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Quantum quenches in two spatial dimensions using chain array matrix product states

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We describe a method for simulating the real time evolution of extended quantum systems in two dimensions (2D). The method combines the benefits of integrability and matrix product states in one dimension to avoid several issues that hinder other applications of tensor based methods in 2D. In particular, it can be extended to infinitely long cylinders. As an example application we present results for quantum quenches in the 2D quantum [(2 + 1)-dimensional] Ising model. In quenches that cross a phase boundary we find that the return probability shows nonanalyticities in time.

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Introduction. The advent of ultracold atomic gas experiments has led to a surge of interest in the time evolution and out-of-equilibrium behavior of many-body quantum systems. Much effort has been focused on one-dimensional (1D) problems because these can be tackled by analytically tractable or highly accurate numerical methods. Key questions that these studies have sought to elucidate are whether and how such systems thermalize after a sudden change, or “quantum quench” of a system’s Hamiltonian, with particular emphasis on the role played by conserved charges in 1D integrable systems [1–11].

Experiments, however, are not limited to 1D and it is interesting to explore similar questions in two dimensions (2D) and above [12]. Unfortunately there is no analog in 2D of the aforementioned analytically exact 1D methods. Numerical approaches using matrix product state (MPS) representations, so successful in 1D, suffer in 2D due to the “area law” growth of entanglement [13,14]. This growth reduces the efficiency of MPS (and related “tensor”) algorithms and limits them to smaller system sizes.

Nonetheless, MPS algorithms can be applied in 2D, by labeling lattice sites (usually in a zigzag fashion) to map to a 1D system [15]. The cost is that nearest neighbor interactions in 2D are mapped to increasingly long ranged 1D interactions, imposing an increasing numerical burden. Recently, progress has been made in performing real time evolution on MPS with such long ranged Hamiltonians by two different routes [16,17]. Algorithms based on generalizations of MPS to higher dimensions, such as projected entangled pair states (PEPS) [18,19], make use of imaginary time evolution to find ground states [20]. However, these higher dimensional tensor methods have not been applied to real time evolution.

In this Rapid Communication we demonstrate that real time evolution is possible for large 2D systems by combining information coming from exactly solvable models with a highly anisotropic MPS formulation. Such an approach retains the contraction efficiency of matrix product states over other tensor methods, while avoiding the build up of long ranged interactions. Our setup will be similar to that used in the density matrix renormalization group (DMRG) studies described in Refs. [21,22] except that here we are explicit in our use of MPS. This change allows for straightforward implementation of algorithms other than DMRG, including those for time evolution and for accurately working with the thermodynamic limit. In particular, using time evolving block decimation (TEBD) [23] we demonstrate that we can study the time evolution after a quench of infinitely long cylinders, with sufficient circumference that we approach the 2D thermodynamic limit. This includes strong quenches where we cross phase boundaries of a 2D quantum system.

Method. At the core of our method is the wish to maximize the analytically exact input going into our MPS algorithm, while simultaneously controlling the growth of entanglement entropy. The construction we use is depicted in Fig. 1: a coupled array of exactly solvable 1D subunits. For each subunit, we have exact knowledge of the spectrum and matrix elements. This exact knowledge means that we begin with the numerics already having accounted for much of the strong correlations of the system. We emphasize our use of exactly solvable models as a building block is not much of a limitation to the method. Such models are ubiquitous in 1D, including Heisenberg spin chains, Luttinger liquids, and Hubbard models to name but a few [24,25]. In this framework, a state of a system of $N$ chains is written in MPS form via

$$|\Psi\rangle_{2D} = \sum_\sigma A^{\sigma[1]} \cdots A^{\sigma[N]} |\sigma_1 \cdots \sigma_N\rangle,$$

where each matrix $A^{\sigma,i}$ is labeled by a chain $i$ and an eigenstate of that individual chain $\sigma_i$. Like the single sites used in 1D MPS algorithms, we are able to manipulate these chain eigenstates because we know their energies and matrix elements for any relevant operator.

For ground and low-lying states of the system the entanglement entropy $S_E$ scales as the boundary “area,” that is to say, the chain length. By keeping the chain length finite we can throttle the growth of $S_E$. By partnering this with the fact that for the systems that we will study, finite size effects are exponentially suppressed, we are able to keep $S_E$ small while remaining in the 2D thermodynamic limit. We have previously demonstrated the effectiveness of this
methodology in equilibrium by studying a 2D quantum [i.e., (2 + 1)-dimensional] critical point [21,22].

The continuum 1D subunits will necessarily have an infinitely large Hilbert space. However, if the system size $R$ is finite the spectrum is discrete, and we may truncate at a cutoff energy $E_c$. This step is justified by appeal to the truncated conformal spectrum approach [26] where it has been observed over a wide body of examples [27–29] that for relevant (in the renormalization group sense) interchain interactions, the low energy sector of a perturbed integrable system is formed primarily from (possibly strong) admixtures of low-lying states of the unperturbed system. Here we will focus on exactly such interchain perturbations.

Equation (1) differs from a MPS for a 1D system only in that the "physical indices" $\sigma$ may be large (see Table I of [30]), requiring strict use of sparse matrices to maximize computational resources. It is also important to take advantage of good quantum numbers and to perform matrix operations (e.g., singular value decompositions) in a block diagonal manner, to help preserve the sparse nature of the matrices and increase numerical efficiency.

MPS time evolution algorithms may then be implemented just as for a 1D system, including TEBD [23] and its infinite counterpart (iTEBD) [31–34]. For the former we may work with a torus or open cylinder geometry; the latter corresponds to a cylinder joined together at its ends to study toroidal systems. For the former we may work in that the "physical indices" $\sigma$ are large (see Table I of [30]), requiring strict use of sparse matrices to maximize computational resources. It is also important to take advantage of good quantum numbers and to perform matrix operations (e.g., singular value decompositions) in a block diagonal manner, to help preserve the sparse nature of the matrices and increase numerical efficiency.

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is a region, \( t_{\Delta,t_{Jz}} < t < t_R \), where we may expect the time evolution to be representative of the 2D thermodynamic limit. But for \( t > t_R \) the finite nature of the chains’ circumferences will play a role. We stress that \( t_R \) does not govern the time scale for revivals in the system. Instead these occur on a much longer time scale, \( t_{\text{revolved}} \sim N t_J \), where \( N \) is the number of chains in the system. Thus in our iTEBD simulations, we never expect to see strict revivals.

To illustrate these time scales in operation, we consider the occupation number, \( n_i(x) \), scaled by interchain coupling, \( J_z \). We indicate the time scale \( t_R \) at which we expect the system postquench to see the effects of the finite circumference of the system. Inset: \( R = 10 \) iTEBD data compared with the perturbative result (P.T.) (dashed line).

In Fig. 2, we see that for a given chain length, \( R \), we can find cutoffs, \( E_c \) such that the time evolution is converged.

It is also possible to calculate postquench correlations between the chains. We show the nearest neighbor spin-spin correlation function as a function of time, \( \langle \sigma_z^{R,i}(x,t) \sigma_z^{R,j}(x,t) \rangle \), for a selection of \( R \) and \( j_z \). Our choice of \( j_z > 0 \) favors antiferromagnetic correlations, producing the overall negative sign. An expansion in small \( t \) shows that this quantity is proportional to \( t^2 \) allowing us to collapse the results onto a single curve at short times. Here we see signatures of both the \( t_{Jz} \) and \( t_R \) scales. In the inset we have marked the intrachain scattering time \( t_{Jz} \), for the system with \( R = 8 \) and \( j_z = 0.1 \). It is visible as the time that the \( j_z = 0.1 \) and \( j_z = 0.01 \) data begin to diverge. We also mark the time scale \( t_R \) at which the data for chains with \( R = 8 \), \( j_z = 0.01 \) begins to diverge from that of \( R = 10 \), \( j_z = 0.01 \).

To show that our method can handle nontrivial aspects of quenching through the critical coupling of the coupled chain system, we search for nonanalyticities in the Loschmidt echo as a function in time. The “Loschmidt echo” or overlap probability at a particular \( t \) is the modulus squared of the overlap between the initial and time evolved state:

\[
G(t) = |\langle \Psi_0 | e^{-iH_{\text{iso}} t} | \Psi_0 \rangle|^2,
\]

where \( \Psi_0 \) is the ground state of the uncoupled chain system. In 1D it is useful to define a per site rate function, \( \ell(t) \) via \( G(t) = \exp[-N \ell(t)] \). Nonanalyticities in \( \ell(t) \) have been interpreted as “dynamical phase transitions,” following an exact calculation of this quantity for the 1D TFIM [41–43]. The general association of such nonanalytic points with equilibrium critical phenomena is contested [44,45], but we demonstrate analytically in low order perturbation theory [30] that for quenches to \( j_z > 0.27 \) we expect nonanalyticities in \( G(t) \). While this estimate for the value of \( j_z \) is larger than \( j_z \)—because of the low order to which we took the computation—it does suggest that simple perturbation theory for the quantity \( G(t) \) can be used to estimate the phase boundaries in some 2D quantum systems.
corresponding quench to $t/\Delta_1$ for a quench to $R = 10$
near the edge of a plateau, whereas for a finite number of chains it takes the
TEBD. The first nonanalytic point for the infinite cylinder forms the
scales with system volume $V$. We are able to simulate, and see that the nonanalyticity has the
comparison we plot log $G(t)$ for a quench to $j_\perp = 0.1$—a value of $j_\perp$ where we should see nonanalyticities. In 2D this quantity scales with system volume $RN$, as does its 1D counterpart \cite{41}. We also observe that it scales with $j^2_\perp$. As expected we find nonanalytic behavior for this quench, within the time window we are able to simulate, and see that the nonanalyticity has the same qualitative structure for both $E_c = 7|\Delta|$ and $8|\Delta|$. For comparison we plot log $G(t)$ for a quench to $j_\perp = 0.1$, where in contrast we find that this quantity is smooth within our simulation window. We remark that nonanalyticities appear for
the same quantity with $j_\perp = 0.2$ (not plotted), just above $j_\perp = 0.185$, but they first occur only at the edge of the attainable times with iTEBD.

Finally we consider the case of finite length and open boundary conditions. The TEBD algorithm is slower by approximately a factor of $N$ due to the loss of translational invariance along the cylinder. We find negligible effect, for finite $N \gtrsim 10$ and $i$ away from the ends of the cylinder, on the results for local quantities such as $n_i(x)$ (up to the time scales we reach). However, this is not true for the Loschmidt echo (a global measure), especially when $|j_\perp| > j_c$. The inset of Fig. 4 shows the difference between the iTEBD and $N = 100$ results for $R = 6$, $j_\perp = 0.5$. While there is excellent agreement up to $t \sim t_\Delta$ (not shown), afterwards there is a clear difference in the nonanalytic point structure. We also find that this effect is even more pronounced for very small $R$ and large $N$ (where our model reduces to a single 1D TFIM), suggesting that boundary conditions have a non-negligible effect on the Loschmidt echo even for large systems. This last result has important consequences for possible experimental investigations.

Conclusions. We have demonstrated a robust method to compute dynamical behavior in 2D quantum ($d = 2 + 1$) systems after a quench, which we intend to use to study other systems including coupled quantum wires (i.e., coupled Luttinger liquids) and Heisenberg chains. The algorithm should prove especially useful when interpreting nonequilibrium cold atom \cite{46,47} and pump-probe experiments in the cuprates \cite{48,49}.

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[40] A sudden quench pumps more energy into the system relative to a ramped quench, and therefore will populate higher energy modes, reducing the efficiency of the algorithm.