

Is the efficiency of classical simulations of quantum dynamics related to integrability?

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Efficiency of time evolution of quantum observables, and thermal states of quenched Hamiltonians, is studied using *time-dependent density-matrix renormalization group* method in a family of generic quantum spin chains which undergo a transition from integrable to nonintegrable-quantum chaotic case as control parameters are varied. Quantum states (observables) are represented in terms of matrix-product operators with rank $D_\epsilon(t)$, such that evolution of a long chain is accurate within fidelity error ϵ up to time t . We found that the rank generally increases *exponentially* $D_\epsilon(t) \propto \exp(\text{const } t)$, unless the model system was integrable in which case we found *polynomial* increase.

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In the theory of classical dynamical systems there is a fundamental difference between integrable and chaotic systems. Chaotic systems, having positive algorithmic complexity, unlike the integrable ones, cannot be simulated for arbitrary times with a finite amount of information about their initial states. Computational complexity of individual chaotic trajectories is linear in time, however, if one wants to describe statistical states (phase space distributions) or observables of chaotic classical systems, up to time t , exponential amount of computational resources $N(t) \sim \exp(ht)$ is needed, where h is the Kolmogorov's dynamical entropy related to exponential sensitivity to initial conditions. For example, one needs to expand the solution of the Liouville equation into the lowest $N(t)$ Fourier modes.

How difficult is it to simulate isolated and bounded quantum systems of many interacting particles using classical resources? In analogy with the classical (chaotic) case, we might expect that the best classical simulation of typical quantum systems [in thermodynamic limit (TL)] is exponentially hard. Even though there is no exponential sensitivity to initial conditions in quantum mechanics, there is a tensor-product structure of the many-body quantum state space which makes its dimension to scale exponentially with the number of particles, as opposed to linear scaling in the classical case. Furthermore, due to intricate quantum correlations (entanglement) generic quantum time evolution cannot be reduced to (efficient) classical computation in terms of non-entangled (classical like) states. However, it is not known what amount and form of quantum entanglement is needed in order to prevent efficient classical simulation.

Recently, a family of numerical methods for the simulation of interacting many-body systems has been developed [1] which is usually referred to as time-dependent density-matrix renormalization group (*t*-DMRG), and which has been shown to often provide an efficient classical simulation of certain interacting quantum systems. Simulations of locally interacting one-dimensional quantum lattices were actually shown rigorously to be efficient in the number n of particles [2] [i.e., computation time and memory resources scale as polynomial functions of n at fixed t , or up to $t = O(\ln n)$], whereas the scaling of computation time and memory with physical time t (in TL $n = \infty$), later on referred to as *time efficiency*, has not been systematically studied.

t-DMRG was shown to be time efficient [3] only in rather special cases of exactly solvable dynamics (generated with XY spin chain Hamiltonian) and/or for particular choices of initial states, lying either in low-energy sectors or in low-dimensional invariant subspaces. However, for applications in nonequilibrium statistical mechanics and condensed matter theory, e.g., in transport phenomena, it is of primary importance to understand long-time dynamics of generic interacting quantum systems [4].

In this paper we address the question of time efficiency implementing an up-to-date version of *t*-DMRG for a family of Ising spin- $\frac{1}{2}$ chains in arbitrary oriented magnetic field, which undergoes a transition from integrable (transverse Ising) to nonintegrable quantum chaotic regime as the magnetic field is varied. We focus on evolution of density operators of *mixed states*, starting from a thermal state of a quenched Hamiltonian, and evolution of *local* or *extensive* initial observables in Heisenberg picture. Note that time evolution of pure states is often ill defined in TL [5]. As a quantitative measure of time efficiency we define and compute the minimal dimension $D_\epsilon(t)$ of matrix product operator (MPO) representation of quantum states and/or observables which describes time evolution up to time t within fidelity $1 - O(\epsilon)$. Our central result states that in generic nonintegrable cases computation resources grow exponentially $D_\epsilon(t) \propto \exp(h_q t)$, except in the integrable case of transverse Ising chain, where the growth is typically linear $D_\epsilon(t) \propto t$. Constant h_q , asymptotically independent of n , depends only on the evolution (Hamiltonian) and not on the details of the initial state observable or error measures, and can be interpreted as a kind of *quantum dynamical entropy*. We conjecture that integrability (solubility) of one-dimensional (1D) interacting quantum systems is in one-to-one correspondence with the efficiency of their classical simulability.

We also studied time efficiency of simulation of *pure states* in Schrödinger picture, for which many examples of efficient applications exist, however all for initial states of rather particular structure typically corresponding to low energy sectors. Treating other, typical states, e.g., eigenstates of unrelated Hamiltonians, linear combinations of highly excited states, or states chosen randomly in the many-particle Hilbert space, we found that, irrespective of integrability of dynamics, *t*-DMRG is *not* time efficient, i.e., $D_\epsilon(t)$ grows

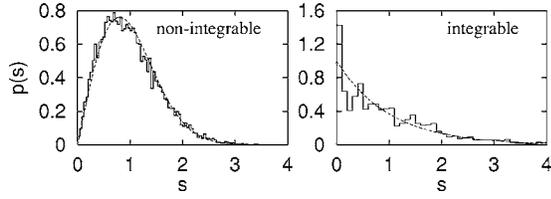


FIG. 1. Nearest neighbor LSD for H_C (left-hand side) and H_R (right-hand side) for $n=12$. Dashed curves are $p(s) = s\pi/2 \exp(-\pi^2 s^2/4)$ (left-hand side) and $p(s) = \exp(-s)$ (right-hand side), typical for chaotic and regular systems, respectively [8]. Eigenenergies $\in[-9,9]$ were used and statistics for even and odd parity states were combined.

exponentially even in the integrable case of transverse field (consistently with a linear growth of entanglement entropy [6]). In view of this fact, our finding that t -DMRG can be time efficient for integrable systems when implemented for time-evolved operators or high-temperature thermal states, provides a new paradigm for a successful application of t -DMRG.

Let us briefly review t -DMRG for evolution of density matrices and operators [7] which generalizes t -DMRG for pure states [1]. One defines a superket corresponding to an operator O expanded in the *computational basis* of products of local operators. Concretely, for a chain of n qubits we use a basis of 4^n Pauli operators $\sigma^{s_0} \otimes \dots \otimes \sigma^{s_{n-1}}$, with $s_j \in \{0, x, y, z\}$ and $\sigma^0 = \mathbb{1}$. The key idea of t -DMRG is to represent any operator in a matrix product form, $O = \sum_{s_j} \text{tr}(A_0^{s_0} \dots A_{n-1}^{s_{n-1}}) \sigma^{s_0} \otimes \dots \otimes \sigma^{s_{n-1}}$, in terms of $4n$ matrices $A_j^{s_j}$ of fixed dimension D . The number of parameters in the MPO representation is $4nD^2$ and for sufficiently large D it can describe any operator. In fact, the minimal D required is equal to the maximal rank of the reduced super density matrix over all bipartitions of the chain. The advantage of MPO representation lies in the fact that doing an elementary local one or two qubit unitary transformation $O' = U^\dagger O U$ can be done locally, affecting only a pair of neighboring matrices $A_j^{s_j}$.

In order to study the role of integrability on the efficiency of t -DMRG we take antiferromagnetic Ising chain in a general homogeneous magnetic field,

$$H(h^x, h^z) = \sum_{j=0}^{n-2} \sigma_j^x \sigma_{j+1}^x + \sum_{j=0}^{n-1} (h^x \sigma_j^x + h^z \sigma_j^z), \quad (1)$$

where $\sigma_j^s = \mathbb{1}^{\otimes j} \otimes \sigma^s \otimes \mathbb{1}^{\otimes (n-1-j)}$. We will analyze evolution for two different magnetic field values: (i) an integrable (regular) case $H_R = H(0, 2)$ with transverse magnetic field and (ii) non-integrable (quantum chaotic) case $H_C = H(1, 1)$ with tilted magnetic field. Particular value of $h^z = 2$ in the case of H_R plays no role. H_R can be solved by Jordan-Wigner transformation which maps H_R to a system of noninteracting fermions. To confirm that H_C , and H_R , indeed represent generic quantum chaotic, and regular system, respectively, we calculated level spacing distribution (LSD) of their spectra (shown in Fig. 1). LSD is a standard indicator of quantum chaos [8]. It displays characteristic level repulsion for strongly nonintegrable quantum systems, whereas for integrable systems

there is no repulsion due to existence of conservation laws and quantum numbers.

Evolution by t -DMRG proceeds by splitting Hamiltonian (1) into even and odd terms, $H = H_e + H_o$, such that terms within H_e or H_o commute between each other. An approximate propagator for short time step is then written using Trotter-Suzuki formula as $U(\delta t) = e^{-iH_e \delta t/2} e^{-iH_o \delta t} e^{-iH_e \delta t/2}$, where each of the three terms can be written as a series of commuting one and two qubit operations. There are two sources of errors in t -DMRG scheme. One is Trotter error scaling as $\propto (\delta t)^3$ per time step, or $\propto (\delta t)^2$ in total, and the other, usually dominating one, is due to truncation.

The truncation error arises because after performing two qubit transformation on MPO the required dimension of the new matrices increases to $4D$. In order to prevent the exponential growth of D with time we truncate the resulting matrices back to dimension D [1]. Truncation after application of a single gate U_i introduces a norm error $\eta(U_i)$ equal to the sum of squares of discarded singular values. As an estimate for the total truncation error $\eta_{\text{tot}}(t)$ at time t we will use a sum of all truncation errors $\eta(U_i)$ for two qubit gates U_i applied up to time t , $U(t) = \prod_i U_i$ (the number of such gates scales as $\sim t/\delta t$). If $\lambda_k^2(U_i), k=0, \dots, 4D-1$, denote decreasingly ordered eigenvalues of the reduced super-density matrix after the application of a gate U_i , then $\eta(U_i)$ and η_{tot} are given by

$$\eta(U_i) = \sum_{j=D}^{4D-1} \lambda_j^2(U_i), \quad \eta_{\text{tot}}(t) = \sum_i \eta(U_i). \quad (2)$$

Simple perturbation argument shows that for small time step δt , single gate truncation error scale as $\eta(U_i) \propto (\delta t)^2$, so the total error $\eta_{\text{tot}}(t) \propto \delta t$. We use the same time step $\delta t = 0.01$ in all our simulations. One may hope that $\eta_{\text{tot}}(t)$ gives a good measure of fidelity

$$F(t) = \frac{|\text{tr}[O_{\text{MPO}}(t) O_{\text{exact}}(t)]|^2}{|\text{tr}[O_{\text{MPO}}^2(t)]| |\text{tr}[O_{\text{exact}}^2(t)]|}, \quad (3)$$

where $O_{\text{MPO}}(t)$ is an operator obtained from the initial O with t -DMRG evolution with a given fixed D , while $O_{\text{exact}}(t) = U^\dagger(t) O U(t)$ is obtained with an exact evolution. Indeed, by comparing to exact numerical simulations of small systems of size $n=6, 8, 10$ and several different D we find quite generally (see Fig. 2 for an example) that up to good numerical approximation $1 - F(t) \approx c \eta_{\text{tot}}(t)/\delta t$, where c is some numerical constant of order 1 which does not depend on δt , D , or n .

The central quantity we are going to study is $D_\epsilon(t)$ which is the minimal dimension D of matrices $A_i^{s_j}$ in order for the total truncation error $\eta_{\text{tot}}(t)$ to be less than some error tolerance ϵ , or fidelity (3) to be bigger than $1 - (c/\delta t)\epsilon$, for evolution to time t . We use $\epsilon = 10^{-4}$ for local and extensive operators and $\epsilon = 10^{-6}$ for thermal states. The central question is the following: does $D_\epsilon(t)$ grow exponentially or polynomially with t ? If it grows polynomially we can say that t -DMRG is time efficient.

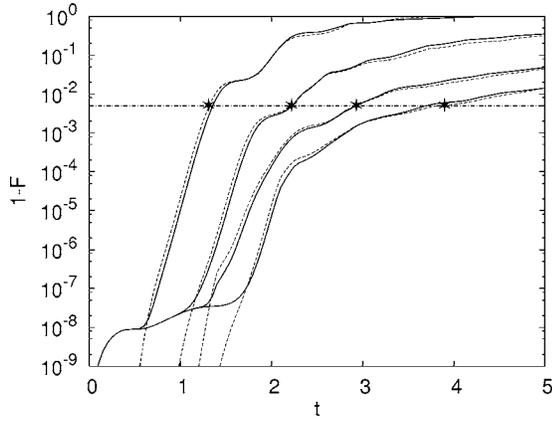


FIG. 2. Fidelity (3) of t -DMRG evolution (full curves) and scaled truncation errors $c\eta_{\text{tot}}(t)/\delta t$ with $c=0.5$ (dashed curves), for $O(0)=\sigma_{n/2}^y$, Hamiltonian H_R and $n=10$. Different sets of curves are for $D=10, 20, 30, 40$ (top to bottom). Chain line marks the threshold where the truncation error $\eta_{\text{tot}}(t)=10^{-4}$ (indicated by stars for different D 's).

Let us first study the case where the initial operator is a local operator in the center of the lattice $O(0)=\sigma_{n/2, s}^x, s \in \{x, y, z\}$. In the integrable case time evolution $O(t)$ can be computed exactly in terms of Jordan-Wigner transformation and Toeplitz determinants [9], however for initial operators with infinite index [10], like, e.g., for $\sigma_{n/2}^{x,y}$, $n \rightarrow \infty$, the evolution is rather complex and the effective number of terms (Pauli group elements) needed to span $O(t)$ grows exponentially in t . In spite of that, our numerical simulations shown in Fig. 3 strongly suggest the linear growth $D_\epsilon(t) \sim t$ for initial operators with infinite index. Quite interestingly, for initial operators with finite index, $D_\epsilon(t)$ saturates to a finite value, for example [11] $D_\epsilon(\infty)=4$ for $\sigma_{n/2}^z$, or $D_\epsilon(\infty)=16$ for $\sigma_{n/2-1}^z \sigma_{n/2}^z$. In nonintegrable cases the rank has been found to grow exponentially, $D_\epsilon(t) \sim \exp(h_q t)$ with exponent h_q which

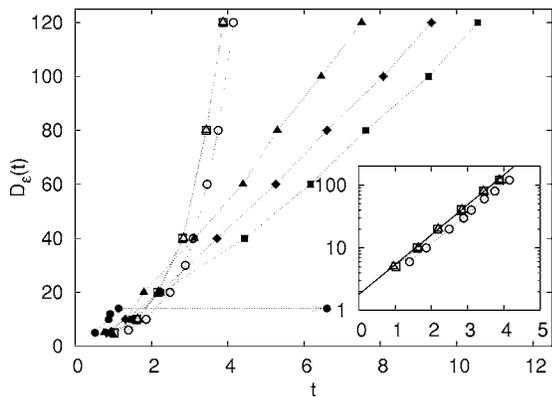


FIG. 3. $D_\epsilon(t)$ for local initial operators. We consider three cases $O(0)=\sigma_{n/2}^{x,y,z}$ (empty circles, squares, and triangles), for nonintegrable evolution H_C , and four cases, $O(0)=\sigma_{n/2}^{x,y}$ (full squares, diamonds), $\sigma_{n/2-1}^z \sigma_{n/2}^z$ (full triangles) with infinite index, and $O(0)=\sigma_{n/2-1}^z \sigma_{n/2}^z$ (full circles) with index 2, for integrable evolution H_R . Full line in the inset illustrates exponential growth $\propto e^{1.1t}$ in the nonintegrable case. Full squares and diamonds are for $n=40$, otherwise $n=20$.

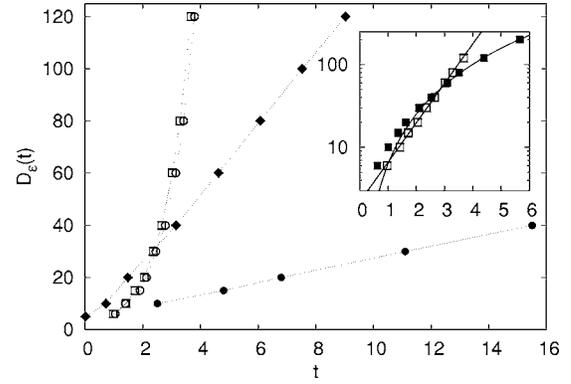


FIG. 4. $D_\epsilon(t)$ for extensive initial operators. For both Hamiltonians H_C, H_R we take $O(0)=\sum_j \sigma_j^x$ (empty, full squares) with infinite index, and $O(0)=H(0,1)$ (empty, full circles) with index 1. For H_R we also show case $O(0)=\sum_j \sigma_j^z \sigma_{j+1}^z + \sigma_j^y \sigma_{j+1}^y$ (full diamonds) with index 1 and 2. In the semilog inset we illustrate exponential increase $\propto e^{1.1t}$ (full straight line) for H_C and polynomial $\sim t^2$ (full curve) for H_R . For full circles $n=64$, otherwise $n=32$.

does not depend on ϵ , properties of $O(0)$ or n , for big n . For $H=H_C$ we find $h_q=1.10$.

In physics it is often useful to consider extensive observables, for instance translational sums of local operators, e.g., the Hamiltonian H or the total magnetization $M^s = \sum_{j=0}^{n-1} \sigma_j^s$. As opposed to local operators, extensive initial operators, interpreted as W-like super states, contain some long-range entanglement so one may expect that t -DMRG should be somewhat less efficient than for local operators. Indeed, in the integrable case we find for extensive operators with finite index that $D_\epsilon(t)$ does no longer saturate but now grows linearly, $D_\epsilon(t) \sim t$, whereas for extensive operators with infinite index the growth may be even somewhat faster, most likely quadratic $D_\epsilon(t) \sim t^2$ but clearly slower than exponential. In the nonintegrable case, we again find exponential growth $D_\epsilon(t) \sim \exp(h_q t)$ with the same exponent h_q as for local initial observables. The results are summarized in Fig. 4. Note that for local as well as for extensive observables $\eta_{\text{tot}}(t)$ asymptotically does not depend on n . Therefore the results shown in Figs. 3 and 4, for which convergence with n has been reached, are already representative of TL.

In the last set of numerical experiments we consider time efficiency of the evolution of a thermal initial state $O(t) = Z^{-1} \exp(-\beta H_0)$ under a sudden change of the Hamiltonian at $t=0$, namely $H(t<0)=H_0=H(0,1), H(t>0)=H_1$. Again, we treat two situations: in the first case we consider change after which the Hamiltonian remains integrable, $H_1=H(0,2)=H_R$, while in the other case the change breaks integrability of the Hamiltonian, $H_1=H(1,1)=H_C$. Initial state is prepared from identity super state using imaginary time t -DMRG with the same MPO rank D as it is later used for real time dynamics. We find, consistently with previous results, that at high temperature ($\beta \ll 1$) the rank $D_\epsilon(t)$ grows very slowly, perhaps slower than linear, in the integrable case, and exponentially $D_\epsilon(t) \sim \exp(h_q t)$, in the nonintegrable case. Interestingly, at lower temperatures we find exponential growth in both cases, even in the integrable one. This is not unreasonable as the initial (thermal) state can be expanded in

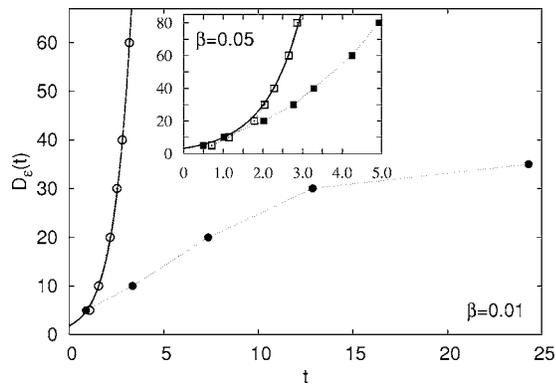


FIG. 5. $D_e(t)$ for thermal states of H_0 with $\beta=0.01$ ($\beta=0.05$ in inset), for evolution with H_C (open symbols) and H_R (full symbols) at $n=40$. Solid curves again indicate exponential increase $\propto e^{1.1t}$.

a power series in β and the higher orders H_0^p become less local with longer entanglement range as we increase the power p . These results are summarized in Fig. 5. In contrast

to local and W-like observables, the total truncation error $\eta_{\text{tot}}(t)$ is for thermal states proportional to n . Therefore, the fidelity at fixed t and D of t -DMRG simulation of thermal states decreases in TL.

In conclusion, we have presented numerical experiments suggesting that the scaling of classical computation resources in t -DMRG simulations of quantum 1D lattices with local interaction may sensitively depend on the integrability of the Hamiltonian, and on whether we propagate pure states or mixed states and/or observables. For the latter we find universal exponential growth of the minimal rank of the matrix product representation in physical time, unless we propagate by an integrable Hamiltonian from the initial state and/or observable which can be related to (sums of) local operators, in which case the growth is polynomial, or even saturates for a specific class of initial operators.

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- [10] Index of a product operator O [Sec. 2, first of Refs. [9]] is one-half the number of Fermi operators in Jordan-Wigner transformation of O and is a conserved quantity for H_R .
- [11] Based on numerical results and intuitive arguments we conjecture that if $O(0)$ is a superposition of finite number of product operators, such that only a single term has the maximal index ν , then the rank saturates at $D_e(\infty)=4^\nu$.