Disentangling sources of quantum entanglement in quench dynamics

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Quantum entanglement may have various origins ranging from solely interaction-driven quantum correlations to single-particle effects. Here, we explore the dependence of entanglement on time-dependent single-particle basis transformations in fermionic quantum many-body systems, thus aiming at isolating single-particle sources of entanglement growth in quench dynamics. Using exact diagonalization methods, for paradigmatic nonintegrable models we compare to the standard real-space cut various physically motivated bipartitions. Moreover, we search for a minimal entanglement basis using local optimization algorithms, which at short to intermediate postquench times yields a significant reduction of entanglement beyond a dynamical Hartree-Fock solution. In the long-time limit, we identify an asymptotic universality of entanglement for weakly interacting systems, as well as a crossover from dominant real-space to momentum-space entanglement in Hubbard models undergoing an interaction quench. Finally, we discuss the relevance of our findings for the development of tensor-network-based algorithms for quantum dynamics.

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Entanglement as one of the most fundamental traits of quantum mechanics plays a key role in various physical contexts, ranging from the characterization of complex many-body states [1,2] to its use as a resource for quantum technologies [3–7]. On the other hand, strong entanglement in body states [1,2] to its use as a resource for quantum technologies, ranging from the characterization of complex many-body states to its use as a resource for quantum technologies. Using exact diagonalization methods, for paradigmatic nonintegrablemodels we compare to the standard real-space cut various physically motivated bipartitions. Moreover, we search for a minimal entanglement basis using local optimization algorithms, which at short to intermediate postquench times yields a significant reduction of entanglement beyond a dynamical Hartree-Fock solution. In the long-time limit, we identify an asymptotic universality of entanglement for weakly interacting systems, as well as a crossover from dominant real-space to momentum-space entanglement in Hubbard models undergoing an interaction quench. Finally, we discuss the relevance of our findings for the development of tensor-network-based algorithms for quantum dynamics.

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Eqs. (4) and (5) far from equilibrium. Different curves correspond to a basis of dispersing Wannier orbitals, in comparison to a standard real-space basis of the interacting model defined in Eqs. (4) and (5) far from equilibrium. Different curves correspond to different entanglement cuts (see plot legend). Inset: Basis optimization of entanglement beyond the dynamical Hartree-Fock cut. Parameters are $L = 24$, $n_p = 12$, $U = J = 1.0$, $W = 0$, $m_i = 1.8$, $m_f = 0.2$. 

state of $H_i$ at $t < 0$. Using numerically exact Krylov time-propagation methods [38,39], for several examples of $H_i$ and $H_f$ representing quenches into nonintegrable systems, we then compute the time-evolved wave function ($\hbar = 1$)

$$\left| \psi(t) \right> = e^{-iH_i t} \left| \psi(0) \right>.$$  

(2)

In order to study the dynamics of the (von Neumann) entanglement entropy $S(t)$, we decompose the system into two subsystems, $A_i$ and $B_i$, each containing $L/2$ orbitals and on average $n_p/2$ particles. However, we do not restrict this decomposition (entanglement cut) to the real-space lattice space, but consider time-dependent basis orbitals $\xi_i = u_i c$, resulting from the real-space lattice representation by an arbitrary $U(L)$ transformation $u_i$ [with $U(L)$ denoting the group of $L \times L$ unitary matrices].

To represent the time-evolved wave function in an arbitrary orbital basis, we need to express $u_i$ in many-body Hilbert space, where it is denoted by $U_i$.

Naively applying $U_i$ to the real-space representation $\psi(t)$ of the state vector $\left| \psi(t) \right>$ would generate an unfeasible computational cost $\sim N^2$, where $N$ is the dimension of the many-body Hilbert space of $n_p$ particles.

However, exploiting that $U_i$ formally may be seen as a “time evolution” with respect to the free Hamiltonian $H_i = \sum_{j<\ell}(i \log u_{j,\ell} c_j^\dagger c_\ell)$ yields

$$\tilde{\psi}(t) = U_i \psi(t) = e^{-iH_i t} \psi(t),$$  

(3)

which naturally allows for the efficient $[O(N)]$ computation of the transformed representation $\tilde{\psi}(t)$, again using Krylov time propagation with respect to the fictitious Hamiltonian $\tilde{H}$.

In the following, we present exact numerical data on the quench dynamics of systems with up to $L = 24$ sites and $n_p = 12$ fermions, where $N \approx 2.7 \times 10^9$. Concretely, we study two examples of nonintegrable ergodic model systems, (i) a one-dimensional (1D) two-band band insulator that is quenched to a topological insulator (TI) phase with weak to modest interactions, and (ii) a metallic single-band Fermi-Hubbard model with next-nearest-neighbor (NNN) interactions. By comparison of these physically quite different scenarios, we will identify various features relating to the basis dependence of entanglement in quantum quench dynamics.

(i) Weakly interacting topological insulator: We first discuss a one-dimensional (1D) two-band system similar to the celebrated Su, Schrieffer, and Heeger (SSH) model [40,41]. There, the lattice index $j = 1, \ldots, L$ is decomposed into a unit-cell index $i = 1, \ldots, L/2$ and a sublattice index $\alpha = a, b$ such that $j = 2i - 1$ for site $a$ in cell $i$ and $j = 2i$ for site $b$ in cell $i$, respectively. In reciprocal space, the two-band Bloch Hamiltonian at lattice momentum $k = 4\pi p/L$, $p = 0, \ldots, L/2 - 1$ of the system is defined as

$$h(k) = [m(t) + J \cos(k)] \sigma_i + J \sin(k) \sigma_i \sigma_j,$$  

(4)

where $\sigma_i$ are the standard Pauli matrices acting on $a/b$ sublattice space, $m(t)$ plays the role of a Dirac mass parameter that is quenched from $m_i$ to $m_f$ at $t = 0$, and $J$ is the hopping strength between neighboring unit cells. For $|m| < |J|$, the model is in a topological insulator phase protected by the chiral symmetry $\sigma_i h(k) \sigma_j = -h(k)$, while at $|m| = |J|$ a topological quantum phase transition to a trivial band insulator phase extending over the parameter regime $|m| > |J|$ occurs. Here, we focus on quenches which change the topological phase of the system Hamiltonian, by choosing $m_i$ in the trivial and $m_f$ in the nontrivial phase, respectively.

For the (standard) real-space entanglement cut, even the noninteracting system is found to exhibit linear entanglement growth at small times. However, this entanglement is readily seen to be entirely basis dependent: The exact solution $\left| \psi(t) \right>$ remains a single Slater determinant at all times, leading to zero entanglement in a suitable basis obtained from time-evolved Wannier functions or Bloch functions representing the initial uncorrelated state. This provides a conceptually simple example for how strongly the entanglement of a system far from equilibrium may depend on the chosen representation.

We now address the natural question as to how an integrability breaking interaction term affects this phenomenology. To this end, we add to the free model (4) the interaction Hamiltonian

$$H_i = \sum_{i} \left[ U n_{i,a} n_{i,b} + W (n_{i,a} n_{i+1,b} + n_{i,b} n_{i+1,a}) \right],$$  

(5)

with $n_{i,a} = c^\dagger_{i,a} c_{i,a}$ ($\alpha = a, b$), where already a nonzero $U$ or $W$ individually is sufficient to make the model nonintegrable, and both terms preserve the protecting chiral symmetry.
We first discuss the case on $U = J$, $W = 0$ for transient times [see Fig. 1(b)]. For the Bloch and Wannier entanglement cut, in which the noninteracting solution would exhibit zero entanglement, $S$ is lower than in the real-space cut, for short to intermediate times. Interestingly, evolving the Wannier basis with respect to a dynamical Hartree-Fock Hamiltonian, thus accounting for interactions at the mean-field level leads to a substantial reduction of $S$ for quite long times. Searching for an optimal entanglement cut by treating the translation-invariant Hermitian matrix $\hat{H}_t$ as a variational ansatz generating the basis transformation $U_t$ [see Eq. (3)] [39], we are able to further reduce $S$ significantly below the dynamical Hartree-Fock basis [see the inset of Fig. 1(b)] by using local optimization algorithms such as Gradient Descent and ADAM [42]. We now switch on $W > 0$ which is generally found to speed up the process of thermalization in 1D topological insulator models [43], thus allowing us to look at the long-time (close to equilibration) behavior of our model. For weak to modest interactions, we observe a quite remarkable universal aspect of entanglement in the long-time limit, namely, that $S$ becomes largely independent of the choice of basis (see Fig. 2). This behavior exemplifies a quite generic mechanism that can be understood with the following physical picture [39].

When a system is quenched far from equilibrium by changing its gapped single-particle Hamiltonian, weak interactions are expected to lead to thermalization at an effective temperature $\beta_e$ of the system with respect to the close to noninteracting postquench Hamiltonian. However, the thermal entropy of a free Hamiltonian [such as Eq. (4)] generically is independent (up to nonextensive boundary effects) on the basis of a bipartition with an average of $n_p/2$ particles in each subsystem. Thus, the basis dependence of the entanglement entropy in this scenario is a transient effect, even though it might last to long times. This basis independence in weakly interacting thermalizing insulators also affects the margin to be gained by entanglement minimization: By optimizing the aforementioned basis-change Hamiltonian $\hat{H}_t$, starting from the set of Wannier orbitals in the long-time limit, here it is not possible to significantly reduce the entanglement entropy.

We conclude by putting our present results into a broader perspective from several angles. Generally speaking, nonintegrable ergodic systems are known to exhibit a generic dynamical behavior for the entanglement (ii) Spinless NNN Fermi-Hubbard model. As a second nonintegrable model system, we consider a spinless single-band Fermi-Hubbard model with a NNN interaction at filling $v = n_p/L$, defined by the Hamiltonian

$$H = \sum_j [-J(c_j^\dagger c_{j+1} + \text{H.c.)} + V(t)(n_j - v)(n_{j+2} - v)],$$

where $J$ (fixed to 1 in the simulations) denotes the hopping strength, $n_j = c_j^\dagger c_j$, and $V(t) \geq 0$ represents the repulsive NNN interaction strength which is suddenly changed from 0 to a finite value over the quench at $t = 0$. We focus on $v = 1/3$ in the following, where the model (6) at zero temperature is known to stay in a metallic Luttinger liquid phase up to large $V > 0$ [44], and has been found to exhibit strongly ergodic behavior [45]. When comparing the long-time entanglement entropy of this model in real space and momentum space, we find an interesting basis dependence that persists even in the long-time limit: For weak to modest $V$, the long-time entanglement in momentum space is lower than in real space, whereas at strong correlations ($V \gtrsim 3J$), the real-space cut leads to lower entanglement entropy (see Fig. 3). This behavior may be interpreted as a dynamical manifestation of the generic competition between an interaction term that is diagonal in real space and a free band structure that is diagonal in momentum space in Hubbard models [39]. At short times, by contrast, entanglement for all $V$ grows steeper in the momentum cut, owing to the nonlocal nature of the interaction in reciprocal space. In both cuts, entanglement clearly exhibits extensive (volume law) scaling for long times, as expected for an equilibrating ergodic system (see the inset of Fig. 3).

**Conclusion.** We conclude by putting our present results into a broader perspective from several angles. Generally speaking, nonintegrable ergodic systems are known to exhibit a generic dynamical behavior for the entanglement...
entanglement than generic states has been crucial for systems, e.g., with the advent of tensor-network methods [24–37], where the basis dependence of entanglement has been successfully exploited in the context of spin-boson models [48] and quantum chemistry settings [49–51]. However, far from equilibrium, generally the dynamical proliferation of entanglement eventually builds up an exponential wall even for the most powerful known computational methods. In this context, our results provide systematic insights addressing the question as to what extent both transient entanglement growth and long-time entanglement may be made computationally manageable, e.g., by extending tensor-network methods to a flexible representation of the physical degrees of freedom that allows for time-dependent basis choices.

In this Rapid Communication, we have been concerned with the influence of single-particle basis rotations on entanglement dynamics. At a conceptual level, our search for an optimal basis in which $S$ is lowest may be interpreted as an entanglement-based dynamical mean-field approach aimed at minimizing the single-particle contributions to $S$. Thinking further along these lines, it is readily conceivable to consider more elaborate approximate solutions based on genuine many-body methods as a starting point for the choice of a correlated basis, which may eliminate even some higher-order quantum correlations from the system. Quantitatively exploring this approach and constructing hybrid numerical methods, where a physically motivated approximate solution serves as the starting point to be augmented by an unbiased tensor-network simulation, represents an interesting subject of future work.

Note added in proof. Recently, we became aware of two related papers [52,53]. The authors of Ref. [52] have applied the idea of a dynamical single-particle basis rotations on matrix product states (MPS), optimizing at each step a sequence of unitary two-site gates acting on the MPS. In Ref. [53], the authors have chosen the frequency basis as a computationally advantageous single-particle basis for a MPS transport calculation.

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