Studies of the quantum dynamics of isolated systems are providing fundamental insights into how statistical mechanics emerges under unitary time evolution \[1\,4\]. Thermalization seems ubiquitous, but experiments with ultracold gases have shown that it need not always occur \[2\,3\], particularly near an integrable point \[7–9\]. A fascinating consequence of unitary dynamics is revealed by calculating the infinite-time average of \(O(\tau)\),

\[
\overline{O(\tau)} = \lim_{\tau \to \infty} 1/\tau \int_0^\tau d\tau O(\tau) = \text{Tr}[\hat{\rho}(\tau) \hat{O}],
\]

where \(\hat{\rho}(\tau) = \exp[-i\hat{H}\tau/\hbar] \hat{\rho} \exp[i\hat{H}\tau/\hbar]\). A major goal in those studies is to understand how to describe observables after relaxation. If the initial state is characterized by a density matrix \(\hat{\rho}\) and the dynamics is driven by a time-independent Hamiltonian \(\hat{H}\), then the time evolution of an observable \(\hat{O}\) is given by \(O(\tau) = \text{Tr}[\hat{\rho}(\tau) \hat{O}]\), where \(\hat{\rho}(\tau) = \exp[-i\hat{H}\tau/\hbar] \hat{\rho} \exp[i\hat{H}\tau/\hbar]\).

A thermal equilibrium in contact with a reservoir, so that thermalization occurs in the nonintegrable regime but fails at integrability. A phase transition-like behavior separates the two regimes.

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We introduce a linked-cluster based computational approach that allows one to study quantum quenches in lattice systems in the thermodynamic limit. This approach is used to study quenches in one-dimensional lattices. We provide evidence that, in the thermodynamic limit, thermalization occurs in the nonintegrable regime but fails at integrability. A phase transition-like behavior separates the two regimes.
are the eigenstates (eigenvalues) of the initial Hamiltonian $\hat{H}_c$ in $c$, and $n^c_a$ is the number of particles in \langle a \rangle (\hat{N}_c | a \rangle = n^c_a | a \rangle$, when $[\hat{N}_c, \hat{H}_c] = 0$). $\mu$, $T_I$, and $Z^l_c = \sum_{\alpha} e^{-(E^c_{\alpha} - \mu n^c_{\alpha})/T_I}$ are the initial chemical potential, temperature, and partition function, respectively. At the time of the quench $\hat{H}_c' \rightarrow \hat{H}_c$, the system is detached from the reservoir so that the dynamics is unitary. Writing the eigenstates of $\hat{H}_c'$ in terms of the eigenstates of $\hat{H}_c$, one can define the DE in each cluster. Its density matrix reads $\hat{\rho}^\text{DE}_c = \sum_\alpha W^c_\alpha | \alpha \rangle \langle \alpha |$, where $W^c_\alpha = (\sum_\alpha e^{-(E^c_{\alpha} - \mu n^c_{\alpha})/T_I}) | \alpha \rangle \langle \alpha | / Z^l_c$, and $| \alpha \rangle$ are the eigenstates of $\hat{H}_c$ ($\hat{H}_c | \alpha \rangle = E^c_{\alpha} | \alpha \rangle$). Taking $\hat{\rho}^\text{DE}_c$ in the calculation of $\mathcal{O}(c)$ to be $\hat{\rho}^\text{DE}_c$, NLCEs can be used to compute observables in the DE.

We use these NLCEs to study quenches of hard-core bosons in one-dimensional lattices, with nearest (next-nearest) neighbor hopping $t$ (\(t'\)) and repulsive interaction $V$ ($V'$) \[21\]. This model is integrable if $t' = V' = 0$ and nonintegrable otherwise \[22\]. It has been previously considered in quenches in finite lattices \[8\], and in studies of the integrability to quantum chaos transition \[23\]. After the quench, we take $V = t = 1$ ($t = 1$ sets our unit of energy), while $t' = V'$ are tuned between 0 and 1. Unless otherwise specified, the initial state is taken to be in thermal equilibrium with temperature $T_I$ for $t_I = 0.5$, $V_I = 1.5$, and $t'_I = V'_I = 0$. We restrict our analysis to half-filling (the average number of particles is one half the number of lattice sites). Given the particle-hole symmetry of our model, this is enforced by taking $\mu = 0$. The NLCE is done using maximally connected clusters, i.e., for any given number of lattice sites $l$, only the cluster with $l$ contiguous sites is used \[21\]. We denote as $\mathcal{O}_l$ the result obtained for an observable $\mathcal{O}$ after the contributions from all clusters with up to $l$ sites are added.

After a quench, it is important to accurately determine the mean energy per site in the DE ($E^{\text{DE}}$). It defines, along with the mean number of particles per site (fixed here to be $1/2$), the thermal ensemble used to determine whether observables thermalize. Since observables within NLCEs are computed using a finite number of clusters, we denote as $\mathcal{O}^{\text{ens}}_l$ the result obtained when adding the contribution of all clusters with up to $l$ sites (the superscript "ens" is used for DE or GE). To assess how close $\mathcal{O}^{\text{ens}}_l$ is to the thermodynamic limit result, we compute the difference between $\mathcal{O}^{\text{ens}}_l$ and the result for the highest order available ($l = 18$ in our calculations)

$$\Delta(\mathcal{O}^{\text{ens}})_l = |\mathcal{O}^{\text{ens}}_l - \mathcal{O}^{\text{ens}}_{18}|.$$  

When $\Delta(\mathcal{O}^{\text{ens}})_l$ becomes independent of $l$, and zero within machine precision, we expect that $\mathcal{O}^{\text{ens}}_l$ has converged to the thermodynamic limit result.

The accuracy of our calculation for $E^{\text{DE}}$ can be inferred from Fig. 1 where we plot $\Delta(E^{\text{DE}})|_{17}$ vs $T_I$ for several quenches. For $T_I \gtrsim 0.7$, $E^{\text{DE}}_{17} = E^{\text{DE}}_{18}$ within machine precision. The insets in Fig. 1 depict $\Delta(E^{\text{DE}})_{l}$ vs $l$ for $T_I = 1$ and 2. These plots show that, (i) $E^{\text{DE}}$ approaches $E^{\text{DE}}_{18}$ exponentially fast with $l$, and (ii) with increasing $T_I$, fewer orders are required for $E^{\text{DE}}$ to converge to an $l$-independent result (expected to be $E^{\text{DE}}$ in the thermodynamic limit) within machine precision.
Once $E^{\text{DE}}$ is known, one can define an effective temperature after the quench ($T$, as that of a grand-canonical ensemble such that $E^{\text{GE}} = E^{\text{DE}}$. (Here, all effective temperatures are computed enforcing that the relative energy difference between $E^{\text{DE}}_{18}$ and $E^{\text{GE}}_{18}$ is smaller than $10^{-11}$.) A question that arises is whether one can make simple measurements in a system after a quench that will distinguish it from one in thermal equilibrium. The fluctuations of the energy per site $\Delta E^2 = \langle (\hat{H}^2) - \langle \hat{H} \rangle^2 \rangle / L$ are a good candidate (see Ref. [21] for another one). In thermal equilibrium they depend on the ensemble used to compute them. $\Delta E^2 = 0$ in the microcanonical ensemble while $\Delta E^2 \geq 0$ in the canonical ensemble and the GE. $\Delta E^2$ is also of interest because, in the latter two ensembles, the specific heat $C_v = (1/L)\partial \langle \hat{H} \rangle / \partial T \propto \Delta E^2$.

In what follows, in order to quantify how order by order the DE prediction for an observable compares to the GE result in the last order, we define the relative difference

$$
\delta(O)_l = \frac{|O_{18}^{\text{DE}} - O_{18}^{\text{GE}}|}{|O_{18}^{\text{GE}}|}.
$$

We make sure that, for all results reported for $\delta(O)_l$, the analysis of $\Delta(O^{\text{GE}})_l$ suggests that $O_{18}^{\text{GE}}$ has converged to the thermodynamic limit result.

In the main panel in Fig. 2 we plot $\Delta E^2$ in the DE (empty symbols) and in the GE (filled symbols) vs $T$ for quenches with $T_f \geq 1$. These results, particularly the ones at the lowest temperatures, make it apparent that $\Delta E^2$ is different in the DE and the GE. Moreover, as shown in Fig. 2 for quenches with different initial states but the same final Hamiltonian $(t' = V' = 0.5)$, $\Delta E^2$ in the DE depends on the initial state. The relative differences $\delta(\Delta E^2)_l$, between $\Delta E^2$ in the DE for order $l$ and in the last order in the GE are plotted in the insets in Fig. 2(a) vs $l$. They show that the nonzero differences seen in the main panels between $\Delta E^2$ in the DE and the GE are fully converged and are thus expected to be the ones in the thermodynamic limit. The fact that $\Delta E^2$ in the DE and the GE agree with each other as $T_f \rightarrow \infty$ (main panel in Fig. 2) is universal. This is because as $T_f \rightarrow \infty$, the initial thermal ensemble becomes a completely random ensemble. Consequently, the DE after a quench and the corresponding GE also become completely random ensembles and give identical results for all observables independently of the model [21, 30].

The question we address next is whether experimentally relevant observables, which are ensemble independent in thermal equilibrium in the thermodynamic limit, thermalize after a quench. Specifically, we consider the momentum distribution $m_k$ [21] and the kinetic energy associated with nearest neighbor hoppings $K = -i \sum_i (\hat{b}_i^\dagger \hat{b}_{i+1})$. In Fig. 3(a), we show $m_k$ in the initial state $(T_f = 2)$, and in the DE and the corresponding GE after quenches with $t' = V' = 0$ (integrable) and $t' = V' = 0.5$ (nonintegrable). The DE and GE results are indistinguishable in the nonintegrable case, indicating thermalization, while they are clearly different at integrability, indicating the lack thereof.

When quantifying the differences between $m_k$ in the DE and the GE, we find that while the convergence of $m_k^{\text{GE}}$ is qualitatively similar to that of the observables...
certainty in the thermodynamic limit. The convergence un-
greater than $\Delta(S_1)$ for finite values as $l \to \infty$. Hence, our
calculations provide strong evidence that, in the ther-
quenches in lattice systems in the thermodynamic limit.

In summary, we have introduced NLCEs for the DE and
shown that they can be used to study generic quenches in lattice systems in the thermodynamic limit.

In the quenches studied here, NLCEs provided strong
evidence that nonintegrable systems thermalize while inte-
grable systems do not, and that a phase transition to
thermalization may occur as soon as one breaks integrabil-
ability. We plan to explore next whether NLCEs can be
used to study dynamics, which would allow one to ad-
ress fundamental questions related to prethermalization
and to the time scales needed to observe thermalization in isolated systems.

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Supplementary Materials:
Quantum Quenches in the Thermodynamic Limit

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Hamiltonian. The hard-core boson Hamiltonian reads
\[
\hat{H} = \sum_i \left\{ -t \left( \hat{b}^\dagger_i \hat{b}_{i+1} + \text{H.c.} \right) + V \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_{i+1} - \frac{1}{2} \right) - t' \left( \hat{b}^\dagger_i \hat{b}_{i+2} + \text{H.c.} \right) + V' \left( \hat{n}_i - \frac{1}{2} \right) \left( \hat{n}_{i+2} - \frac{1}{2} \right) \right\},
\]
where \( \hat{b}^\dagger_i (\hat{b}_i) \) denote the hard-core boson creation (annihilation) operators, and \( \hat{n}_i = \hat{b}^\dagger_i \hat{b}_i \) the number operator. In addition to the bosonic commutation relations \([\hat{b}_i, \hat{b}^\dagger_j] = \delta_{ij}\), those operators satisfy the constraints \(\hat{b}^\dagger_i^2 = \hat{b}_i^2 = 0\), which prevent multiple occupancies of lattice sites in all physical states.

Momentum distribution \( m_k \). The momentum distribution function is defined as the Fourier transform \( m_k = (1/L) \sum_{j,j'} e^{ik(j-j')} \hat{\rho}_{jj'} \) of the one-particle density matrix \( \hat{\rho}_{jj'} = \hat{b}^\dagger_j \hat{b}_{j'} \). In our calculations, we compute \( m_k \) in 100 equidistant \( k \) points between \( k = 0 \) and \( \pi \). For \( m_k \), in the same spirit of Eq. (1) in the main text, define
\[
\Delta(m^{\text{ens}})_l = \left\{ m_k \right\}^{\text{ens}}_{\text{ens}} - \left\{ m_k \right\}^{\text{ens}}_{18},
\]
where by "ens" we mean DE or GE, and, in the same spirit of Eq. (2) in the main text, we define
\[
\delta(m)_l = \left\{ m_k \right\}^{\text{DE}} - \left\{ m_k \right\}^{\text{GE}}_{18}.
\]

Linked-cluster expansions. In a linked-cluster expansion \[20\], the expectation value of an extensive observable \( \hat{O} \) per lattice site \( O = \langle \hat{O} \rangle / L \) (\( L \) is the number of lattice sites), in the thermodynamic limit, is computed as the sum over the contributions from all clusters \( c \) that can be embedded on the lattice
\[
O = \sum_c M(c) \times W_O(c).
\]
\( M(c) \) is the number of ways per site in which cluster \( c \), with all sites connected, can be embedded on the lattice. \[M(c) \] is known as the multiplicity of \( c \]. \( W_O(c) \) is the weight of that cluster for the observable \( O \), which is calculated using the inclusion-exclusion principle:
\[
W_O(c) = O(c) - \sum_{s \subset c} W_O(s),
\]
where the sum runs over all connected sub-clusters of \( c \) and
\[
O(c) = \text{Tr}(\hat{O} \hat{\rho}_c) / \text{Tr}(\hat{\rho}_c)
\]
is the expectation value of \( \hat{O} \) calculated for the finite cluster \( c \), with many-body density matrix \( \hat{\rho}_c \).

**Effective temperature \( T \) after the quench.** In Fig. 5, we show \( T \) for the quenches in Fig. 1 in the main text. While \( T \) can be seen to be greater than \( T_l \) in those quenches, this need not always occur. A quench, if \( T_l > 0 \), can effectively cool a system. As an example, in Fig. 5 we also show \( T \) for quenches in which \( t' = V' = 0 \) after the quench, while \( t_l = 1.5, V_l = 0.5 \) (\( t'_l = V'_l = 0 \) and \( t = V = 1 \), as in all other quenches), which illustrates that \( T \) can be lower than \( T_l \). The straight line depicts \( T = T_l \).

**NLCE with maximally connected clusters.** An important feature of NLCEs, which is not present in other linked-cluster expansions, is that one has quite some freedom in the selection of the building blocks used to carry out the expansion. One can use sites, bonds, and even squares or triangles depending on the geometry of the lattice \[22, 23\]. (A pedagogical introduction to NLCEs and their implementation can be found in Ref. \[24\].) Here, we use the maximally connected clusters. For \( l \) sites, the maximally connected cluster is the cluster with \( l \) contiguous sites in which all nearest and next-nearest neighbor hoppings and interactions defined by the Hamiltonian are included. It is the only connected cluster with \( l \) sites if \( t' = V' = 0 \). Such an expansion is expected to be best suited when \( t' = V' \) are small compared to \( t \) and \( V \). In our calculations, we carry out the NLCE computing observables in all maximally connected clusters with up to \( l = 18 \).

Quantum fluctuations of the density. In addition to the fluctuations of the energy discussed in the main text, the fluctuations of the density per site, \( \Delta N^2 = (\langle N^2 \rangle - \langle N \rangle^2) / L \), also allow one to distinguish the DE from the GE. In thermal equilibrium, they depend on the ensemble used to compute them. \( \Delta N^2 = 0 \) in the microcanonical and canonical ensembles, while it can be different from...
and in the last order in the GE are plotted vs differences
for quenches with different initial states but the same 
the ones at the lowest temperatures, make it apparent 
compressibility of interest because, in the grand-canonical ensemble, the 
for quenches with different initial 
T (empty symbols) and in the GE (filled symbols) vs 
differences between results obtained using full exact
diagonalization (ED) in systems with periodic boundary
conditions (l = 18, 20, and 22 sites) and the NLCE results for l = 18

\[
\delta(O^{\text{ED}})_L = \left|\frac{O^{\text{ED}}_L - O^{\text{GE}}_L}{|O^{\text{GE}}_L|}\right|
\]  
and

\[
\delta(m^{\text{ED}})_L = \frac{\sum_k |(m_k)^{\text{ED}}_L - (m_k)^{\text{GE}}_L|}{\sum_k (m_k)^{\text{GE}}_L},
\]

where the sum in Eq. (10) is restricted to the values of 
that are available in the specific cluster with periodic 
boundary conditions used in the exact diagonalization 
calculation. These differences exhibit a scaling that is 
consistent with 1/L, as expected. They make evident 
that the scaling (and ultimately the accuracy) of the 
results obtained using NLCEs and ED are fundamentally 
different, namely, exponential (NLCEs) vs power law (ED).

In the main panel in Fig. 6, we plot \(\delta(N^2)\) for 
for the same quenches as in the main panel.

zero only in the grand-canonical ensemble. \(N^2\) is also 
of interest because, in the grand-canonical ensemble, the 
compressibility \(\kappa = (1/L)\partial(N)/\partial\mu = N^2/T\).

In the main panel in Fig. 6, we plot \(\delta(N^2)\) in the 
DE (empty symbols) and in the GE (filled symbols) vs 
for quenches with \(T_l \geq 1\). These results, particularly 
the ones at the lowest temperatures, make it apparent 
that \(\delta N^2\) is different in the DE and the GE. Moreover, 
for quenches with different initial states but the same 
final Hamiltonian (with \(t'=V'=0.5\)), \(\delta N^2\) in the DE 
can be seen to depend on the initial state. The relative 
differences \(\delta(N^2)_l\) between \(\delta N^2\) in the DE for order \(l\) 
and in the last order in the GE are plotted vs \(l\) in the 
inset in Fig. 6. They show that the nonzero differences 
seen in the main panel between \(\delta N^2\) in the DE and the 
GE are fully converged and are thus expected to be the 
ones in the thermodynamic limit.

Convergence of NLCEs vs exact diagonalization. In 
Fig. 7 we show relative differences between NLCE results 
for four observables when all contributions from clusters 
with up to \(l\) sites are added and the results for \(l = 18\) 
(the highest order in the NLCE calculation that we have 
computed) vs \(l\). Those relative differences were defined 
in Eq. (1) in the main text and in Eq. (5) here. We took 
Hamiltonian Eq. (3) when \(t'=0\), which was systematically 
studied using exact diagonalization in Ref. [31]. 
One can see in all panels in Fig. 7 that the relative 
differences decrease exponentially fast with the order \(l\) 
of the NLCE calculation (note that results are presented 
for two temperatures \(T = 1\) and \(T = 5\)).

In the insets in Figs. 7(a), 7(c), and 7(d), we report rel-

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FIG. 7. Open (filled) symbols report the relative differences $\Delta(E^{GE})_l$ (a), $\Delta(\Delta E^{GE})_l$ (b), $\Delta(K^{GE})_l$ (c), and $\Delta(m^{GE})_l$ (d) vs $l$ for $T = 1$ ($T = 5$). Results are presented for $V' = 0$ (circles) and $V' = 1.0$ (squares). In all cases one can see an exponential decrease of the differences with increasing cluster size. In the insets in (a), (c), and (d) we show log-log plots of relative differences between results of full exact diagonalization in systems with periodic boundary conditions ($L = 18, 20$ and $22$ sites) and NLCE results with $l = 18$. In this case one can see that, as expected, the results are consistent with power law scaling in $L$. We have included straight lines in the insets explicitly depicting $1/L$ scaling.

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