Open System Tensor Networks and Kramers’ Crossover for Quantum Transport

Gabriela Wójtowicz,1 Justin E. Elenewski,2,3 Marek M. Rams,1,* and Michael Zwolak2,*

1Jagiellonian University, Marian Smoluchowski Institute of Physics, Łojasiewicza 11, 30-348 Kraków, Poland
2Biophysics Group, Microsystems and Nanotechnology Division, Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD, USA
3Maryland Nanocenter, University of Maryland, College Park, MD, USA

Tensor networks are a powerful tool for many-body ground states with limited entanglement. These methods can nonetheless fail for certain time-dependent processes — such as quantum transport or quenches — where entanglement growth is linear in time. Matrix product state decompositions of the resulting out-of-equilibrium states require a bond dimension that grows exponentially, imposing a hard limit on simulation timescales. However, in the case of transport, if the reservoir modes of a closed system are arranged according to their scattering structure, the entanglement growth can be made logarithmic. Here, we extend this ansatz to open systems via extended reservoirs that have explicit relaxation. This enables transport calculations that can access true steady-states, time-dynamics, and periodic driving. We demonstrate the approach by calculating the transport characteristics of an open, interacting system. These results open a path to rigorous, many-body transport calculations.

Many-body quantum systems are characterized by complex ground and dynamic states, yielding emergent phenomena that span from superconductivity to exotic magnetic phases. Furthermore, for non-equilibrium properties, systematic excitations can yield a response that diverges markedly from ground state behavior [1]. The theoretical treatment of many-body systems is thus challenging, as analytical solutions are difficult to derive for most problems of interest. This situation has driven the development of numerical methods such as quantum Monte Carlo [2,3], dynamical mean field theory (DMFT) [4,5], and tensor network approaches [6–10], which now lie at the forefront of many-body theory. Among these, tensor networks leverage the structure of correlations and entanglement to provide a local, numerically controllable description of many-body systems — limiting computation to a submanifold of Hilbert space that captures the underlying physical characteristics.

While tensor networks methods, such as matrix product states (MPS), have proven extremely successful for correlated ground states, their application to time-dependent behavior can be stifled by a rapid growth of entropy in time [11,12]. In the context of quantum transport, this is due to scattering at impurity sites, which generates entangled electron–hole pairs in the adjacent contact regions [13]. For a pair of electrodes, L and R, held at a bias μ, the attempt frequency for scattering events is μ/2π [14]. The bipartite entanglement entropy S between them will then grow linearly as $S \approx \log D$. Increasing the simulation duration requires an exponentially larger D and thus exponentially larger computational requirements (see Ref. [13]).

Despite its physical origin, this exponential barrier can be mitigated by working in a basis that reflects the natural scattering structure of current–carrying states [13]: An incoming particle of frequency ωk will be transmitted from one reservoir, through the system, and into an outgoing state of the same frequency (up to some characteristic spread in energy). Entanglement is thus highly local in the energy domain, provided that the (nearly) iso–energetic modes in L and R are arranged adjacent to

---

* marek.rams@uj.edu.pl
  * mpz@nist.gov
each other on a 1D lattice, a mixed energy–spatial basis that preserves the structure of correlations. We recently leveraged this observation to develop a time-dependent MPS approach for closed systems. This approach shifts the temporal growth of entanglement from linear to logarithmic [13]. The energy basis, alternatively known in literature as the ‘star–geometry’, has been employed in MPS impurity solvers for non-equilibrium DMFT [18,19] due to the smaller entanglement present, and in the study of quenched and Floquet states in the Anderson impurity model [20,21], where the latter work also found a large suppression of entanglement when modes were reordered [21]. Nonetheless, our method is unique in pairing the reservoir modes according to the actual entanglement structure and, so far, giving the only demonstration of accurate, extensive simulations (in reservoir size and time) of traditionally entanglement-limited non-equilibrium problems.

Here, we demonstrate that this mixed energy–spatial basis gives a framework for open quantum system MPS simulations where implicit reservoirs offset carrier depletion in the lead/reservoir regions \(\mathcal{L}\) and \(\mathcal{R}\) (Fig. [1]). This method is numerically stable in the physical regime that reflects the transport properties in the infinite reservoir limit [22,23]. We apply the approach to describe transport through a two-site, interacting many-body impurity, demonstrating applicability to a nontrivial example. This approach provides a platform for examining real steady states and will enable problems with long timescales (e.g., due to many-body relaxation) to be controllably studied.

Quantum transport is typically examined via a composite system that contains non–interacting left (\(\mathcal{L}\)) and right (\(\mathcal{R}\)) reservoirs that drive transport through an ‘impurity’ region (the system \(S\)) [24], see Fig. [1]. The Hamiltonian takes the form

\[
H = H_S + H_L + H_R + H_I,
\]

where \(H_S\) is the (many–body) Hamiltonian for \(S\), \(H_L\)\slash{}\(H_R\) = \(\sum_{k \in \mathcal{L}\slash{}\mathcal{R}} \hbar \omega_k a_k^\dagger a_k\) are the explicit reservoir Hamiltonians, and \(H_I = \sum_{k \in \mathcal{L}\mathcal{R}} \sum_{i \in S} \hbar v_{ki} (c_i^\dagger a_k + a_k^\dagger c_i)\) is the interaction Hamiltonian that couples \(S\) to \(\mathcal{LR}\). The \(c_i^\dagger (c_i)\) and \(a_k^\dagger (a_k)\) are fermionic creation (annihilation) operators in \(S\) and \(\mathcal{LR}\), respectively. We take the index \(k\) to implicitly include all relevant reservoir labels (state, spin, etc.), while \(\omega_k\) and \(v_{ki}\) are the reservoir mode frequencies and system–reservoir coupling frequencies.

If there are an infinite number of explicit reservoir modes in each reservoir, then a steady state will form [24]. However, only a finite reservoir can be simulated. While this reservoir may be large, it will never give a true steady state, which will make some parameter regimes and protocols (e.g., dynamic driving) difficult or inaccessible. To rectify this situation, implicit reservoirs can relax the reservoir modes to their equilibrium distribution at different chemical potentials [25]. This requires an evolution for the density matrix \(\rho\) for the \(\mathcal{LSR}\) composite system. A particularly useful equation of motion that includes relaxation is the Markovian master equation

\[
\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \sum_k \gamma_{k+} \left( c_k^\dagger \rho c_k - \frac{1}{2} \{ c_k^\dagger c_k, \rho \} \right) + \sum_k \gamma_{k-} \left( c_k \rho c_k^\dagger - \frac{1}{2} \{ c_k c_k^\dagger, \rho \} \right), \tag{2}
\]

where \{·,·\} is the anticommutator. The first term gives the Liouville–von Neumann evolution of \(\rho\) under a Hamiltonian \(H\), while the second and third term give injection and depletion of the modes \(k\) at a rate \(\gamma_{k+}\) and \(\gamma_{k-}\), respectively. To ensure that the reservoir modes relax to equilibrium in the absence of \(S\), these rates are \(\gamma_{k+} \equiv \gamma f^\alpha(\omega_k)\) and \(\gamma_{k-} \equiv \gamma [1 - f^\alpha(\omega_k)]\), where \(f^\alpha(\omega_k)\) is the Fermi–Dirac distribution in the \(\alpha \in \{L, R\}\) reservoir (in this case, \(\gamma\) is the sole parameter controlling relaxation but it can easily be made \(k\)-dependent).

When the reservoirs are held at different chemical potentials \(\mu_\alpha\) (and/or temperatures), the bias \(\mu = \mu_L - \mu_R\) will drive a current. We refer to \(\mathcal{L}\) and \(\mathcal{R}\), the reservoir modes that are contained explicitly in the dynamics, as the extended reservoirs. This particular Markovian master equation has been widely employed in various guises, see Ref. [23] to describe transport in non–interacting systems [22,23,26,35] and it follows naturally from the generic approach (explicit reservoir/bath states plus Markovian broadening to represent the spectral function) suggested in Ref. [36] for open system dynamics. It is provably correct in both the non–interacting and many-body cases [22,23], and requires \(\gamma\) (and the extended reservoir size) to be in a certain, physical regime [22,23], otherwise the Markovian relaxation will give artifacts not representative of transport or even a proper equilibrium. A related approach within dynamical mean-field theory uses an equation similar to Eq. (2), but optimizing the relaxation (including intermode relaxation) to represent the reservoir spectral function [37,40]. We will examine intermode relaxation in a later contribution. While it can more effectively represent the spectral function, it increases the computational cost of the MPS simulation.

We implement this framework within an MPS approach. While a variety of tensor network techniques exist [41,43], we solve Eq. (2) with the time-dependent variational principle (TDVP) [41,43], where the density matrix is vectorized to represent it within an MPS [46]. TDVP is highly effective for this particular case, as it can accommodate direct time evolution for any Hamiltonian or Lindbladian that may be represented as a matrix product operator (MPO), and the MPO in the mixed-basis transport setup (Fig. [1]) has a small, fixed bond dimension. We note that time-evolving block decimation may also be quite effective [47] and we leave open the question of what is the optimal implementation (via purification schemes, etc. [48]).

Since our approach works with the energy basis of the extended reservoirs, there is no requirement on the spatial dimensionality of the reservoirs: They can be of ar-
bitary dimension, have long-range hopping both within the reservoirs and to \( \mathcal{S} \) (when to multiple sites in \( \mathcal{S} \), a larger MPO is necessary). The only requirements are that the reservoirs are non-interacting and there is not a direct interaction between left and right regions (these can be relaxed, albeit with a loss of efficiency). As an example, we will work with a 1D lattice with nearest neighbor hopping, \( H_{L/R} = \hbar \omega_0 \sum_{j \in L/R} (c_j^\dagger c_{j+1} + \text{h.c.}) \), transformed into its energy basis for \( L \) and \( R \). The energy basis for each extended reservoir separately is given by \( a_k = \sum_{j \in L} U_{kj}^i c_j \), with the canonical transformation \( \mathcal{U}_{kj} = \sqrt{2/(N+1)} \sin(jk\pi/(N+1)) \), frequencies \( \omega_k = 2\omega_0 \cos(k\pi/(N+1)) \), and couplings \( v_k = vU_{kj}^L \). In this example setup, each of the \( N \) reservoir modes in the energy basis couple to the system through a single contact site in real space, located at either end of the system, with coupling constant \( v \) to \( \mathcal{S} \). We calculate the current as \( I = \langle I_{LS} + I_{SR} \rangle / 3 \), where \( I_{ij} \) flows from \( i \) to \( j \) (e.g., at the \( LS \) interface, \( I_{LS}(t) = -4 \sum_{k \in L} v_k \text{Im}(a_k^\dagger c_k) \) where an extra factor of two is included here to account for spin). All three should be the same in the steady state and their deviation gives a measure of simulation error, see Fig. 2. Since the bias is maintained by the implicit reservoirs, i.e., via the Lindblad terms in Eq. (2), the applied bias is not in \( H_{L/R} \). Thus, the mixed basis arranges the modes in \( L \) and \( R \) adjacent to each other according to their energies in the isolated reservoir Hamiltonians (see Fig. 1). The initial state in all simulations is the steady state of Eq. (2) without \( H_T \) in \( H \).

Our TDVP–based approach enforces operator Hermiticity during MPS calculations, explicitly using real arithmetic and a Hermitian operator basis to expand the MPS. Strong correlations between impurity modes substantially increase the required bond dimension, and thus we merge these into a single state. During TDVP calculations, we restrict the MPS bond dimension \( D_n \) at all cuts \( n \) to lie below a maximal value \( D_n \leq D_{\text{max}} \). To account for inhomogeneous nature of the setup, and small entanglement outside of the bias window, we truncate all the singular values below a given threshold \( s_{\text{min}} \). In practice, we take \( s_{\text{min}} = 10^{-6} \), which is set small enough not to influence the accuracy of the results (which is predominantly controlled by \( D_{\text{max}} \)).

As a general rule, entanglement increases the bond dimension \( D \) required to meet a given convergence threshold, limiting the quality of MPS calculations. This does not, however, restrict the simulation times accessible through our computational approach, as depicted in Fig. 2. In this case, the transient current \( I(t) \) rapidly reaches a steady–state at modest reservoir relaxation \( \gamma \), in tight correspondence with propagation of the exact correlation matrix for a non–interacting system. The time to do so can also increase with the many–body coupling strength (as we will discuss). However, at a given coupling, convergence is ultimately mediated by the reservoir relaxation time \( \gamma^{-1} \), which sets the scale to reach the steady state.

Although convergence is sluggish for weak relaxation (small \( \gamma \)) and rapid for strong relaxation (large \( \gamma \)), the choice of this parameter is not arbitrary – it must be judiciously chosen to give physical behavior [23]. Nonethe-

![FIG. 2. Non–interacting benchmark simulations. a. Transient current for a non–interacting, spinless, two-site system \( H_S = \hbar \omega_0 (c_1^\dagger c_1 + c_1 c_2 + \text{h.c.}) \). Data are given for two system-site couplings \( v_S \) at fixed relaxation \( \gamma = 0.1\omega_0 \). Mixed basis MPS dynamics (black, dashed line) match the exact result (solid, colored lines) even at a modest upper limit on the bond dimension \( D_{\text{max}} \). b. Steady–state current \( I(t = \infty) \) versus \( \gamma \) from diagonalizing the exact Lindbladian (solid lines) and the long–time limit of MPS propagation (data points), up to time \( t_{\text{max}} \). Exact and MPS data compare well, with deviations only in the small \( \gamma \) regime. c. Relative deviation \( (I_{\text{MPS}} - I_{\text{Corr}})/I_{\text{Corr}} \) between exact and MPS results as a function of \( D_{\text{max}} \) at \( \gamma = 0.1\omega_0 \). All calculations have a bias of \( \mu = \omega_0/2 \) across implicit reservoirs of \( N = 128 \) modes, starting from Fermi–Dirac occupations \( (k_B T = \hbar \omega_0/40) \), a system frequency \( \omega_S = 0.1\omega_0 \) and a system–reservoir coupling \( v = \omega_0/2 \) (between \( L \) and site 1 of \( \mathcal{S} \), and \( R \) and site 2). In a and b, the MPS bond dimension may grow up to \( D_{\text{max}} = 256 \) during time evolution. The steady state current from MPS simulations is taken as an average over last \( \Delta t = t_{\text{max}} / 10 \). The error bars are \( \pm \sigma \) with \( \sigma_r^2 = \sigma_1^2 + \sigma_2^2 \), where \( \sigma_1 \) is the fluctuations of \( I \) in \( \Delta t \) and \( \sigma_2^2 = \sum_{i} (|I_i - I|)^2/3 \) is the mismatch of currents at different interfaces \( i \in \{LS, SS, RR\} \). The latter gives a measure of the error from truncating the MPS to finite bond dimension \( D \), which, for the mismatch values here, is likely the bulk of the finite-\( D \) contribution to the error.
less, the long simulation times required at small $\gamma$ limit the ability to exhaustively map these transport regimes through long–timescale simulations. To partially circumvent this limitation, we introduce a protocol in which the terminal MPS state from a given TDVP evolution is used as the starting state for a successively smaller relaxation $\gamma_m$. At each stage of this process, we adopt a timestep $\Delta t_m = \min[1, 1/\gamma_m]$ and maximal simulation time $t_{\text{max}} = 10\Delta t_m \max[1/\gamma_m, 100]$ which are defined in terms of $\gamma_m$, accelerating convergence to the steady–state. Alternatively, the steady state could be targeted directly with the density matrix renormalization group approach [49].

The results of the open system approach depend on the relaxation strength $\gamma$, see Fig. 2b. The steady state current has three qualitatively distinct regimes [22, 23, 34]: It will initially increase linearly with $\gamma$, then plateau, and then decrease as $1/\gamma$ [50]. At small $\gamma$, the ‘replenishing’ of particles controls the current, and thus the current is proportional to $\gamma$. At large $\gamma$, the development of coherence — a necessary condition for current to flow — is suppressed by strong relaxation, resulting in the $1/\gamma$ behavior. Only in between — the plateau regime — can the current represent the physical scenario of interest. These regimes are well–understood, see Ref. [22, 23] and [34] and also occur in thermal transport [51–53]. They are a simulation analog of Kramers problem in solution–phase chemical reaction rates [54].

There are additional requirements to properly represent transport in the plateau regime. Namely, Markovian relaxation is not inherently a physical process [22, 23], as it occupies modes according to their energies in isolation rather than properly broadened energies due to the contact with the implicit reservoirs. Thus, $\gamma$ needs to be sufficiently lower than the broadening of the occupation, $\gamma \ll k_B T/\hbar$. The relaxation must also be strong enough to be on the plateau, which occurs at $\gamma \approx W/N$, where $W$ is the reservoir bandwidth ($W = 4\omega_0$ in our example). This requires that $N \approx hW/k_B T$ for physical simulations [22, 23]. Thus, for ideal values we would consider $N > 160$ and $\gamma < \omega_0/40$ (having in mind characteristic $\omega_0 \approx 1$ eV and room temperature). In practice, we have taken $N = 128$ and $\gamma = \omega_0/10$, which is on the plateau but slightly outside of the physical regime, and computed errors due to the variation of $N$ and $\gamma$. The MPS simulations work very well from large $\gamma$ down to intermediate $\gamma$. As $\gamma$ goes off the plateau ($\gamma < W/N$), long-time coherence of particles flowing back and forth in the LSR system make MPS simulations difficult (to which we will return). In the plateau regime (where the duration of simulation has little effect), the error arising from MPS truncation decays steadily with $D$ (the exact solution will, of course, be reached if $D \to \infty$), but with some non–monotonic structure related to the interplay of multiple error sources.

The robust performance of our MPS simulations for intermediate to large $\gamma$ is reflected in the mutual information across a bipartite split of the lattice, which we adopt as a measure of correlation since we have a globally mixed state (as taken in either the spatial basis or the mixed basis of Fig. 3b). Upon splitting the lattice into subsystems $A$ and $B$, the mutual information is $I(A : B) = S_A + S_B - S_{AB}$, where $S_A = -\text{tr}\rho_A \log\rho_A$ is the von Neumann entropy of subsystem $A$ with density matrix $\rho_A$. As a reference point, Figure 3c shows the mutual information when a split is taken in the spatial basis of a non-interacting system. Substantial correlations exist among states in $\mathcal{L}$ and $\mathcal{R}$ from the outset — a consequence of the initial state distributions. Furthermore, during time evolution, we observe a light–cone like spread of correlations from $\mathcal{S}$, albeit at a lower magnitude than for the closed system [13]. These factors place a computational limit on MPS evolution. Figure 3c presents the same profile for the mixed basis, where the lattice is now arranged with state above the system energy on the right and below the system energy on the left (isoenergetic pairs are placed side–by–side, and state

**FIG. 3. Mutual information.** a. Mutual information versus time $t$ and cut location $n$ in the spatial basis, where states in $\mathcal{L}$ are on the left and those in $\mathcal{R}$ are on the right, for the system in Fig. 2 with $v_b = (1 + \sqrt{2})v^2/\omega_0$ and $\gamma = 0.1\omega_0$. b. The same as a but with a mixed basis. In this case, states on the left have an energy below 0, while those on the right above 0, with sites in $\mathcal{S}$ put in the middle. The mutual information is highly suppressed and only located in the bias window. c. The mutual information versus $\gamma$ and cut location for the steady state in the mixed basis. The physical regime (generally the small $\gamma$ side of the plateau) has the largest mutual information, as the relaxation interferes least with particle transport. Oscillations in $I(n)$ reflect the mixed–basis pairing, increasing when a cut is taken between paired current–carrying states and decreasing between pairs. We merge the states in $\mathcal{S}$ for all cases, thus no bipartite cut through the system is present. The bias window ($\pm \mu/2$) is shown for reference.
energies increase with increasing \( n \). Correlations (except for a very small spread in energy) are localized to modes in the bias window and highly suppressed, as seen in Fig. 3b. This underscores the physics of the nonequilibrium state, where correlations are generated between pairs of current–carrying modes in the bias window.

The mutual information also depends on the relaxation strength \( \gamma \), as seen in Fig. 3a, for the steady state. When \( \gamma \) is very large, correlations are highly suppressed, since the \( LSR \) composite system remains near a product state with \( L \) and \( R \) close to their isolated equilibrium state (the current is suppressed as \( 1/\gamma \), prohibiting the generation of correlated pairs across \( L \) and \( R \)). The contribution from entangled, current–carrying modes becomes apparent on the plateau, where the mutual information becomes larger and more broadly distributed among reservoir modes. Furthermore, the largest mutual information coincides with physical region of \( \gamma \), where the current corresponds to the Landauer limit. The MPS simulations become more difficult in the physical regime, although they remain modest.

The simulations become most difficult when \( \gamma \) is off the plateau (\( \gamma < W/N \)). This is likely due to factors not captured by the mutual information. The correlations are more moderate than in the physical regime. However, relative to their maximum, which occurs in the bias window, the correlations are more diffuse. Moreover, the small \( \gamma \) regime is also difficult due to the timescales needed to reach the steady state and due to the small current being buried in the background (i.e., difficult to extract without a very large \( D \)). For the simulations here, though, the truncation gives the major error in the state for the small \( \gamma \) regime. Since this regime is not of practical interest, we forgo a detailed analysis of its behavior.

As a final — and nontrivial — demonstration, we give the first instance of the Kramers turnover for a many–body, quantum system. We examine the same two–site impurity but with a nearest–neighbor, many–body interaction \( U n_1 n_2 \) in \( S \), where \( n_i \) is the number operator at site \( i \). Figure 4a shows \( I(t) \) for several values of the interaction strength \( U \). After a short transient regime, tied to both the intrinsic dynamics [55] and \( \gamma \)–dependent relaxation, the current rapidly converges to its steady state. While the timescale for relaxation increases with a progressively more negative \( U \), a higher bond dimension is not required for convergence. Figure 4b shows the steady state current versus \( \gamma \). The turnover behavior is similar to the non–interacting system, as expected from its physical origin involving a transition from \( \gamma \)–limited current to plateau to coherence–suppressed transport behavior. Nonetheless, the many–body interaction does influence the convergence to a smooth plateau. Moreover, the small \( \gamma \) regime remains difficult for MPS, but does take on a linear relationship, \( I \propto \gamma \).

For this many–body model, the transport characteristics exhibit non–monotonic behavior versus \( U \). In the non–interacting system, there are two eigenstates the isolated \( S \) at \( \pm v_S \). When \( U \) is sufficiently large and negative, there is a bound state of two fermions in \( S \) lying outside the bias window, blocking the current (i.e., it will decay to zero as \( U \to \infty \)). When \( U \) approaches zero, but is still less than zero, the system mode at \( -v_S \) remains nearly occupied and the higher energy mode is effectively pulled down in energy by the many–body interaction. Ne-
glecting the lower energy mode, other than than a mean-field effect on the higher energy mode, gives a peak current at $U = -4v_S/3$. This is in reasonable agreement with the full many-body result. As $U$ becomes repulsive, the system will begin to have only a single particle present. Nevertheless, this can sustain a finite current (half the value of the $U = 0$ current) even as $U \to \infty$, giving rise to the asymmetry between very attractive and very repulsive interactions.

While MPS approaches have been previously employed to study transport in interacting (spatially) 1D models in real-time \cite{11, 3} or in linear response via an equilibrium correlation function \cite{66, 67}, the mixed-basis has eliminated constraints on the reachable time- and spatial-scales \cite{13}. The open system approach demonstrated here enables a direct computation of steady-state currents, allowing it to be treated in a manner analogous to ground states (i.e., finding a stationary state), and makes use of the mixed-basis to limit correlations that would otherwise make the simulations prohibitive. This approach will also be useful for finding Floquet states and the effect of artificial gauge fields, examining time-dependent processes that perturb the system around its stationary state, and handling transport when long timescales appear (e.g., due to many-body interactions), as well as giving the right framework for coarse-graining reservoir modes \cite{68}. It may also help in solving other boundary driven problems (e.g., 1D lattices driven by Markovian processes only at the ends). Overall, the approach will permit the accurate simulation of challenging many-body systems, ones where larger and more complex interacting impurities give rise to intricate behavior.

J. E. E. acknowledges support under the Cooperative Research Agreement between the University of Maryland and the National Institute for Standards and Technology Physical Measurement Laboratory, Award 70NANB14H209, through the University of Maryland. We acknowledges support by National Science Center (NCN), Poland under Projects No. 2016/23/B/ST3/00830 (GW) and No. 2016/23/D/ST3/00384 (MMR).

\begin{thebibliography}{99}
\bibitem{1} J. Eisert, M. Friesdorf, and C. Gogolin, Nature Phys. \textbf{11}, 124 (2015).
\bibitem{2} W. M. C. Foulkes, L. Mitra, R. J. Needs, and G. Rajagopal, Rev. Mod. Phys. \textbf{73}, 33 (2001).
\bibitem{3} L. K. Wagner and D. M. Ceperley, Rep. Prog. Physics \textbf{79}, 1 (2016).
\bibitem{4} A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys \textbf{68}, 13 (1996).
\bibitem{5} G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev. Mod. Phys. \textbf{78}, 865 (2006).
\bibitem{6} F. Verstraete, V. Murg, and J. I. Cirac, Adv. Phys. \textbf{57}, 143 (2008).
\bibitem{7} J. I. Cirac and F. Verstraete, J. Phys. A: Math. Theor. \textbf{42}, 504004 (2009).
\bibitem{8} J. Haegeaman and F. Verstraete, Annu. Rev. Cond. Mat. Phys. \textbf{8}, 355 (2017).
\bibitem{9} S. Ran, E. Tirrito, C. Peng, X. Chen, G. Su, and M. Lewenstein, arxiv:1708.09213.
\bibitem{10} R. Orús, arXiv:1812.04011.
\bibitem{11} N. Schuch, M. M. Wolf, K. G. H. Vollbrecht, and J. I. Cirac, New J. Phys. \textbf{10}, 033032 (2008).
\bibitem{12} J. Eisert, Modeling and Simulation \textbf{3}, 520 (2013), arXiv:1308.3318.
\bibitem{13} M. M. Rams and M. Zwolak, arXiv:1904.12793.
\bibitem{14} L. S. Levitov and G. B. Lesovik, JETP Letters \textbf{58}, 230 (1993).
\bibitem{15} C. J. W. Beenakker, in Proc. Int. School Phys. E. Fermi, Vol. 162 (IOS Press, Amsterdam, 2006) p. 307.
\bibitem{16} I. Klich and L. Levitov, Phys. Rev. Lett. \textbf{102}, 100502 (2009).
\bibitem{17} C.-C. Chien, M. Di Ventra, and M. Zwolak, Phys. Rev. A \textbf{90}, 023624 (2014).
\bibitem{18} F. A. Wolf, T. P. McCulloch, and U. Schollwöck, Phys. Rev. B \textbf{90}, 235131 (2014).
\bibitem{19} D. Bauernfeind, M. Zingl, R. Triebel, M. Aichhorn, and H. G. Evertz, Phys. Rev. X \textbf{7}, 031013 (2017).
\bibitem{20} Z. He and A. J. Millis, Phys. Rev. B \textbf{96}, 085107 (2017).
\bibitem{21} Z. He and A. J. Millis, Phys. Rev. B \textbf{99}, 205138 (2019).
\bibitem{22} D. Gruss, K. A. Velizhanin, and M. Zwolak, Sci. Rep. \textbf{6}, 24514 (2016).
\bibitem{23} J. E. Elenewski, D. Gruss, and M. Zwolak, J. Chem. Phys. \textbf{147}, 151101 (2017).
\bibitem{24} A.-P. Jauho, N. S. Wingreen, and Y. Meir, Phys. Rev. B \textbf{50}, 5528 (1994).
\bibitem{25} There will, though, still be a trade-off of relaxation time and accurate representation of long-time processes.
\bibitem{26} Y. Dubi and M. DiVentra, Nano Lett. \textbf{9}, 97 (2009).
\bibitem{27} A. A. Dzhioev and D. S. Kosov, J. Chem. Phys. \textbf{134}, 044121 (2011).
\bibitem{28} T. Zelovich, L. Kronik, and O. Hod, J. Chem. Theory Comput. \textbf{10}, 2927 (2014).
\bibitem{29} T. Zelovich, L. Kronik, and O. Hod, J. Chem. Theory Comput. \textbf{11}, 4861 (2015).
\bibitem{30} T. Zelovich, L. Kronik, and O. Hod, J. Phys. Chem. C \textbf{120}, 15052 (2016).
\bibitem{31} T. Zelovich, T. Hansen, Z.-F. Liu, J. B. Neaton, L. Kronik, and O. Hod, J. Chem. Phys. \textbf{146}, 092331 (2017).
\bibitem{32} S. Ajisaka, B. Žukovič, and Y. Dubi, Sci. Rep. \textbf{5}, 8312 (2015).
\bibitem{33} O. Hod, C. A. Rodriguez-Rosario, T. Zelovich, and T. Frauenheim, J. Phys. Chem. A \textbf{120}, 3278 (2016).
\bibitem{34} D. Gruss, A. Smolyanitsky, and M. Zwolak, J. Chem. Phys. \textbf{147}, 141102 (2017).
\bibitem{35} D. Gruss, A. Smolyanitsky, and M. Zwolak, arxiv:1804.02701.
\bibitem{36} M. Zwolak, \textit{Dynamics and Simulation of Open Quantum Systems}, Ph.D. thesis (2008).
\bibitem{37} E. Arrigoni, M. Knap, and W. von der Linden, Phys. Rev. Lett. \textbf{110}, 086403 (2013).
\bibitem{38} A. Dorda, M. Nuss, W. von der Linden, and E. Arrigoni, Phys. Rev. B \textbf{89}, 165105 (2014).
\bibitem{39} A. Dorda, M. Ganahl, H. G. Evertz, W. von der Linden,
and E. Arrigoni, Phys. Rev. B 92, 125145 (2015).
[40] A. Dorda, M. Sorantin, W. v. d. Linden, and E. Arrigoni, New J. Phys. 19, 063005 (2017).
[41] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003); 93, 040502 (2004).
[42] P. Schmitteckert, Phys. Rev. B 70, 121302 (2004).
[43] M. P. Zaletel, R. S. K. Mong, C. Karrasch, J. E. Moore, and F. Pollmann, Phys. Rev. B 91, 165112 (2015).
[44] J. Haegeman, J. I. Cirac, T. J. Osborn, I. Pizorn, H. Verschelde, and F. Verstraete, Phys. Rev. Lett. 107, 070601 (2011).
[45] J. Haegeman, C. Lubich, I. Oseledets, B. Vandereycken, and F. Verstraete, Phys. Rev. B 94, 165116 (2016).
[46] M. Zwolak and G. Vidal, Phys. Rev. Lett. 93, 207205 (2004).
[47] D. Bauernfeind, M. Aichhorn, and H. G. Evertz, arXiv:1906.09077 (2019).
[48] D. Jaschke, S. Montangero, and L. D. Carr, Quantum Sci. Technol. 4, 013001 (2018).
[49] J. Cui, J. I. Cirac, and M. C. Bañuls, Phys. Rev. Lett. 114, 220601 (2015).
[50] There are some exceptions to the γ and 1/γ regimes, depending on the presence of energy gaps and symmetries, see Ref. [51] for a discussion of some of these.
[51] K. A. Velizhanin, C. C. Chien, Y. Dubi, and M. Zwolak, Phys. Rev. E 83, 050906 (2011).
[52] C. C. Chien, K. A. Velizhanin, Y. Dubi, and M. Zwolak, Nanotechnology 34, 095704 (2013).
[53] K. A. Velizhanin, S. Sahu, C.-C. Chien, Y. Dubi, and M. Zwolak, Sci. Rep. 5, 17506 (2015).
[54] H. A. Kramers, Physica 7, 284 (1940).
[55] M. Zwolak, J. Chem. Phys. 149, 241102 (2018).
[56] M. A. Cazalilla and J. B. Marston, Phys. Rev. Lett. 88, 256403 (2002).
[57] M. Zwolak and G. Vidal, Phys. Rev. Lett. 93, 207205 (2004).
[58] K. A. Al-Hassanieh, A. E. Feiguin, J. A. Riera, C. A. Bsser, and E. Dagotto, Phys. Rev. B 73, 195304 (2006).
[59] P. Schmitteckert and G. Schneider, in High Performance Computing in Science and Engineering, edited by W. E. Nagel, W. Jäger, and M. Resch (Springer, Berlin, 2006) pp. 113–126.
[60] G. Schneider and P. Schmitteckert, arXiv:cond-mat/0601389 (2006).
[61] L. G. G. V. Dias da Silva, F. Heidrich-Meisner, A. E. Feiguin, C. A. Bsser, G. B. Martins, E. V. Anda, and E. Dagotto, Phys. Rev. B 78, 195317 (2008).
[62] F. Heidrich-Meisner, A. E. Feiguin, and E. Dagotto, Phys. Rev. B 79, 235336 (2009).
[63] A. Branschdel, G. Schneider, and P. Schmitteckert, Ann. Phys. (Berlin) 522, 657 (2010).
[64] C.-C. Chien, D. Gruss, M. Di Ventra, and M. Zwolak, New J. Phys. 15, 063026 (2013).
[65] D. Gruss, C.-C. Chien, J. T. Barreiro, M. D. Ventra, and M. Zwolak, New J. Phys. 20, 115005 (2018).
[66] D. Bohr, P. Schmitteckert, and P. Wölfle, Europhys. Lett. 73, 246 (2006).
[67] D. Bohr and P. Schmitteckert, Phys. Rev. B 75, 241103 (2007).
[68] M. Zwolak, J. Chem. Phys. 129, 101101 (2008).