Dynamical simulation of integrable and non-integrable models in the Heisenberg picture

Dominik Muth, Razmik G. Unanyan, and Michael Fleischhauer

1 Fachbereich Physik und Forschungszentrum OPTIMAS, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany
2 Graduate School Materials Science in Mainz, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany

(Dated: December 22, 2010)

The numerical simulation of quantum many-body dynamics is typically limited by the linear growth of entanglement with time. Recently numerical studies have shown, however, that for 1D Bethe-integrable models the simulation of local operators in the Heisenberg picture can be efficient as the corresponding operator-space entanglement grows only logarithmically. Using the spin-1/2 XX chain as generic example of an integrable model that can be mapped to free fermions, we here provide a simple explanation for this. We show furthermore that the same reduction of complexity applies to operators that have a high-temperature auto correlation function which decays slower than exponential, i.e., with a power law. This is amongst others the case for models where the Blombergen-De Gennes conjecture of high-temperature diffusive dynamics holds. Thus efficient simulability may already be implied by a single conservation law (like that of total magnetization), as we will illustrate numerically for the spin-1 XXZ model.

PACS numbers: 02.70.-c, 67.80.dk, 75.10.Pq

White’s Density Matrix Renormalization Group (DMRG) and its more recent generalizations to time evolution using the Time Evolving Block Decimation (TEBD) or t-DMRG algorithms are indispensable tools in the numerical simulation of one-dimensional quantum many body systems. They permit high-accuracy calculations, provided that the entanglement between any two complementary partitions remains small. For finite-range interactions this is the case for the ground state. However in real time evolution the entanglement often grows linear in time, limited only by the Lieb-Robinson upper bound. E.g. for the spin-1/2 XY chain the evolution of the entanglement entropy was investigated in showing explicitly the linear growth in time.

However the evolved state contains a lot of information which is of little interest. Experimental measurements as well as theories are almost solely concerned with few particle properties, i.e., quantities that can be expressed in terms of expectation values of only a small number of elementary operators. This suggests to go to the Heisenberg picture (HP) instead, and to simulate the dynamics of these operators. Prosen et al. where the first to pursue this approach. They observed an exponential speed up in numerical simulations of local operators for integrable systems. So far there is however no general understanding of why this is the case and whether or not integrability is crucial. In the present paper we provide an explanation of the speed-up for integrable models that can be mapped to free fermions. We also argue that integrability is not necessary and that the existence of a conservation law may suffice for the efficient simulation of the dynamics of local operators that constitute the conserved quantity. We will discuss the spin-1/2 and spin-1 XXZ models as specific examples supporting and illustrating our arguments.

In order to do HP simulations using e.g. the TEBD scheme, the operator $\hat{O}(t)$ at time $t$ is expressed in terms of a matrix product operator (MPO). For typical observables this is straightforward for the initial time $t = 0$. Time evolution is then calculated by updating the matrices according to the Heisenberg equation of motion using a Trotter decomposition. Efficient simulation requires that the matrix dimension of the MPO’s (called bond dimension) is limited to a maximum value $\chi$. This means that only the $\chi$ largest Schmidt values in the Hilbert space of operators are kept, corresponding to a small operator-space (OS) entanglement between any two complementary partitions of the lattice. To quantify the entanglement of an operator $\hat{O}(t)$, which after proper normalization can be viewed as state vector in OS, we use the OS Rényi entropies (OSRE):

$$ S_\alpha = \frac{\log_2 \mathrm{Tr} \hat{\kappa}^\alpha}{1 - \alpha} \geq S_\beta, \quad \beta > \alpha > 0 \quad (1) $$

Here $\hat{\kappa}$ is the corresponding reduced density matrix in OS resulting from tracing out the left or right partition at a given bond. In the limit $\alpha \to 1$, $S_\alpha$ is the well known von Neumann entropy, which is a good measure of bi-partite entanglement. For $\alpha \to 0$, $S_\alpha$ gives the dimension of the Hilbert space. Clearly for an MPO of bond dimension $\chi$, the maximum for all Rényi entropies is $\log_2 \chi$. Although it is not yet fully established when a quantum state or an operator is faithfully represented by a matrix product with finite bond dimension, one can employ the results of Schuch et al. to show that efficient simulation is impossible if the Rényi entropies with $\alpha > 1$ scale faster than logarithmically with time. If $S_{\alpha>1}$ grows linearly in time, we must expect that the computational cost required to reach a certain accuracy, which is polynomial in $\chi$, will grow exponentially with time (note that this is not necessarily true for $S_\alpha$ with $\alpha \leq 1$). In fact for the time evolution of typical state vectors in the Schrödinger picture this is very often the case. On the other hand an at most logarithmic growth of $S_{\alpha>1}$ is a necessary condition for an efficient simulability. Although not sufficient, it also gives good indication when such a simulation is possible. In the following we will discuss the time evolution of the OSRE for a generic model, the XXZ chain,
\[ \hat{H} = -\frac{i}{\hbar} \sum_j \left( \hat{\sigma}_x^j \hat{\sigma}_x^{j+1} + \hat{\sigma}_y^j \hat{\sigma}_y^{j+1} + \Delta \hat{\sigma}_z^j \hat{\sigma}_z^{j+1} \right), \] where \( \hat{\sigma}_x, \hat{\sigma}_y, \) and \( \hat{\sigma}_z \) denote the Pauli matrices in the spin-\( \frac{1}{2} \) case and the spin-1 matrices (eigenvalues \(-1, 0, 1\)) in the spin-1 case respectively. The spin-\( \frac{1}{2} \) case is integrable for any value of the anisotropy \( \Delta \). For the special case of \( \Delta = 0 \) (spin-\( \frac{1}{2} \) XX model) this model can be mapped to free fermions.

**Integrable models equivalent to free fermions:** Let us consider the spin-\( \frac{1}{2} \) XXZ model as a general example of a 1D integrable model. We have calculated the time evolution of the OSRE \( S_2 \) for different types of simple operators using the TEBD scheme with open boundary conditions and a fourth order Trotter decomposition \([12]\). The restriction to open boundary conditions is not an issue for local operators as long as the time is shorter than the propagation time to reach the boundaries \([5]\). Although not shown the OS von-Neumann entropy \( S_1 \) has the same scaling behavior. One clearly notices the three types of interactions in the XXZ-super-Hamiltonian \( H \) which can be mapped to free fermions.

![FIG. 1: (Color online) OSRE dynamics for the 40 site spin-\( \frac{1}{2} \) XXZ model for a split in the center. The legend gives initial operator and anisotropy in the order in which the arrow cuts the graphs. Dashed lines mark infinite index operators (see text). \( \chi = 1000 \) is used in all cases and the numerical error is negligible on the time scale shown.](image)

In the following we will provide an explanation of the entropy scaling for the case of the XX-model, i.e., for \( \Delta = 0 \), which can be mapped to free fermions. This will be done by reexpressing the XXZ model in terms of Majorana-fermion operators \([14]\), which turns out to be more convenient than the more common Wigner-Jordan transformation: \( \hat{w}_{2j-1} = \left( \prod_{l<j} \hat{\sigma}_z^l \right) \hat{\sigma}_x^j \hat{w}_{2j} \left( \prod_{l<j} \hat{\sigma}_z^l \right) \hat{\sigma}_y^j \). The Majorana operators are Hermitian and fulfill anti-commutation relations \( \{ \hat{w}_j, \hat{w}_{j'} \} = 2 \delta_{jj'} \). The three types of interactions in the XXZ-model can be reexpressed as

\[
\begin{align*}
\hat{\sigma}_x^j \hat{\sigma}_x^{j+1} &= -i \hat{w}_{2j} \hat{w}_{2j+1} - 1, \\
\hat{\sigma}_y^j \hat{\sigma}_y^{j+1} &= i \hat{w}_{2j-1} \hat{w}_{2j+1}, \\
\hat{\sigma}_z^j \hat{\sigma}_z^{j+1} &= -\hat{w}_{2j-1} \hat{w}_{2j} \hat{w}_{2j+1} \hat{w}_{2j+2} - 1.
\end{align*}
\]

A complete basis in the OS is given by \( \hat{P}_\alpha = \prod_j \hat{a}_j^{\alpha-1} \hat{a}_j^\dagger \), where \( \alpha = (\alpha_1, \alpha_2, \ldots) \) and \( \{ \alpha_1 \} \in \{0,1\}^N \). We can now define adjoint-fermion annihilators and creators via \( \hat{a}_j \hat{P}_\alpha = \alpha_j \hat{w}_j \hat{P}_\alpha \), \( \hat{a}_j^\dagger \hat{P}_\alpha = (1 - \alpha_j) \hat{w}_j \hat{P}_\alpha \), with \( \{ \alpha_j, \alpha_j^\dagger \} = \delta_{jj} \). Associating the adjoint vacuum \( \hat{P}_0 \) with the unity operator \( 1 \), i.e., \( |1\rangle = |\hat{P}_0\rangle \), we can express all operators in terms of adjoint-fermion excitations \([13]\): \( |\hat{P}_\alpha\rangle = \prod_j (\hat{a}_j^\dagger \hat{a}_j^{\alpha-1} \hat{a}_j^\dagger \hat{a}_j^{\alpha/2}) \). Mapping the Heisenberg equation then gives a Schrödinger like equation for the evolution in OS,

\[
i \frac{d}{dt} \hat{P}_\alpha = [\hat{P}_\alpha, \hat{H}] \rightarrow i \frac{d}{dt} [\hat{P}_\alpha, \hat{H}] = [\hat{P}_\alpha, \hat{H}] = \hat{H}(\hat{P}_\alpha),
\]

with a “super”-Hamiltonian \( \hat{H} \). Explicitly calculating the terms in the commutator for the XX-model via \( |[\hat{P}_\alpha, \hat{a}_j^\dagger \hat{a}_j^{\alpha-1} \hat{a}_j^\dagger \hat{a}_j^{\alpha/2}]\rangle = 2i (\hat{a}_j \hat{a}_j^{\alpha-1} \hat{a}_j^\dagger \hat{a}_j^\dagger - \text{h.a.}) |\hat{P}_\alpha\rangle \), and \( |[\hat{P}_\alpha, \hat{a}_j^\dagger \hat{a}_j^{\alpha-1} \hat{a}_j^\dagger \hat{a}_j^{\alpha/2}]\rangle = -2i (\hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j^{\alpha-1} - \text{h.a.}) |\hat{P}_\alpha\rangle \) yields the XX super-Hamiltonian

\[
\hat{H}_{XX} = i \sum_j \left( \hat{a}_j^\dagger \hat{a}_j \hat{a}_{2j+1} + \hat{a}_j \hat{a}_{2j+1}^\dagger \hat{a}_{2j+2} \right) - \text{h.a.}
\]

This Hamiltonian corresponds to two uncoupled chains of free fermions. The total number of adjoint fermions, \( \sum_{m=1}^{2N} \hat{a}_m^\dagger \hat{a}_m \), is conserved. Note that the anisotropy \( \Delta \) in the original XXZ Hamiltonian would introduce recombination and pair creation across the chains. Although the above mapping is non local, operators acting only left of a given site \( j \) will be mapped to fermions that are again only left of this very site. So the OSRE of the original XX-model will be the same as the corresponding state vector Rényi entropy of two uncoupled chains of free fermions. Thus we have to calculate the entanglement dynamics of the two uncoupled chains with an initial state given by the operator in questions to get the OSRE in the XX model. The key point is that local operators are equivalent to very special, simple initial states in the corresponding fermion chains. We here have to distinguish between finite index operators (those that involve only a finite number of adjacent fermions after the mapping) and infinite index operators (involving a number proportional to the system size \( L \)). An example of the first kind is \( |\hat{\sigma}_y^\alpha\rangle = -i \hat{a}_j^\dagger \hat{a}_{2j-1} |1\rangle \). Examples of the second kind arise either from local operators like \( |\hat{\sigma}_x^\alpha\rangle = i^{j-1} (\prod_{l=1}^{2j-1} \hat{a}_l^\dagger \hat{a}_l) \hat{a}_{2j-1} |1\rangle \) or non local ones like \( |\hat{F}\rangle = (\prod_{l=1}^{2j-1} \hat{a}_l^\dagger) |\alpha\rangle \).

We proceed by showing that the bi-partite Rényi entropy \( S_2 \) for a system of free fermions in 1D is strictly related to the number fluctuations in any one of the two partitions assuming a fixed total number. We can assume that the initial state of the fermions corresponding to the local operators of interest is a Gaussian state. Due to the free evolution it remains Gaussian and can be transformed into a product form \( \hat{\theta} = \otimes_j \hat{\theta}_j \) where the \( \hat{\theta}_j \) correspond to site \( j \) and have eigenvalues \( |\eta_j| \leq 1 \). The square of the variance of the total particle number in each partition is then
\[ \Delta N^2 = \sum_{j \in A} (1 - \eta_j^2) / 4 = \Delta N^2 \quad \Box. \] On the other hand \[ S_2 = - \log_2 \text{Tr} \rho^2 = - \sum_j \log_2 \left( 1 - (1 - \eta_j^2) / 2 \right). \] Using \[ \frac{2}{\ln 2} \frac{x}{2 - x} \leq - \log_2 (1 - x) \leq \frac{1}{\ln 2} \frac{x}{2 - x}, \] where \(0 \leq x \leq \frac{1}{2}\), one obtains \[ \frac{4}{\ln 2} \Delta N^2 \geq S_2 \geq \frac{2}{\ln 2} \Delta N^2. \quad (5) \]

For finite index operators we find saturation as can be seen in Fig. 1. This reflects the fact, that there is only a finite number \(M\) of free particles present in both chains together. Thus a finite \(\chi\) of \(2^M\) yields the exact solution \[ \Box. \] For infinite index operators we observe logarithmic growth of \(L\) super state corresponding to an infinite index operator like \(|F\rangle\) (a finite size example of which is shown in Fig. 1) is filled up completely with fermions in the left part of the chains. Inside these regions the Pauli principle prevents hopping of fermions and thus only particles at the edge where the effective band-insulator is connected to the vacuum can move and fill the empty parts of the double chain. For the half filled chain Antal et al. have shown that \(\Delta N^2 \approx (\ln t + D) / 2\pi^2\) in the limit of large \(t\) with a known constant \(D > 0\) \[14\]. Other infinite index operators that result in a initial occupation of the two chains different from that of \(|F\rangle\) only on a finite number of sites show the same logarithmic long time behavior of the OSRE, see \[\Box\] This explains the dynamics of the OSRE in the XX model as a generic example of an integrable model that can be mapped to free fermions.

**non-integrable models:** We now show that there is another class of systems and operators which may allow an efficient simulation of dynamics in the HP. We construct an upper bound for the OSRE \(S_\alpha\), \(\alpha > 1\), in terms of the infinite-temperature auto-correlation function (ITAC). Without loss of generality we assume a normalized operator, i.e.

\[ \frac{1}{\Delta} \text{Tr} \left[ \hat{O}^\dagger \hat{O} \right] = 1, \] where \(\Delta\) is the local dimension of the chain.

With respect to a splitting of the chain of length \(L\) into two parts here and below all \(\bar{A}\) act on the sub chain A of length \(L_A\) and all \(\bar{B}\) on B of length \(L_B\). Any operator can be represented as \(\hat{O} = \sum_{m,n} \Lambda_{mn} (t) \hat{A}_m \otimes \hat{B}_n\) with orthonormal bases \(\frac{1}{\Delta} \text{Tr} \left[ \hat{A}_n^\dagger \hat{A}_m \right] = \frac{1}{\Delta} \text{Tr} \left[ \hat{B}_n^\dagger \hat{B}_m \right] = \delta_{nm}\). \(\Lambda\) is a matrix and its singular values \(\sqrt{\lambda_n}\) are the eigenvalues of \(\hat{\kappa}\) are coefficients of a Schmidt decomposition \(\hat{O}(t) = \sum_{n=1}^\chi \sqrt{\lambda_n} \hat{A}_n(t) \otimes \hat{B}_n(t)\), where now the Schmidt rank \(\chi\) is at most \(\Delta^2 \min(L_A, L_B)\). This allows to express the infinite-temperature auto-correlation function in terms of Schmidt coefficients. We find for \(\alpha > 1\)

\[ \left| \left< \hat{O}^\dagger(t) \hat{O} \right>_{t=\infty} \right| = \left| \text{Tr} \left[ \Lambda^\dagger(t) \Lambda(0) \right] \right| \leq \sum_{k=1}^\chi \sqrt{\lambda_k \lambda_k(0)} \quad (6) \]

\[ \leq \text{Tr} \sqrt{\kappa(0)} \left( \sum_{k=1}^\chi \frac{\sqrt{\lambda_k(0)}}{\text{Tr} \sqrt{\kappa(0)}} \right)^{\frac{1}{\alpha}} \quad (7) \]

\[ = \left( \text{Tr} \sqrt{\kappa(0)} \right)^{1 - \frac{1}{\alpha}} \left( \sum_{k=1}^\chi \lambda_k^\alpha \right)^{\frac{1}{\alpha}} \quad (8) \]

In (6) we made use of von Neumann’s trace inequality (see e.g. \[\Box\]). Furthermore Jensen’s inequality can be used because \(x^\alpha\) is a concave function in \(x\). Finally (8) is true by the Cauchy-Schwarz inequality. We thus obtain the following estimate for Rényi entropies, assuming an initial product operator, \(\text{Tr} \sqrt{\kappa(0)} = 1\), for simplicity:

\[ S_\alpha \leq \frac{2\alpha}{1 - \alpha} \log_2 \left| \left< \hat{O}^\dagger(t) \hat{O} \right>_{t=\infty} \right| \quad \text{for } \alpha > 1. \quad (9) \]

If the ITAC decays with a power law and slower in time, \(S_\alpha\) will grow at most logarithmically for \(\alpha > 1\). The ITAC has been studied over decades in condensed matter physics as it is measured in nuclear magnetic resonance and neutron scattering experiments in magnetic spin chains. While not proved rigorously, it is believed that the Blomberg-de Gennes conjecture \[19\] of spin diffusion holds: If \(\sum_{j=1}^L \hat{O}_j\) is a conserved quantity, then the ITAC of \(\hat{O}_j\) will show diffusive behavior (i.e. \(\sim 1/\sqrt{t}\) in 1D). To our knowledge there is no counter example except for integrable models, where this diffusive behavior can turn into a ballistic one (i.e. \(\sim 1/t\) in 1D) \[20, 21\]. Nevertheless it always remains slower than exponential. We conclude that in the HP TEBD we can expect \(S_2\) to grow at most logarithmically in time, even if the model is non-integrable, if the initial operator belongs to a conservation law (for integrable systems there is an infinite number of those, but one is sufficient). This in turn indicates that an efficient classical simulation should be possible for large times.

The spin-1 XXZ chain is an example of a non-integrable system, although extension to additional higher-order nonlinear terms may turn it into an integrable one \[22, 23\]. However the total \(z\)-magnetization \(\sum_{j=1}^L \hat{\sigma}_j^z\) is conserved. This conservation law will lead to a logarithmic scaling of \(S_2\) for \(\hat{\sigma}^z\). Fig. 2 shows numerical indication for this. It should be noted that the spin-1 model is computationally much harder than the spin-\(1/2\) model since the local Hilbert space dimension is increased. Although we do observe logarithmic scaling of the OSRE corresponding to \(\hat{\sigma}^z\), the prefactor is large, such that we cannot go to far in time. The plot shows data for different matrix dimension \(\chi\) up to the point where the cutoff error becomes substantial. A clear tendency is visible: On the logarithmic scale \(S_2\) approaches a straight line, while in the linear plot a sub-linear scaling is evident. This is consistent with the expected logarithmic scaling of the OSRE. For \(\hat{\sigma}^+\) Fig. 2 shows logarithmic scaling of \(S_2\) only for \(\Delta = 1\) because only then the total \(x\)- and \(y\)-magnetization are also conserved. Otherwise it indicates linear growth of \(S_2\) with time. We can understand this now as a direct consequence of the Blomberg-de Gennes conjecture, which predicts a power law rather than an exponentially decaying ITAC in the isotropic case (see in-
we have also been investigated numerically. The OSRE shows the expected time dependence, i.e., logarithmic scaling in the regular and linear scaling in the chaotic case. From the numerical results we can also extract the von Neumann entropy as a function of time. It scales exactly as $S_2$ in the spin-$\frac{1}{2}$ model for all operators we looked at. The results are not conclusive in the spin-1 case however, since the dependence on the matrix dimension $\chi$ used in the simulations is much stronger. At least they do not contradict the presumption, that again the scaling is the same as for $S_2$.

In summary we have given a simple explanation of the at most logarithmic time dependence of the OSRE $S_2$ for the spin-$1/2$ XX model as a generic integrable model that can be mapped to free fermions. The operator dynamics in that model is equivalent to two uncoupled chains of free fermions with an initial state corresponding to the operator under consideration. For local operators these initial states are rather simple. E.g. an operator $\sigma_j^+$ corresponds to a single fermion in each chain. We have shown that the bi-partite OSRE $S_2$ is strictly related to the fluctuations of the fermion number in the two partitions, which in turn allowed a simple understanding of the entropy dynamics. We have shown furthermore that for any model, integrable or not, $S_2$ in OS can be bound by the infinite-temperature auto-correlation function of the considered operator. This in turn means that for systems and observables for which the Blombergen-de Gennes conjecture of spin diffusion holds, an at most logarithmic growth of the OS entanglement is expected. The latter applies e.g. for local operators that constitute a global conservation law.

We are indebted to Thomaš Prosen, Jesko Sirker, and Frank Verstraete for valuable discussions, the SFB TRR49 of the DFG and the Excellence Initiative (DFG/GSC 266) for financial support, and the Erwin Schrödinger Institute, Vienna, for hospitality.

sets of Fig. 2. We note, that the regular and chaotic Hamiltonians used in the original work by Prosen and Žnidarič [8] have also been investigated numerically. The OSRE shows the expected time dependence, i.e. logarithmic scaling in the regular and linear scaling in the chaotic case.

From the numerical results we can also extract the von Neumann entropy as a function of time. It scales exactly as $S_2$ in the spin-$\frac{1}{2}$ model for all operators we looked at. The results are not conclusive in the spin-1 case however, since the dependence on the matrix dimension $\chi$ used in the simulations is much stronger. At least they do not contradict the presumption, that again the scaling is the same as for $S_2$.

In summary we have given a simple explanation of the at most logarithmic time dependence of the OSRE $S_2$ for the spin-$1/2$ XX model as a generic integrable model that can be mapped to free fermions. The operator dynamics in that model is equivalent to two uncoupled chains of free fermions with an initial state corresponding to the operator under consideration. For local operators these initial states are rather simple. E.g. an operator $\sigma_j^+$ corresponds to a single fermion in each chain. We have shown that the bi-partite OSRE $S_2$ is strictly related to the fluctuations of the fermion number in the two partitions, which in turn allowed a simple understanding of the entropy dynamics. We have shown furthermore that for any model, integrable or not, $S_2$ in OS can be bound by the infinite-temperature auto-correlation function of the considered operator. This in turn means that for systems and observables for which the Blombergen-de Gennes conjecture of spin diffusion holds, an at most logarithmic growth of the OS entanglement is expected. The latter applies e.g. for local operators that constitute a global conservation law.

We are indebted to Thomaš Prosen, Jesko Sirker, and Frank Verstraete for valuable discussions, the SFB TRR49 of the DFG and the Excellence Initiative (DFG/GSC 266) for financial support, and the Erwin Schrödinger Institute, Vienna, for hospitality.

* Electronic address: muth@physik.uni-kl.de