  $\omega = 0$  are because the FI scheme yields a noncausal self-energy, which is fixed by minimally adjusting the coefficients  $\alpha$  to fulfill the constraint of causality; see Ref. [60].
- [69] Consider that the self-energy assumes large values, leading to large absolute differences.
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