

Semigroup Influence Matrices for Nonequilibrium Quantum Impurity Models

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We introduce a framework for describing the real-time dynamics of quantum impurity models out of equilibrium which is based on the influence matrix approach. By replacing the dynamical map of a large fermionic quantum environment with an effective semigroup influence matrix (SGIM) which acts on a reduced auxiliary space, we overcome the limitations of previous proposals, achieving high accuracy at long evolution times. This SGIM corresponds to a uniform matrix-product state representation of the influence matrix and can be obtained by an efficient algorithm presented in this Letter. We benchmark this approach by computing the spectral function of the single impurity Anderson model with high resolution. Further, the spectrum of the effective dynamical map allows us to obtain relaxation rates of the impurity toward equilibrium following a quantum quench. Finally, for a quantum impurity model with on-site two-fermion loss, we compute the spectral function and confirm the emergence of Kondo physics at large loss rates.

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Introduction—Quantum impurity models (QIMs) describe a small interacting system coupled to a large noninteracting environment. Fermionic QIMs exhibit a variety of correlated phenomena such as the Kondo effect [1,2]. These models continue to be widely studied due to their relevance to quantum transport in mesoscopic systems [3–5] and because of their central role in the computational methods for correlated materials such as dynamical mean-field theory (DMFT) [6–8].

Experimental advances in synthetic quantum systems such as ultracold atoms enable probing real-time dynamics of QIMs [9–11]. Recently, a realization of the Kondo effect in a nonequilibrium, experimentally accessible setting, where the impurity site is subject to strong dissipation, has been proposed [12,13]. In such highly nonequilibrium regimes the conventional methods suited for equilibrium QIMs break down, calling for the development of new numerically exact approaches.

In this direction, a novel class of methods for out-of-equilibrium QIMs exploits the structure of temporal correlations encoded in the environment’s influence matrix (IM) [14–21]. The IM is a large multitime tensor encoding the

effect of the environment on the impurity, and in essence, these methods aim to approximate the IM by a matrix product state (MPS). The promise of such an approach is supported by rigorous results that establish a polynomial scaling of complexity with evolution time [22,23]. While the existing IM algorithms for fermionic QIMs [17,19,21] are competitive with methods such as diagrammatic Monte Carlo [24–26], hierarchical equations of motion [23,27–30], and time-dependent numerical renormalization group [31–33], they still require significant computational resources.

In this Letter, we demonstrate how temporal translation invariance can be exploited to achieve a representation of the IM as a compressed uniform MPS. This approach effectively generates a dynamical semigroup where the environment is replaced by compressed auxiliary degrees of freedom [20]. We introduce an efficient algorithm for constructing this semigroup influence matrix (SGIM), achieving accurate and controlled computations of nonequilibrium QIM dynamics for long evolution times. In particular, as we show below, the SGIM method allows for computing a spectral function of the single-impurity Anderson model with high resolution across all frequencies. Furthermore, we study the dynamical formation of Kondo correlations following a quantum quench and, finally, investigate the dissipative Kondo effect [12,13] using this numerically exact method.

Method—We consider a QIM where the impurity (I) consists of fermionic modes labeled by an index σ . Each of these modes is coupled to an independent Gaussian fermionic environment (E) via the Hamiltonian

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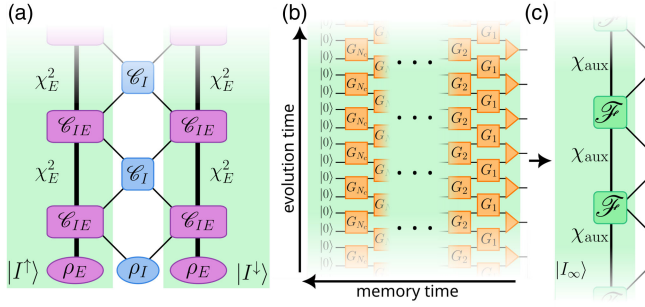


FIG. 1. (a) Real-time evolution of a QIM with two baths $\sigma = \uparrow, \downarrow$ expressed as tensor contraction corresponding to Eq. (3). (b) Tensor network representation of an infinite Gaussian IM corresponding to Eq. (6), decomposed into nearest neighbor gates. (c) Semigroup influence matrix as obtained from contracting (b) using iTEDB.

$$H_{IE}^\sigma = \sum_k (v_{\sigma k} d_\sigma^\dagger f_{\sigma k} + v_{\sigma k}^* f_{\sigma k}^\dagger d_\sigma) + \sum_k \epsilon_{\sigma k} f_{\sigma k}^\dagger f_{\sigma k}. \quad (1)$$

Here, d_σ and $f_{\sigma k}$ are the annihilation operators for the fermions in the impurity and the environment, respectively. Each environment is fully characterized by its spectral density $J_\sigma(\omega) = \sum_k |v_{\sigma k}|^2 \delta(\omega - \epsilon_{\sigma k})$, inverse temperature β , and chemical potential μ [34].

For a small time step δt , the dynamical map or *quantum channel* of the QIM dynamics can be expressed within second order Trotter approximation as

$$\mathcal{C}_{QIM}[\delta t] = \mathcal{C}_I[\delta t/2] (\Pi_\sigma \mathcal{C}_{IE}^\sigma[\delta t]) \mathcal{C}_I[\delta t/2] + O(\delta t^3), \quad (2)$$

where $\mathcal{C}_I[\delta t/2]$ is a channel for a local, interacting evolution on the impurity (half step $\delta t/2$) and the evolution $\mathcal{C}_{IE}^\sigma[\delta t] = e^{-iH_{IE}^\sigma \delta t} \otimes e^{iH_{IE}^\sigma \delta t}$ describes the coupling with the environment via Hamiltonian (1). The channel (2) can be used to express the evolution of the impurity state for N time steps [cf. Fig. 1(a)]:

$$\rho_I(N\delta t) = \text{tr}_E[(\mathcal{C}_{QIM}[\delta t])^N \rho_{QIM}(0)], \quad (3)$$

where tr_E denotes the trace over all environment modes. We can collect all terms in Eq. (3) that correspond to a single environment in one object [green shaded area in Fig. 1(a)]. This defines the *influence matrix* [15],

$$|I_N^\sigma\rangle = \text{tr}_E[(\mathcal{C}_{IE}^\sigma[\delta t])^{\otimes N} \rho_E^\sigma], \quad (4)$$

where $\otimes_I$ denotes the tensor product over the impurity degrees of freedom, while the environment degrees of freedom are contracted. In the context of characterizing non-Markovian dynamics, a similar object is known as *process tensor* [35]. Time evolution as in Eq. (3) can be expressed in terms of overlaps of IMs [17,18], which can be computed efficiently if the IM is parametrized as a

matrix product state with low bond dimension. However, for any given MPS-IM, the maximal number of time steps which can be computed is limited by N .

On the other hand, using Eq. (3) directly for numerical computations is impractical because the channels $\mathcal{C}_{IE}^\sigma$ act on the large environment density matrix space. The central idea of our approach is to find an efficient algorithm to replace these channels by a different linear map $\mathcal{F}$ that faithfully reproduces the local impurity dynamics when used in Eq. (3), but acts on a much smaller *auxiliary space*. This linear map defines a *semigroup influence matrix* (SGIM) and is a representation of the effective dynamical semigroup of the environment time evolution [36]. The accuracy of this representation as well as the numerical cost is controlled by the dimension of the auxiliary space χ_{aux} . By substituting $\mathcal{F}^\sigma$ into Eq. (4), we can understand it as a uniform MPS representation of an IM with an infinite number of time steps [Fig. 1(c)].

Previous works [17–19] has shown that, for Gaussian fermionic environments in QIMs, the IM can, in a vectorized form, be expressed as a Gaussian many-body state:

$$|I_N^\sigma\rangle = \prod_{n=1}^N \prod_{m=1}^n \exp(\vec{c}_n^\dagger \cdot G_{n,m}^\sigma \vec{c}_m^\dagger) |0\rangle, \quad (5)$$

where $G_{n,m}$ are 4×4 correlation matrices and $\vec{c}_n$ are fermionic annihilation operators with four fermionic modes per time step n (see Ref. [37]). Various algorithms exist to directly generate a finite MPS representation of states in the form (5) [19,38–40], resulting in an efficient algorithm for short time dynamics of QIMs [17,19].

Looking at the correlation matrices $G_{m,n}^\sigma$ closely, we note that in the bulk, for $1 \ll n, m \ll N$, the temporal correlations become effectively translationally invariant $G_{n,m}^\sigma = G_{n-m}^\sigma$. Furthermore, the correlations of continuous environments decay at large time differences. This allows us to neglect correlations for time differences larger than some bath-dependent effective memory time N_c . We can formally express an “infinite IM” as

$$|I_\infty^\sigma\rangle = \prod_{n=-\infty}^{+\infty} \prod_{k=0}^{N_c} \exp(\vec{c}_n^\dagger \cdot G_k^\sigma \vec{c}_{n-k}^\dagger) |0\rangle. \quad (6)$$

This state is translationally invariant and can thus be efficiently represented as a uniform MPS, allowing us to find an effective SGIM $\mathcal{F}^\sigma$. Note that, even though the SGIM is time translation invariant, it still can be used to compute nonstationary impurity dynamics such as local quenches by using appropriate time-dependent evolution on the impurity. To construct an SGIM, we first derive an exact tensor network representation of Eq. (6), which is depicted in Fig. 1(b). Briefly, each network layer introduces correlations G_k^σ corresponding to a given memory time step k in Eq. (6), starting from the memory time cutoff $k = N_c$

and going to $k = 0$. Details on this construction are provided in Supplemental Material [37]. Structurally, our result resembles the network used in the TEMPO method for bosonic Gaussian environments [20,41].

Contracting the tensor network [see Fig. 1(c)] to uniform MPS using conventional infinite time-evolving block decimation (iTEBD) [42] yields an SGIM. Truncation with a fixed singular value decomposition (SVD) truncation tolerance is highly efficient because entanglement, and hence the MPS bond dimension, will build up only toward the end of the contraction. This allows us to set the memory time cutoff N_c so large that all correlations beyond the cutoff fall below the truncation tolerance, eliminating the memory time cutoff as a parameter which needs to be monitored for convergence.

Compared to finite-MPS approaches, the SGIM method allows for significantly longer evolution times with lower demands in computation time and memory. The construction of the SGIM is dominated by singular value decompositions in the last few layers of the network and is independent of the number of time steps. This is in contrast to the construction of a finite MPS for N time steps which requires, depending on the approach, $O(N)$ [17] or $O(N^2)$ [19] SVD computations with a large bond dimension. An alternative method to construct an infinite MPS-IM within an auxiliary mode expansion [43] relies on infinite density matrix renormalization group, which is likewise computationally very demanding. With our algorithm, IM simulations are no longer limited by the compression step.

Owing to the semigroup structure, the SGIM is very well suited for computing dynamical properties of QIMs in the stationary regime. For this we first compute the stationary state corresponding to the leading eigenvector of the auxiliary dynamical map, either by Krylov methods [44] or by simply running the time evolution until convergence (power iteration). The stationary state is then used as initial condition to compute the real-time Green's function from time evolution, which can be Fourier transformed to obtain the spectral function. Since our method captures the full continuum bath, no postprocessing such as spectral broadening [45] is required.

Equilibrium benchmark—To benchmark our method we first consider the single impurity Anderson model (SIAM) [46] where spin-1/2 fermions ($\sigma = \uparrow, \downarrow$) interact on a single site with a Hubbard interaction in an otherwise noninteracting system. The impurity Hamiltonian for this model is given by

$$H_1 = U n_{\uparrow} n_{\downarrow} - \frac{U}{2} n_{\uparrow} - \frac{U}{2} n_{\downarrow}. \quad (7)$$

Equilibrium properties of the SIAM can be computed with a variety of established approaches [2,7,47], so excellent reference data is available.

In Fig. 2 we display the spectral function for a benchmark problem considered in Refs. [48,49]. The spectral function shows the Kondo resonance at low frequencies, Hubbard

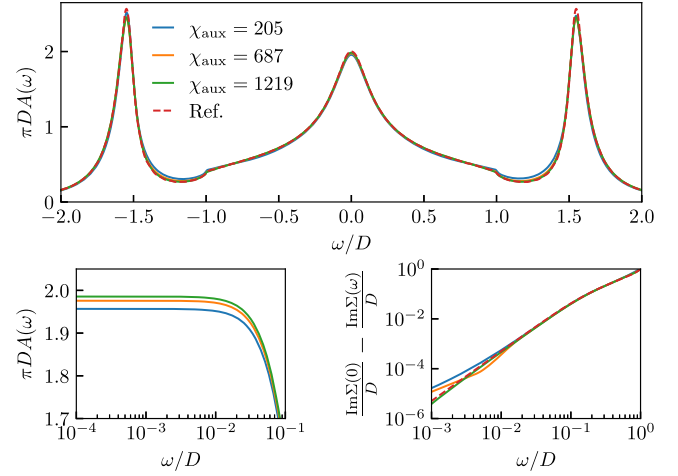


FIG. 2. Upper: spectral function $A(\omega)$ of the SIAM (7) with semicircular bath $J_{\uparrow/\downarrow}(\omega) = D/(2\pi)\sqrt{1 - \omega^2/D^2}$, $\mu = 0$, $\beta = 100/D$, and $U = 2D$. Lower left: spectral function at low frequencies. Friedel sum rule requires $\pi DA(0) = 2$ at $\beta = \infty$. Lower right: imaginary part of the self energy $\Sigma(\omega)$ at low frequencies (reference data from Ref. [49]). We used a Trotter time step $\delta t = 0.05/D$.

resonances at high frequencies, and the sharp band edges. The agreement with the reference is already very good at moderate auxiliary space dimensions χ_{aux} . Crucially, using higher accuracy representations we obtain excellent low-frequency resolution for the spectral function, recovering almost the entire spectral weight at $\omega = 0$, with an error below 1% for the Friedel sum rule $\pi DA(0) = 2$ [50]. The expected Fermi-liquid behavior of the self energy is also fulfilled up to small frequencies, with consistent improvement when the auxiliary space dimension is increased.

Quench and Kondo physics—We now turn to a non-equilibrium situation where dynamics is triggered by a quench from an initially polarized impurity. In Fig. 3 we consider a flatband environment particularly well suited to study Kondo physics. Real-time dynamics of this model was considered previously in Refs. [17,51] for limited evolution times. With our approach, we are now able to describe the spin relaxation for long times, while retaining high accuracy for the fast initial quench dynamics. To characterize the asymptotic decay, we can make use of semigroup formalism by extracting dynamical properties from the spectrum of our effective dynamical map. For example, we can extract the longest time scale of the problem directly as the logarithm of the next-to-leading eigenvalue. In the SIAM this time scale is the asymptotic spin relaxation rate Γ_D , which corresponds to the Kondo scale [52,53]. The next-to-leading eigenvalue, or spectral gap, can be computed efficiently using Krylov methods [44]. As displayed in Fig. 3 (inset), the extracted rate indeed predicts the slow spin relaxation at long times. We reproduce the exponential dependence of the relaxation rate on the interaction strength U , finding an excellent fit

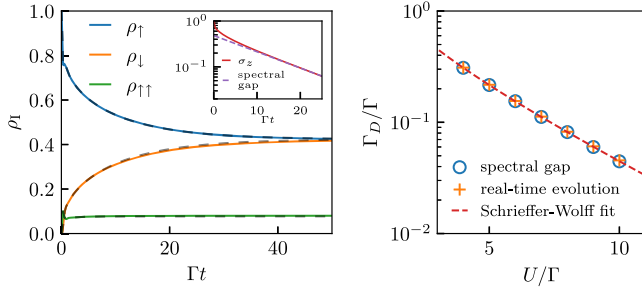


FIG. 3. SIAM dynamics for a flatband bath $J_{\uparrow/\downarrow}(\omega) = 2\Gamma/[2\pi(1 + e^{\nu(\omega-\omega_c)})(1 + e^{-\nu(\omega+\omega_c)})]$ with $\nu = \omega_c = 10\Gamma$, $\beta = 100/\Gamma$, $\mu = 0$. Left: quench from a polarized impurity with $U = 8\Gamma$. We achieve convergence with $\delta t = 0.025/\Gamma$, $\chi_{\text{aux}} = 305$ (dashed: $\chi_{\text{aux}} = 154$). Inset: asymptotic exponential decay of $\sigma_z = \rho_{\uparrow} - \rho_{\downarrow}$ compared with the prediction from the spectral gap. Right: spin relaxation rate Γ_D (computed via the spectral gap and real-time evolution) for different interaction strengths U and fit to the Schrieffer Wolff formula [2,49].

with the functional form $\Gamma_D(U) = \sqrt{a/U}e^{-bU}$ expected for the Kondo scale in the Schrieffer-Wolff limit [2,49].

Dissipative impurity model—A key advantage of IM approaches is their ability to seamlessly handle nonunitary impurity dynamics such as Markovian dissipation [54,55] without incurring additional numerical overhead. External dissipation creates a genuine nonequilibrium situation, opening new possibilities to engineer and explore unconventional quantum states [56]. For instance, recent works proposed a way to realize Kondo physics with strong local two-fermion losses [12,13], with local dynamics generated by the Lindbladian,

$$\mathcal{L}_I \rho = -i\epsilon_d[n_{\uparrow} + n_{\downarrow}, \rho] + \gamma L \rho L^{\dagger} - \frac{\gamma}{2}\{L^{\dagger}L, \rho\}, \quad (8)$$

where $L = d_{\uparrow}d_{\downarrow}$. The corresponding local channel is given by $\mathcal{C}_1[\delta t/2] = e^{\mathcal{L}_I \delta t/2}$. In the limit $\gamma \rightarrow \infty$ a double occupancy of the impurity is completely suppressed, and the model reduces to the Anderson impurity model with infinite repulsion, a model known to exhibit Kondo physics. For finite γ , the emergence of the Kondo effect has been explored with adiabatic elimination [12] and a multi-Gaussian variational ansatz [13]. Here, we compute the *exact* spectral function of the model for different values of γ with a flatband bath, shown in Fig. 4. Crucially, our method can cover the full crossover at all frequencies without restrictive approximations. At small γ the spectral function is close to the noninteracting case, with a single peak centered at the impurity energy ϵ_d , broadened by the interaction with the bath. As the loss rate is increased, a sharp Kondo peak develops at $\mu = 0$, corresponding to the slow spin relaxation also present in the unitary SIAM (Fig. 3).

Conclusions—The SGIM construction introduced here is an efficient approach to studying out-of-equilibrium QIMs, giving access to long evolution times with low

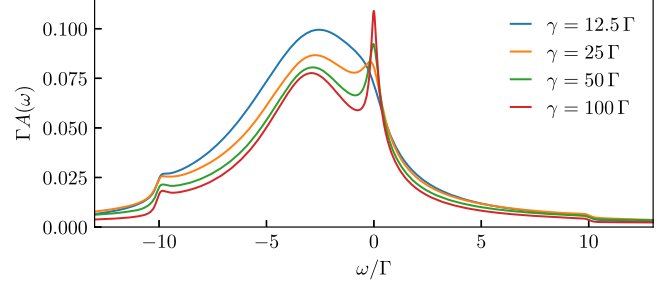


FIG. 4. Spectral function for the dissipative SIAM with the same bath used in Fig. 3 and on-site energy $\epsilon_d = -3\Gamma$. As the loss rate γ is increased, a sharp Kondo peak appears at $\mu = 0$. For these computations we used a Trotter time step of $\delta t = 0.002/\Gamma$ and an auxiliary dimension of $\chi_{\text{aux}} = 239$.

computational demands. The underlying *temporal* MPS representation provides a significantly more effective compression of the environment compared to direct time evolution of QIMs via chain mappings [57] in combination with regular spatial MPS [58–61], which requires large bond dimensions to achieve convergence at low frequencies [49]. In the future, our method can be applied to a wide range of problems. In particular, this includes transport phenomena in strongly correlated systems, where real-time dynamics are required to compute nonequilibrium steady states [61]. Further, the IM framework can be used directly for driven impurities beyond the high-frequency limit [62], as well as for feedback and optimal control problems [63] and as impurity solver for nonequilibrium DMFT [8,64]. Finally, the efficient compressed representation of environments could offer a favorable scalability for numerical simulations of multiorbital impurity problems, which remains a central challenge in multiorbital DMFT.

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Data availability—The data that support the findings of this article are openly available [65], embargo periods may apply.

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