Dynamical Simulation of Integrable and Nonintegrable Models in the Heisenberg Picture

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The numerical simulation of quantum many-body dynamics is typically limited by the linear growth of entanglement with time. Recently numerical studies have shown that for 1D Bethe-integrable models the simulation of local operators in the Heisenberg picture can be efficient. Using the spin-1/2 XX chain as generic example of an integrable model that can be mapped to free fermions, we provide a simple explanation for this. We show furthermore that the same reduction of complexity applies to operators that have a high-temperature autocorrelation function which decays slower than exponential, i.e., with a power law. Thus efficient simulability may already be implied by a single conservation law as we will illustrate numerically for the spin-1 XXZ model.

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White's Density Matrix Renormalization Group (DMRG) [1] and its more recent generalizations to time evolution using the time evolving block decimation (TEBD) [2] or t-DMRG [3] 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 [4]. However, in real time evolution the entanglement often grows linear in time, limited only by the Lieb-Robinson upper bound [5,6]. E.g., for the spin-$\frac{1}{2}$ XY chain the evolution of the entanglement entropy was investigated in [7] 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 quantities that can be expressed in terms of only a small number of elementary operators. This suggests going to the Heisenberg picture (HP) and simulating the dynamics of these operators. Prosen *et al.* [8,9] were the first to pursue this approach. They observed an exponential speedup in 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 Letter we provide an explanation of the speedup for 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 local operators that constitute the conserved quantity. We discuss the spin-$\frac{1}{2}$ 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 then means updating the matrices according to the Heisenberg equation using a Trotter decomposition. Efficient simulation requires that the matrix dimension of the MPO's (called bond dimension) is limited to a maximum value χ. I.e., only the χ largest Schmidt values in the Hilbert space of operators are kept, corresponding to a small operator-space (OS) entanglement between any two complementary partitions. 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):

$$S_\alpha = \frac{\log_2 \mathrm{Tr}\hat{\kappa}^\alpha}{1-\alpha} \geq S_\beta, \qquad \beta > \alpha > 0. \tag{1}$$

Here $\hat{\kappa}$ is the corresponding reduced density matrix in OS resulting from tracing out one partition at a given bond. In the limit $\alpha \to 1$, S_α is the well-known von Neumann entropy, which is a good measure of bipartite entanglement. For $\alpha \to 0$, S_α gives the dimension of the Hilbert space. Clearly for an MPO of bond dimension χ, 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.* [10] 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 will grow exponentially with time (note that this is not necessarily true for S_α with $\alpha \leq 1$ [10]). In fact, for the time evolution of typical state vectors in the Schrödinger picture this is often the case [11]. 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 discuss the time evolution of the OSRE for a generic model, the XXZ chain,

$\hat{H} = -\frac{1}{2}\sum_j(\hat{\sigma}^x_j\hat{\sigma}^x_{j+1} + \hat{\sigma}^y_j\hat{\sigma}^y_{j+1} + \Delta\hat{\sigma}^z_j\hat{\sigma}^z_{j+1})$, where $\hat{\sigma}^{x,y,z}$ denote Pauli matrices or 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 Δ. For $\Delta = 0$ (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 generic example of a 1D integrable model. We have calculated the time evolution of the OSRE S_2 for different 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 the boundaries [5]. Although not shown the OS von-Neumann entropy S_1 has the same scaling behavior. One clearly notices that the OSRE of all operators scales at most logarithmically in time, an observation made already by Prosen *et al.* for other integrable models [9,13]. In the special case of $\Delta = 0$ the entropy saturates at a finite value for some operators like $\hat{\sigma}^z$.

In the following we provide an explanation 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 fermions [14], which turns out to be more convenient than the Wigner-Jordan form: $\hat{w}_{2j-1} = (\prod_{l<j}\hat{\sigma}^z_l)\hat{\sigma}^x_j$, $\hat{w}_{2j} = (\prod_{l<j}\hat{\sigma}^z_l)\hat{\sigma}^y_j$. The Majorana operators are Hermitian and fulfill anticommutation relations $\{\hat{w}_j, \hat{w}_l\} = 2\delta_{jl}$. The three types of interactions in the XXZ model can be reexpressed as

$$\begin{aligned}\hat{\sigma}^x_j\hat{\sigma}^x_{j+1} &= -i\hat{w}_{2j}\hat{w}_{2(j+1)-1},\\ \hat{\sigma}^y_j\hat{\sigma}^y_{j+1} &= i\hat{w}_{2j-1}\hat{w}_{2(j+1)},\\ \hat{\sigma}^z_j\hat{\sigma}^z_{j+1} &= -\hat{w}_{2j-1}\hat{w}_{2j}\hat{w}_{2(j+1)-1}\hat{w}_{2(j+1)}.\end{aligned} \tag{2}$$

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

$$i\frac{d}{dt}\hat{P}_\alpha = [\hat{P}_\alpha, \hat{H}] \mapsto i\frac{d}{dt}|\hat{P}_\alpha\rangle = |[\hat{P}_\alpha, \hat{H}]\rangle =: \hat{\mathcal{H}}|\hat{P}_\alpha\rangle, \tag{3}$$

with a "super"-Hamiltonian $\hat{\mathcal{H}}$. Explicitly calculating the terms in the commutator for the XX model via $|[\hat{P}_\alpha, \hat{\sigma}^x_j\hat{\sigma}^x_{j+1}]\rangle = 2i(\hat{a}^\dagger_{2j}\hat{a}_{2(j+1)-1} - \text{H.a.})|\hat{P}_\alpha\rangle$, and $|[\hat{P}_\alpha, \hat{\sigma}^y_j\hat{\sigma}^y_{j+1}]\rangle = -2i(\hat{a}^\dagger_{2j-1}\hat{a}_{2(j+1)} - \text{H.a.})|\hat{P}_\alpha\rangle$ yields

$$\hat{\mathcal{H}}_{XX} = i\sum_j(\hat{a}^\dagger_{2j}\hat{a}_{2j+1} + \hat{a}^\dagger_{2j-1}\hat{a}_{2j+2} - \text{H.a.}). \tag{4}$$

This Hamiltonian corresponds to two uncoupled chains of free fermions. The total number of adjoint fermions, $\sum_{m=1}^{2N}\hat{a}^\dagger_m\hat{a}_m$, is conserved. Note that the anisotropy Δ in the original XXZ Hamiltonian would introduce recombination and pair creation across the chains. Although the above mapping is nonlocal, 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. 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 adjoint fermions) and infinite index operators (involving a number proportional to the system size L). An example of the first kind is $|\hat{\sigma}^z_j\rangle = -i\hat{a}^\dagger_{2j-1}\hat{a}^\dagger_{2j}|\mathbf{1}\rangle$. Examples of the second kind arise either from local operators like $|\hat{\sigma}^x_j\rangle = i^{j-1}(\prod_{l=1}^{2(j-1)}\hat{a}^\dagger_l)\hat{a}^\dagger_{2j-1}|\mathbf{1}\rangle$ or non local ones like $|\hat{F}\rangle = |\prod_{l=1}^{j-1}\hat{\sigma}^z_l\rangle = i^{j-1}(\prod_{l=1}^{2(j-1)}\hat{a}^\dagger_l)|\mathbf{1}\rangle$.

We proceed by showing that the bipartite 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. Because of the free evolution it remains Gaussian and can be transformed into a product form $\hat{\rho} = \bigotimes_j\hat{\rho}_j$ where the $\hat{\rho}_j$ correspond to site j and have eigenvalues $\frac{1\pm\eta_j}{2}$, $|\eta_j| \leq 1$. The square of the variance of the total particle number in each partition is then $\Delta N^2_A = \sum_{j\in A}(1-\eta^2_j)/4 = \Delta N^2_B$ [15]. On the other hand $S_2 = -\log_2\mathrm{Tr}\hat{\rho}^2 = -\sum_j\log_2[1-(1-\eta^2_j)/2]$. Using $\frac{2}{\ln 2}\frac{x}{2-x} \leq -\log_2(1-x) \leq \frac{1}{\ln 2}\frac{x}{1-x}$, where $0 \leq x \leq \frac{1}{2}$, one obtains

$$\frac{4}{\ln 2}\Delta N^2 \geq S_2 \geq \frac{2}{\ln 2}\Delta N^2. \tag{5}$$

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 in both chains together. Thus a finite χ of 2^M yields the exact solution [16] for all times [17]. For infinite index operators we observe logarithmic growth of the OSRE, see Fig. 1. While the infinite number of involved adjoint fermions may suggest a linear growth of ΔN^2, this is not the case. The superstate corresponding to a infinite index operator like $|\hat{F}\rangle$ (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 can move and fill the empty parts of the double chain. For the half-filled chain Antal *et al.* have shown that $\Delta N^2 \cong (\ln t + D)/2\pi^2$ in the limit of large t with a known constant $D > 0$ [18]. Other infinite

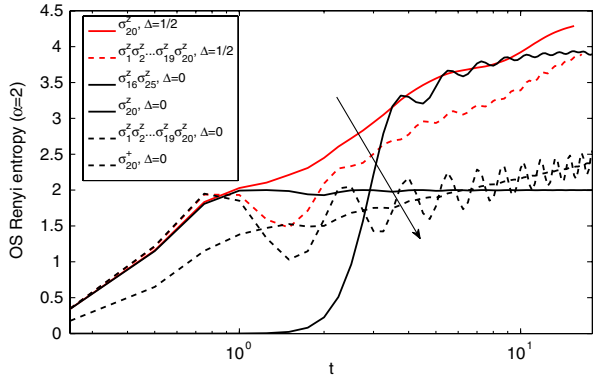

FIG. 1 (color online). OSRE dynamics for the 40 site spin-$\frac{1}{2}$ XXZ model for a split in the center. The legend gives initial operator and anisotropy in the order in which the arrow cuts the graphs. Dashed lines mark infinite index operators (see text). $\chi = 1000$ is used in all cases and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

index operators that result in a initial occupation of the two chains different from that of $|\hat{F}\rangle$ only on a finite number of sites show the same logarithmic behavior of the OSRE, see $|\hat{\sigma}^+\rangle$ at a single site, also shown in Fig. 1. This explains the dynamics of the OSRE in the XX model as a generic example of a model that can be mapped to free fermions.

Nonintegrable models.—We now show that there is another class of systems and operators that may allow an efficient simulation in the HP. We construct an upper bound for the OSRE S_α, $\alpha > 1$, in terms of the infinite-temperature autocorrelation function (ITAC). Without loss of generality we assume a normalized operator, i.e., $\frac{1}{d^L}\mathrm{Tr}[\hat{O}^\dagger\hat{O}] = 1$, where d 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 $\hat{A}$ act on the subchain A of length L_A and all $\hat{B}$ on B of length L_B. Any operator can be represented as $\hat{O}(t) = \sum_{m,n}\Lambda_{mn}(t)\hat{A}_m \otimes \hat{B}_n$ with orthonormal bases $\frac{1}{d^{L_A}}\mathrm{Tr}[\hat{A}_n{}^\dagger\hat{A}_m] = \frac{1}{d^{L_B}}\mathrm{Tr}[\hat{B}_n^\dagger\hat{B}_m] = \delta_{nm}$. Λ is a matrix and its singular values $\sqrt{\lambda_n}$ ($\lambda_1 \geq \lambda_2 \geq \ldots$ are the eigenvalues of $\hat{\kappa}$) are coefficients of a Schmidt decomposition $\hat{O}(t) = \sum_{n=1}^{\chi}\sqrt{\lambda_n}\,\hat{\mathcal{A}}_n(t) \otimes \hat{\mathcal{B}}_n(t)$, where χ is at most $d^{2\min(L_A,L_B)}$. This allows us to express the ITAC in terms of Schmidt coefficients. We find for $\alpha > 1$

$$|\langle\hat{O}^\dagger(t)\hat{O}\rangle_{T=\infty}| = |\mathrm{Tr}[\Lambda^\dagger(t)\Lambda(0)]| \leq \sum_{k=1}^{\chi}\sqrt{\lambda_k\lambda_k(0)} \quad (6)$$

$$\leq \mathrm{Tr}\sqrt{\hat{\kappa}(0)}\left(\sum_{k=1}^{\chi}\frac{\sqrt{\lambda_k(0)}}{\mathrm{Tr}\sqrt{\hat{\kappa}(0)}}\lambda_k^{\alpha/2}\right)^{1/\alpha} \quad (7)$$

$$= (\mathrm{Tr}\sqrt{\hat{\kappa}(0)})^{1-(1/\alpha)}\left(\sum_{k=1}^{\chi}\lambda_k^\alpha\right)^{1/2\alpha}. \quad (8)$$

In (6) we made use of von Neumann's trace inequality (see, e.g., [19]). Furthermore, Jensen's inequality can be used because $x^{1/\alpha}$ is concave in x. Finally (8) is true by the Cauchy-Schwarz inequality. Assuming an initial product operator, $\mathrm{Tr}\sqrt{\hat{\kappa}(0)} = 1$, for simplicity, we obtain

$$S_\alpha \leq \frac{2\alpha}{1-\alpha}\log_2|\langle\hat{O}^\dagger(t)\hat{O}\rangle_{T=\infty}| \quad \text{for } \alpha > 1. \quad (9)$$

If the ITAC decays with a power law or slower in time, S_α 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 proofed rigorously, it is believed that the Blombergen–de Gennes conjecture [20] 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 counterexample except for integrable models, where this diffusive behavior can turn into a ballistic one (i.e., $\sim 1/t$ in 1D) [21,22]. 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 nonintegrable, 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 nonintegrable system, although extension to additional higher-order nonlinear terms may turn it into an integrable one [23,24]. The total z magnetization $\sum_{j=1}^{L}\hat{\sigma}_j^z$ is conserved. This will lead to a logarithmic scaling of S_2 for $\hat{\sigma}^z$. Figure 2 shows numerical indication for this. It should be noted that the spin-1 model is computationally much harder than the spin-$\frac{1}{2}$ 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 too far in time. The plot shows data for different matrix dimension χ 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 sublinear 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 Blombergen–de Gennes conjecture, which predicts a power law rather than an exponentially decaying ITAC in the isotropic case (see insets 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

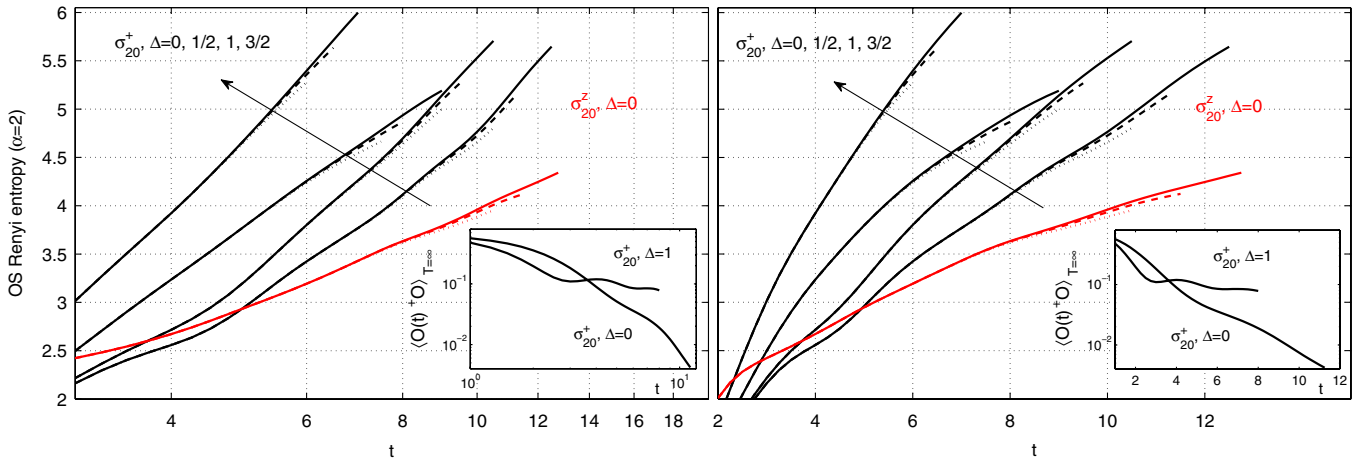

FIG. 2 (color online). OSRE dynamics for the 40 site spin-1 XXZ model for a split in the center. Dotted, dashed, and solid lines indicate simulations using $\chi = 300$, $\chi = 500$, and $\chi = 1000$, respectively. The left panel features a logarithmic, the right panel a linear time scale. The curves show clear indication of the predicted long-time scaling. The insets show two corresponding ITAC curves for $\hat{\sigma}^{+}_{20}$ (note the logarithmic vertical scaling).

the dependence on the matrix dimension χ 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 $\hat{\sigma}^{z}_{j}$ corresponds to a single fermion in each chain. We have shown that the bipartite 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 ITAC 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.

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