Entanglement dynamics in harmonic-oscillator chains

R. G. Unanyan and M. Fleischhauer
Fachbereich Physik und Forschungszentrum OPTIMAS, Technische Universität Kaiserslautern, D-67663 Kaiserslautern, Germany
(Received 7 March 2014; published 26 June 2014)

We study the long-time evolution of the bipartite entanglement in translationally invariant one-dimensional harmonic lattice systems. We show that for Gaussian states, in quadratic interactions with periodic boundary conditions, there exists a lower bound for the von Neumann entropy which increases linearly in time. This implies that the dynamics of harmonic lattice systems can in general not efficiently be simulated by algorithms based on matrix-product decompositions of the quantum state, and interactions are needed to suppress the entanglement growth with time.

DOI: 10.1103/PhysRevA.89.062330 PACS number(s): 03.67.Bg, 05.50.+q, 03.65.Ud, 05.70.Jk

I. INTRODUCTION

In recent years so-called matrix product states (MPS) have received much attention for the numerical simulation of one-dimensional (1D) quantum many-body systems [1,2] (see for review [3]). This is because the ground state of fermionic and bosonic lattice systems with finite-range interactions and an excitation gap usually implies an area law of entanglement [4–8], stating that the von Neumann entropy of a partition scales with the surface size. In 1D the surface area is independent of the size of the system, resulting in a weakly entangled ground state, which can thus faithfully be represented by MPS. Even when the excitation gap vanishes, e.g., for free fermions [9,10] and bosons [13–16], i.e., for critical systems, there is only a correction which is at most logarithmic in the system size. The situation is, however, quite different for nonequilibrium problems as here the scaling not only with size but also with time is relevant. With respect to the latter only an upper bound derived by Lieb and Robinson exists [17], which states that the von Neumann entropy increases at most linearly in time. Being an upper bound, it does not allow us to draw any conclusion about the approximability of the long-time dynamics of quantum many-body systems by MPS. However, it is very often found that the bipartite entropy does indeed scale linear in time, which implies that the required computational resources increase exponentially. For example it has been shown for the spin-$\frac{1}{2}$ XY model that the entropy grows linearly with time after a global quench [18]. On the other hand, it was found for the case of free fermions that the entropy may grow only logarithmically in time [19], showing that for certain initial states the long-time dynamics is accessible with MPS-based methods. To the best of our knowledge, there are no such studies for the entanglement entropy of bosons.

In the present paper we study the time evolution of the entropy in 1D bosonic systems that evolve under translationally invariant quadratic Hamiltonians with local or finite-range couplings. It should be noted that this model is an exactly solvable one, and the dynamics of logarithmic negativity and correlation functions between spatially separated oscillators have been studied in Refs. [11,12]. To separate the problem of size scaling from the scaling with time, which is the subject of interest in this paper, we consider a specific class of 1D systems and initial conditions where the bipartite entropy becomes independent of system size. Specifically we choose as the initial state of the time evolution the ground state $\Phi$ of some local, gapped Hamiltonian $H_0$. One can intuitively expect that under such initial conditions the bipartite entanglement entropy of the time-evolved state will be independent of system size for the following reasons: For the ground state of local Hamiltonians the presence of an excitation gap is sufficient for an area law of entanglement [8], hence the entropy of the initial state is size independent. Furthermore it is easy to see that the state time-evolved under a Hamiltonian $H, \Psi(t) = \exp[-i H t]\Phi$, which is the ground state of a time-dependent Hamiltonian $H'[t] = \exp[-i H_0] H_0 \exp[i H t]$. The spectrum of $H'[t]$ is identical to that of $H_0$, i.e., it too has an excitation gap. Finally the Lieb-Robinson bounds guarantee that for any fixed time $t$ its coupling matrix elements between sites $i$ and $j$ are exponentially small beyond a certain distance $l_*$. Hence for $|i-j| > l_*$ the growth of $H'[t]$ is also of finite range [20]. As a consequence we can expect that the entanglement entropy of the time-evolved state will saturate with increasing system size. However, it is not possible to draw any conclusion about the time-scaling of entanglement beyond the limits set by the Lieb-Robinson upper bounds.

In the present paper we show that in contrast to free fermions the entropy of the time-evolved quantum state of free bosons always grows linearly in time. This means that contrary to intuition for bosonic systems interactions are crucial to suppressing the increase of entanglement with time and to making long-time simulations with MPS-based methods possible.

II. TRANSLATIONALLY INVARIANT HARMONIC OSCILLATORS

To be specific we consider a one-dimensional system of $N$ bosonic oscillators described by $N$ pairs of canonical operators $\mathbf{x} = (x_1,x_2,\ldots,x_N)$ and $\mathbf{p} = (p_1,p_2,\ldots,p_N)$. The oscillators are coupled by a quadratic Hamiltonian of the form

$$H = \frac{1}{2} \mathbf{p}^2 + \frac{1}{2} \mathbf{x} | V | \mathbf{x} ,$$

where $V$ is a real, symmetric, positive definite, time-independent matrix. We assume translational invariance, implying that $V$ is a Toeplitz matrix. Furthermore we consider periodic boundary conditions, such that $V$ is circulant. Circulant matrices form a commutative algebra. Moreover the elements of a circulant matrix can be generated from the...
spectral function $\lambda(\theta) > 0$: 

$$
V_{kk} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, \lambda(\theta) \, e^{-i(k-k')\theta}.
$$

The square root of the spectral function $\lambda(\theta)$ can be interpreted as a dispersion relation, $\lambda^{1/2}(\theta)$ being the frequency of a wave with wave number $\theta$.

We now want to determine the scaling of the entanglement entropy with time. To this end we have to find the time evolution under the local Hamiltonian (1). The system is assumed to start its evolution at $t = 0$ from a Gaussian state, i.e.,

$$
\Phi(x) = a_0 \exp \left(-\frac{1}{2} |x| B |x| \right), \quad a_0 = \left(\det B / \pi^n \right)^{1/4},
$$

where $B$ is a real, symmetric, and positive definite Toeplitz matrix. Periodic boundary conditions imply that $B$ is also a circulant matrix with spectral function $\beta(\theta)$. As the initial state is the ground state of a gapped, local Hamiltonian, $\beta(\theta)$ is nonzero and regular corresponding to a noncritical state. Since the Hamiltonian of the system is quadratic, the time-evolved state remains Gaussian and we have to search for a solution in the form

$$
\Psi(x,t) = \frac{1}{(\pi^N \det \bar{A}^{-1})^{1/4}} \exp \left(-\frac{1}{2} |x| A(t) |x| \right).
$$

Here and in the following a tilde denotes the real part, i.e., $\tilde{X} = \Re X$. By taking into account the symmetry of $B$ and after simple calculations one can easily find that $A(t)$ obeys Riccati’s equation

$$
\frac{\partial A}{\partial t} = A^2 - V, \quad A(0) = B.
$$

Its solution can be written as

$$
A(t) = V^{1/2} \cos(t V^{1/2}) B + i V^{1/2} \sin(t V^{1/2}) \cos(t V^{1/2}) V^{1/2} + i \sin(t V^{1/2}) B',
$$

which is again a circulant matrix. The spectral function $\Lambda(\theta,t)$ of its real part $\Lambda$ can easily be obtained from $\lambda(\theta)$ and $\beta(\theta)$:

$$
\Lambda(\theta,t) = \frac{\beta(\theta) \lambda(\theta)}{\lambda(\theta) \cos^2[\lambda^{1/2}(\theta)] + \beta^2(\theta) \sin^2[\lambda^{1/2}(\theta)]}.
$$

Note that if $B = V^{1/2}$, the spectral function and thus the matrix $A(t)$ becomes time independent, because in this case the initial state is the ground state of the full Hamiltonian.

### III. LOWER BOUNDS TO ENTANGLEMENT GROWTH

Having the solution of the Schrödinger equation we can now calculate the reduced density matrix of a block of $N-n$ oscillators and from this a lower bound to the rate of entanglement growth.

#### A. Reduced density matrix

The reduced density matrix can be obtained by partitioning the symmetric matrices $A(t)$ and $A^{-1}(t)$ into blocks

$$
A(t) = \begin{bmatrix} T & C \\ C^T & R \end{bmatrix}, \quad A^{-1}(t) = \begin{bmatrix} Q & D \\ D^T & P \end{bmatrix},
$$

where $T$ is an $n \times n$ and $R$ an $(N-n) \times (N-n)$ matrix. Similar calculations have been done in Refs. [21,22] for the ground state of a chain of oscillators. After a lengthy but straightforward calculation we find for the matrix elements of the reduced density operator (see for details, e.g., [21,22])

$$
\rho_R(x,x') = N \exp \left[ \frac{x^T}{\Delta} \begin{bmatrix} -\Gamma & \Delta \\ \Delta & -\Gamma^* \end{bmatrix} \frac{x'}{\Delta} \right].
$$

where $x = (x_{n+1}, \ldots, x_N)$, $x' = (x'_{n+1}, \ldots, x'_N)$ are the coordinates of the remaining $N-n$ oscillators,

$$
\Gamma = \frac{R}{2} - \frac{C^T \tilde{T}^{-1} C}{4}, \quad \Delta = \frac{C^T \tilde{T}^{-1} C^*}{4},
$$

and $N = (\det \tilde{P}^{-1/2}/(\pi)^{2n})$ is a normalization with

$$
\tilde{P}^{-1} = \tilde{R} - \tilde{C}^T \tilde{T}^{-1} \tilde{C}.
$$

#### B. Dynamics of von Neumann entropy and purity

We proceed by analyzing the dynamical behavior of the bipartite entanglement. There are several measures of entanglement between parties of a closed system, examples being the von Neumann entropy $S = -\text{tr} \{ \rho \ln \rho \}$ and the purity $\text{tr} \{ \rho^2 \}$, where the following inequality holds: $S \geq -\ln \text{tr} \{ \rho^2 \}$. It should be noted that $-\ln \text{tr} \{ \rho^2 \}$ represents also a lower bound to all Renyi entropies $S_{\alpha} = \frac{1}{1-\alpha} \ln \text{tr} \{ \rho^2 \}$ with $\alpha < 1$ as $S_{\alpha} \geq S_1 = S$.

To derive a lower bound for the entropy we calculate the purity of Eq. (9).

$$
\text{tr} \{ \rho^2 \} = \int dxdx' \rho_R(x,x') \rho_R(x',x).
$$

The Gaussian nature of (9) allows to calculate this integral in a straightforward way

$$
\text{tr} \{ \rho^2 \} = \frac{\det \tilde{P}^{-1}}{\det[\tilde{T} - \Delta] \det[\tilde{T} + \Delta]^{1/2}}.
$$

After simple algebra one obtains

$$
\text{tr} \{ \rho^2 \} = \{ \text{tr} \{ \tilde{P} (\tilde{R} + Z^T \tilde{T}^{-1} Z) \} \}^{-1/2} \leq \{ \text{tr} \{ \tilde{P} \tilde{R} \} \}^{-1/2},
$$

where $Z = (C - C^*)/2i$. The last inequality follows from the fact that $Z^T \tilde{T}^{-1} Z$ is a positive definite matrix. With this we find the following lower bound to the von Neumann entropy:

$$
S \geq -\ln \text{tr} \{ \rho^2 \} \geq \frac{1}{2} \ln \text{det} \{ \tilde{P} \tilde{R} \}.
$$

To facilitate analytical calculations of determinants, we consider the limits $N \gg 1$ and $N > n \gg 1$. It can then be shown [13] that in this limit the elements of matrices $\tilde{R}$ and $\tilde{P}$ can be generated from the spectral functions $\Lambda(\theta,t)$ and $\Lambda^{-1}(\theta,t)$, respectively. Since $\Lambda(\theta,t)$ is a regular function, i.e., $\Lambda(\theta,t) > 0$ for any $t$, we may apply the strong Szegö...
Theorem [23] to calculate the determinants. According to this theorem

\[ S \geq \sum_{k=1}^{\infty} |c_k|^2, \quad (14) \]

where the \( c_k \) are Fourier coefficients of \( \Lambda^{-1}(\theta,t) \), i.e.,

\[ c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \ln \Lambda^{-1}(\theta,t) \exp(-i\theta k). \quad (15) \]

If \( \beta(\theta) \) and \( \lambda(\theta) \) are constant functions, i.e., the oscillators are uncoupled, all Fourier coefficients (15) vanish except for \( c_0 \). In this case Eq. (14) reduces to the trivial bound \( S \geq 0 \) (entanglement is never generated). In what follows we will consider only the nontrivial case when \( \lambda(\theta) \) is not a constant.

In Fig. 1 we have plotted the right-hand side of Eq. (14) numerically evaluated for an initial state with spectral function \( \beta(\theta) = 1 \) and a Hamiltonian \( H \) with spectral function \( \lambda(\theta) = [c - \cos(\theta)]^2 \). If \( c > 1 \), \( H \) has a finite excitation gap since there is no real zeroth of \( \lambda(\theta) \). If the gap vanishes, i.e., for \( c \leq 1 \), the ground state of \( H \) becomes critical. One clearly recognizes a linear increase with time. The insert shows the correction to the initial spectral function is proportional to the difference \( \beta^2(\theta) - \lambda(\theta) \), as was expected. The Fourier coefficients \( c_k \) in Eq. (15) can then easily be calculated as

\[ c_k \approx \xi_k + t^2 \delta_k, \]

where \( \xi_k \) and \( \delta_k \) are some constant numbers. From this, one can calculate the sum (14) for short time, which yields

\[ S \geq x_1 + x_2 t^2. \quad (17) \]

2. Long-time dynamics

In the following we will derive an analytic estimate for the lower bound to the entropy for long times. Note that \( \beta^2(\theta) = \lambda(\theta) \) corresponds to an initial state that is an eigenstate of \( H \) and thus has no time evolution at all. In any real system, the number of oscillators in the chain is finite and therefore in order to neglect boundary effects in the thermodynamic limit it is necessary to consider time intervals \( t \leq L/v \), where \( v \) is the speed of excitation after a quench, the so-called Lieb-Robinson speed [17] (see also [20]), and \( L \) is the system size. For the sake of simplicity of the derivations we consider a Hamiltonian \( H \) with a finite excitation gap. The derivation for a nongapped Hamiltonian is more involved and will not be presented here. As noted above, the presence of a gap is, however, irrelevant. In the following we use an alternative expression for \( \sum_{k=\infty}^{\infty} |c_k|^2 \) which is very useful for numerical and analytical calculations. By Parseval’s theorem this sum can be rewritten as (see the Appendix for details)

\[ \sum_{k=1}^{\infty} |c_k|^2 = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\eta_1 d\eta_2 \ln^2 \frac{\Lambda(\theta_1 - \eta_1, t)}{\Lambda(\theta_1 + \eta_1, t)} \sin^2 \eta_2. \quad (18) \]

Making use of the inequality

\[ \ln \frac{x}{y} > \frac{1}{M} |x - y|, \quad 0 < x, y \leq M, \]

one finds

\[ S \geq \frac{1}{M^2} \sum_{k=1}^{\infty} |b_k|^2, \quad (19) \]

where \( M = \max \Lambda(\theta, t) \), and

\[ b_k = \frac{1}{2\pi} \int_{0}^{2\pi} d\eta \Lambda^{-1}(\theta, t) \exp(-i\eta k). \quad (20) \]

The coefficients \( b_k \) have a simple physical meaning: They determine the correlations in momentum space over a distance \( k \), i.e., \( \langle \Psi(t) | p_k p_{k+l} | \Psi(t) \rangle \sim b_k \). With this we have

\[ S \geq \frac{1}{M^2} \sum_{k=1}^{\infty} \kappa_k + \mu_k(t)^2, \quad (21) \]

where we have decomposed \( \Lambda^{-1}(\theta,t) \) in a time-independent and a time-dependent term

\[ \kappa_k = \frac{1}{4\pi} \int_{0}^{2\pi} d\theta \frac{\lambda(\theta) + \beta^2(\theta)}{\beta(\theta) \lambda(\theta)} \cos(k\theta), \quad (22) \]

\[ \mu_k(t) = \frac{1}{4\pi} \int_{0}^{2\pi} d\theta \frac{\lambda(\theta) - \beta^2(\theta)}{\lambda(\theta) \beta(\theta)} \cos(2\theta \lambda^{1/2}(\theta)) \cos(k\theta). \quad (23) \]
The term proportional to $\zeta_2^2$ in Eq. (21) does not depend on time and can be disregarded. The second term can be estimated using the Cauchy-Schwarz inequality

$$\left| \sum_{k=1}^{\infty} k \zeta_k \mu_k(t) \right| \leq \left( \sum_{k=1}^{\infty} k^2 \zeta_k^2 \right)^{1/2} \left( \sum_{k=1}^{\infty} \mu_k^2(t) \right)^{1/2}.$$  

Applying again the Cauchy-Schwarz inequality we obtain

$$\sum_{k=1}^{\infty} k^2 \mu_k^2(t) = \sum_{k=1}^{\infty} |\mu_k(t)||\mu_k(t)| \leq \left( \sum_{k=1}^{\infty} k^2 |\mu_k(t)|^2 \right)^{1/2} \left( \sum_{k=1}^{\infty} |\mu_k(t)|^2 \right)^{1/2},$$

and by Parseval’s theorem, one has

$$\sum_{k=1}^{\infty} k^2 |\mu_k(t)|^2 = \frac{1}{2\pi} \int_0^{\pi} d\theta \left( \frac{d}{d\theta} \frac{\lambda(\theta) - \beta^2(\theta)}{\lambda(\theta)\beta(\theta)} \cos[2\pi \lambda^{1/2}(\theta)] \right)^2,$$

(24)

and

$$\sum_{k=1}^{\infty} |\mu_k(t)|^2 = -|\mu_0(t)|^2 + \frac{1}{2\pi} \int_0^{\pi} d\theta \left( \frac{\lambda(\theta) - \beta^2(\theta)}{\lambda(\theta)\beta(\theta)} \cos[2\pi \lambda^{1/2}(\theta)] \right)^2.$$

(25)

The time dependence of the sum $|\sum_{k=1}^{\infty} k \zeta_k \mu_k(t)|$ is thus bounded from above by the square root of $t$.

We now show that the term $\sim \mu_k(t)^2$ in Eq. (21) is bounded from below by a function linear in $t$. As the interaction matrix $V$ is of finite range, the spectral function $\lambda(\theta)$ is a trigonometric polynomial of finite degree $K$. We introduce the group velocity of eigenmodes of the quenched Hamiltonian (1)

$$v_g(\theta) = \left| \frac{d\lambda^{1/2}(\theta)}{d\theta} \right| = \frac{1}{2} \left| \frac{d\lambda(\theta)}{d\theta} \right| \lambda^{1/2}.$$

(26)

By the theorem of Bernstein [23] one has max $|\frac{d\lambda(\theta)}{d\theta}| \leq K$ max $\lambda(\theta)$, and therefore

$$v_g(\theta) \leq \frac{K \max \lambda(\theta)}{2\sqrt{\min \lambda(\theta)}} = v_m.$$

(27)

Hence if $k \geq k_{\text{max}} = v_m t$ for any $\alpha > 0$ there exists a constant $C_2$ depending on $\lambda(\theta)$ and $\beta(\theta)$ such that for all $t$ and $k$ with $k > v_g t$

$$|\mu_k(t)| \leq \frac{C_2}{k^\alpha}.$$

(28)

On the other hand, one finds

$$\sum_{k=1}^{\infty} k^2 \mu_k^2(t) > \sum_{k=1}^{v_m} k^2 \mu_k^2(t) > \sum_{k=1}^{v_m} \frac{k^2}{1 + k^2 \mu_k^2(t)}$$

$$> \frac{1}{1 + v_g t} \sum_{k=1}^{v_m} k^2 \mu_k^2(t)$$

$$= \frac{1}{1 + v_g t} \left( \sum_{k=1}^{\infty} k^2 \mu_k^2(t) - \sum_{k=v_m + k_{\text{max}} = v_m t}^{\infty} k^2 \mu_k^2(t) \right).$$

The second term in the brackets vanishes for large $t$ according to the estimation (28). By Parseval’s theorem we arrive at

$$\sum_{k=1}^{\infty} k^2 \mu_k^2(t)$$

$$> \frac{1}{1 + v_g t} \int_0^{\pi} d\theta \left( \frac{d}{d\theta} \frac{\lambda(\theta) - \beta^2(\theta)}{\lambda(\theta)\beta(\theta)} \cos[2\pi \lambda^{1/2}(\theta)] \right)^2$$

for large $t$. By neglecting all highly oscillating terms one eventually finds

$$S > \frac{t}{\pi v_m} \int_0^{\pi} d\theta \left( \frac{\lambda(\theta) - \beta^2(\theta)}{\lambda(\theta)\beta(\theta)} \right)^2 v_g^2(\theta).$$

(29)

Equation (29) is the main result of our paper. We see that the rate of generation of entanglement is proportional to the group velocity of excitations of the quenched Hamiltonian. And the energy difference between initial and quenched states acts as a source of entanglement production.

IV. SUMMARY

We derived a lower bound to the scaling of the entanglement entropy $S_\alpha, \alpha \leq 1$ with time in a one-dimensional system of coupled harmonic oscillators. The main result, Eq. (29), implies that the bond dimension of the matrices used in an MPS representation needs to increase exponentially in time to allow a faithful representation of the dynamical many-body wave function. This means that in contrast to fermionic systems, where at least for certain initial conditions a simulation of the long-time dynamics is possible, for harmonic-oscillator systems this is in general impossible. For bosons, interactions are necessary to suppress the growth.

There are many directions for extending the presented approach. The discussion can be immediately generalized to a two-dimensional array of harmonic oscillators, with an interaction of finite range in one direction and an infinite range in the other direction [25]. Another important study can be investigating the quench dynamics in long-range interacting systems including bosonic and fermionic freedoms in trapped ions [26]. An interesting extension of this work will be to examine the evolution of the entropy starting from a non-Gaussian initial state.

ACKNOWLEDGMENTS

The authors thank J. Eisert for stimulating discussions. The financial support of the DFG through the SFB-TR49 is gratefully acknowledged.
APPENDIX

By definition of Fourier coefficients, we have

$$\ln \Lambda^{-1}(\eta_1 + \eta_2, t) - \ln \Lambda^{-1}(\eta_1 - \eta_2, t) = \sum_{k=-\infty}^{\infty} c_k [\exp(i\eta_2 k) - \exp(-i\eta_2 k)] \exp(i\eta_1 k) = \sum_{k=-\infty}^{\infty} 2i c_k \sin \eta_2 k \exp(i\eta_1 k).$$

By Parseval’s theorem, one has

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\eta_1 |\ln \Lambda^{-1}(\eta_1 + \eta_2, t) - \ln \Lambda^{-1}(\eta_1 - \eta_2, t)|^2 = 4 \sum_{k=-\infty}^{\infty} |c_k|^2 \sin^2 \eta_2,$$

and therefore

$$\frac{1}{8\pi^2} \int_{-\pi}^{\pi} d\eta_1 \int_{-\pi}^{\pi} d\eta_2 |\ln \Lambda^{-1}(\eta_1 + \eta_2, t) - \ln \Lambda^{-1}(\eta_1 - \eta_2, t)|^2 = \frac{1}{2\pi} \sum_{k=1}^{\infty} |c_k|^2 \int_{-\pi}^{\pi} d\eta_2 \frac{\sin^2 k\eta_2}{\sin^2 \eta_2} = \sum_{k=1}^{\infty} |c_k|^2 k.$$

We have used the fact that for $k \geq 1$,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\eta \frac{\sin^2 k\eta}{\sin^2 \eta} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\eta \frac{|e^{2ik\eta} - 1|^2}{|e^{2\eta} - 1|^2} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\eta \left| \sum_{m=0}^{k-1} e^{2im\eta} \right|^2 = k.$$