Exact Relaxation in a Class of Nonequilibrium Quantum Lattice Systems

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A reasonable physical intuition in the study of interacting quantum systems says that, independent of the initial state, the system will tend to equilibrate. In this work we introduce an experimentally accessible setting where relaxation to a steady state is exact, namely, for the Bose-Hubbard model quenched from a Mott quantum phase to the free strong superfluid regime. We rigorously prove that the evolving state *locally* relaxes to a steady state with maximum entropy constrained by second moments—thus maximizing the entanglement. Remarkably, for this to be true, no time average is necessary. Our argument includes a central limit theorem and exploits the finite speed of information transfer. We also show that for all periodic initial configurations (charge density waves) the system relaxes locally, and identify experimentally accessible signatures in optical lattices as well as implications for the foundations of statistical mechanics.

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The study of the nonequilibrium properties of quantum many body systems has recently entered a renaissance era. This has been motivated, in part, by recent experimental developments; the rapid progress of experiments involving ultracold atoms in optical lattices, with their high degree of control and long coherence times, has opened the door to precise experimental studies of the dynamics of strongly interacting quantum systems [1]. In addition, questions of relaxation and thermalization for nonequilibrium systems are again receiving attention from foundational perspectives. This is partly triggered by intuition from quantum information theory where maximally or almost maximally entangled states emerge from appropriate distributions of random states [2–4].

One particularly fascinating setting which has recently received intensive study is that of *quenching*, that is, a sudden change of interaction strength [5–8]. Several explanations for, and numerical studies of, quenched dynamics have gradually led to the formulation of a rather general body of theory and conjectures; it has been mooted that if the system starts in the ground state of one Hamiltonian then certain properties such as correlators of the system should relax to an analogue of the thermal state of the new Hamiltonian after a quench [5]. By these observations we are motivated to formulate a conjecture. This *local relaxation conjecture* states that a system should locally relax to a steady state, respecting conserved quantities.

The local relaxation conjecture may sound suspiciously like a violation of unitarity as the global state must, of course, remain pure throughout the dynamics. However, a reasonable physical intuition which explains why there is no contradiction is that for a small block of sites the rest of a system acts like a reservoir and thus allows the site or the block to equilibrate. Indeed, the full explanation for the emergence of a local steady state during the course of the quench may be intuitively described along these lines: as time evolves the system becomes correlated [6]—from each site a wave front moving at some finite speed emerges, carrying information [8]. As time progresses more and more excitations will have passed through a given site, see Fig. 1. The cumulative effect of these successive excitations results in an effective averaging process; information stored in one site becomes infinitely diluted across the lattice.

In this work we introduce a physical setting where the local relaxation conjecture can be studied analytically. We find an exact convergence to a steady state for long times in the quenched Bose-Hubbard model. Our method is self-contained and physically motivated, and it is valid also for finite system sizes relevant to experimental settings. In the course of the proof we are also able to quantify the dilution of information throughout the lattice. Thus, our approach is considerably simpler and more physically intuitive than a potential approach based on the C^*-algebraic arguments developed in Ref. [9] to study the local relaxation of free fermions and bosons freely moving in $\mathbb{R}^n$ and classical

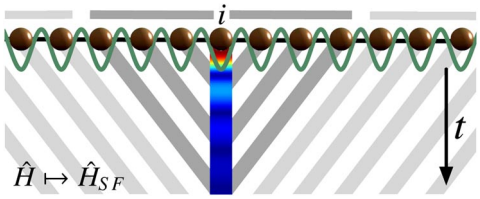

FIG. 1 (color online). Intuitive picture of the relaxation process in the quenched Bose-Hubbard model: for any lattice site i (or any block of sites) within a cone (dark gray) defined by the speed of information transfer excitations significantly contribute to the local mixing of the state at the site. Contributions from outside this cone (light gray) are exponentially suppressed. The incommensurate influence of the lattice sites in the cone gives rise to a relaxation to maximal entropy for large times t.

systems [10]. Interestingly, the convergence is not only true in the *time average*, but actually true for any large instant of time. This is in contrast to the recent approaches developed in quantum information [4], where, in order to study this problem, it would seem necessary to consider the time-averaged local state rather than the local state itself. For blocks of sites we also find a relaxation.

Quenched Bose-Hubbard dynamics.—We start from a Bose-Hubbard Hamiltonian, modeling, e.g., a dilute gas of ultracold atoms in an optical lattice [11]. It reads $\hat{H} = \hat{H}_{\mathrm{SF}} + \hat{U}$, where

$$\hat{H}_{\mathrm{SF}} = -J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j, \hat{U} = \frac{U}{2}\sum_{i=1}^{N} \hat{n}_i(\hat{n}_i - 1) - \sum_{i=1}^{N} \mu_i \hat{n}_i.$$

Here $\hat{b}_1, \ldots, \hat{b}_N$ denote bosonic annihilation operators and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$. The coefficient J governs the strength of hopping to neighboring sites ($\langle i, j\rangle$ indicates summation over nearest neighbors) and U defines the strength of the on-site interaction. Finally, the local chemical potential μ_i controls the particle number and may accommodate, e.g., a trapping potential or the situation occurring when a second lattice with a different wavelength is superimposed [12]. For theoretical simplicity we assume periodic boundary conditions for $\hat{H}_{\mathrm{SF}}$. This system exhibits two distinct phases as J and U are varied. When the hopping dominates, that is $J \gg U$, the system is in a *superfluid phase*. For a dominant on-site repulsion the ground state is a *Mott insulator* [11].

We imagine that the system is in the deep Mott regime (corresponding to $J = 0$), in which the ground state vector is a product $\otimes_{i=1}^{N} |m_i\rangle$ of individual number state vectors $|m_i\rangle$ of $m_i = \max\{0, [\mu_i/U + 1/2]\}$ bosons at each site. Here, $[\cdot]$ denotes the closest integer to the value in brackets. We then imagine that the system is rapidly *quenched*, at $t = 0$, to the strong superfluid regime $J \gg U$. We model this quench by an instantaneous change in the Hamiltonian to the regime $U = 0$. Thus, the system state vector at time t is given by (we set $\hbar = 1$) $|\psi(N, t)\rangle = e^{-it\hat{H}_{\mathrm{SF}}} \otimes_{i=1}^{N} |m_i\rangle$.

Relaxation for a single site.—We are interested in whether subsystems consisting of single sites or blocks thereof equilibrate, and, if so, in what sense. For clarity we start by proving relaxation for the quantum state of a single site and initial states with $m_i = m$, and then extend this result to multiple sites $S \subset L$ and different initial conditions. The state of site i in the lattice $L = [1, \ldots, N]$ is given by a partial trace $\hat{\varrho}_i(N, t) = \mathrm{tr}_{L\setminus\{i\}}[|\psi(N, t)\rangle\langle\psi(N, t)|]$. Throughout this Letter we describe the system in phase space, making use of the characteristic function to represent the state $\hat{\varrho}_i$. It is defined for complex α as $\chi_i(\alpha; N, t) = \mathrm{tr}[\hat{\varrho}_i(N, t) e^{\alpha\hat{b}_i^\dagger - \alpha^*\hat{b}_i}]$ and can be shown to take the form $\chi_i = \exp(-|\alpha|^2/2) \times \prod_{j=1}^{N} L_m(|\alpha|^2 |V(N, t)_{i,j}|^2)$, where L_m are Laguerre polynomials, and $V(N, t) = \exp(-it\mathcal{J})$, $\mathcal{J}_{i,j}(N) = -J\delta_{\mathrm{dist}(i,j),1}$, governs the dynamics of the state. We now show that we indeed locally, *at each site* i, find convergence to a state that maximizes the entropy: we prove that the state $\hat{\varrho}_i(N, t)$ approximates a Gaussian state $\hat{\varrho}_G$ arbitrarily well. We find that the first moments of $\hat{\varrho}_G$ vanish, and its second moments are identical to the initial ones. Gaussian states maximize the local entropy for fixed second moments, which are constants of motion for the initial states $|m\rangle^{\otimes N}$, see below for more general initial states.

Our main result can thus be summarized as $\hat{\varrho}_i(N, t) \to \hat{\varrho}_G$, where the limit of large N is taken first and then the limit of large t is taken. Note that there is no time average involved. More precisely, for any $\varepsilon > 0$ and sufficiently large system size N, we find recurrence and relaxation times $t_{\mathrm{Rec}} > t_{\mathrm{Relax}} > 0$ such that

$$||\hat{\varrho}_i(N, t) - \hat{\varrho}_G||_{\mathrm{tr}} < \varepsilon \quad \text{for } t \in [t_{\mathrm{Relax}}, t_{\mathrm{Rec}}]. \qquad (1)$$

Here, t_{Relax}, t_{Rec} are governed by the hopping strength J, which defines the speed of information transfer, see Fig. 1. For finite N recurrences occur for times larger than t_{Rec}; however, these can be shifted to infinity for large N. Closeness of $\hat{\varrho}_i(N, t)$ and $\hat{\varrho}_G$ is measured in trace norm which of course means that *all* local expectation values are the same as for the relaxed state. Another way of interpreting the relaxation to a Gaussian state is that the entanglement between the site i and the rest of the chain becomes *maximal*.

There are two key insights we use in our rigorous central limit type argument: we divide the lattice system into two domains defined by a causal cone (see Fig. 1), which is specified by the velocity of information propagation. The first insight is that the causal cone defines what sites can have a significant influence at a time: we can neglect the influence of excitations from sites that are too far away to have a causal influence. The second and most significant insight is that inside this cone, the collective influence of excitations truly randomizes the system.

Outside the causal cone.—A "Lieb-Robinson type argument" makes the above intuition rigorous: as $\mathcal{J}_{i,j} = 0$ for $1 < \mathrm{dist}\,(i, j) =: d$, we have that $(\mathcal{J}^k)_{i,j} = 0$ for $d > k$, i.e., $|V_{i,j}| = |\sum_{k\geq d}([-it\mathcal{J}]^k)_{i,j}/k!| \leq |\sum_{k\geq d}(6Jt/k)^k|$, where we made use of the property that matrix entries are bounded by the operator norm of the matrix. This defines the causal cone and an upper bound to the speed of information transfer (this upper bound is sufficient for our purposes): contributions with $d > 6Jt$ are exponentially suppressed: $|V_{i,j}| \leq (6Jt/d)^d/(1 - 6Jt/d)$. For any $\epsilon > 0$ we have $|V_{i,j}| < \epsilon$ for all i, j: $\mathrm{dist}\,(i, j) > L(t)$, where $L(t)$ is given by the solution to $[6Jt/L(t)]^{L(t)} = \epsilon[1 - 6Jt/L(t)]$ and is hence independent of the system size N.

Inside the causal cone.—Also for $\mathrm{dist}\,(i, j) \leq L(t)$ the $|V_{i,j}|$ can be made as small as desired, now due to an averaging process: as $\mathcal{J}$ is a circulant matrix, the $V_{i,j} = V_{i-j}$ can be thought of as Riemann sum approximation to an integral representation of the Bessel function $J_l(x) = \frac{1}{2\pi i^l}\int_0^{2\pi} d\phi e^{ix\cos(\phi)} e^{il\phi}$, up to a phase i^l. Combining the error involved in such approximations with the bound

$|J_l(x)| < x^{-1/3}$, valid for all $x \geq 0$ and all l, we obtain $|V_l| \leq 2\pi^2[2Jt + L(t)]/N + (2Jt)^{-1/3}$ for $l \leq L(t)$. Combining this with the bound on contributions from outside the causal cone, we finally have that $|V_{i,j}| < \epsilon$ for all i, j and $t \in \{4/(J\epsilon^3), N\epsilon^2/[4\pi^2 J(8\epsilon + 6)]\}$.

Central limit type theorem.—We are now in the position to apply a central limit type argument: we can expand the logarithm of the characterisic function, identify certain terms quadratic in α, and then bound higher order terms:

$$\log\chi_i(\alpha; N, t) = -\left(m + \frac{1}{2}\right)|\alpha|^2 + \sum_{j=1}^{N} l_m(|\alpha|^2|V_{i,j}|^2) - \sum_{j=1}^{N}\sum_{k=2}^{\infty}\frac{(1 - L_m(|\alpha|^2|V_{i,j}|^2))^k}{k},$$

where $l_m = L_m + mx - 1$. The remainder terms can be made as small as desired utilizing the bound on $|V_{i,j}|$ derived above. For example, after a number of steps, one finds that the second term can be bounded from above by $|\sum_{j=1}^{N} l_m(|\alpha|^2|V_{i,j}|^2)| \leq l_m(-1)|\alpha|^4 \sup_{i,j}|V_{i,j}|^2$. Along the same lines, but with more technical effort, the third term can be bounded from above in a similar way. Equipped with these bounds, we find that for any complex α, $\chi_i(\alpha; N, t) = e^{-(m+1/2)|\alpha|^2} + f(\alpha; N, t)$, where $|f(\alpha; N, t)|$ can be made arbitrarily small for all $t \in [t_{\mathrm{Relax}}, t_{\mathrm{Rec}}]$, where $t_{\mathrm{Rec}} > t_{\mathrm{Relax}} > 0$ for a suitable choice of the lattice size N. Pointwise closeness for the characteristic functions of two quantum states translates to closeness in trace norm for the states [13,14]; we have completed the argument. We therefore find that the state of a single site, in the limit of large times, maximizes the entropy for the given initial second moments: Gaussian states have this extremal property of having maximal entropy. So subject to this constraint, it is *maximally entangled* with the rest of the chain. Since we can bound the time scale on which relaxation occurs [the single site relaxes to a Gaussian at the rate $(2Jt)^{-1/3}$] our argument is robust under small perturbations. This result gives a clear handle on the situation for finite system sizes: for any finite system size N, there will eventually be recurrences. The time scale for such recurrences to occur in the (N, t) plane is governed by the speed of information transfer and the system size N. For large or *infinite system size*, locally the system appears exactly relaxed for large times, giving the impression of an ''irreversible dynamics''. This *local relaxation* is perfectly consistent with the unitary dynamics of the full system; the whole system never truly relaxes to an equilibrium state as it always preserves the *full memory* of the initial condition.

Relaxation of blocks.—Using arguments essentially identical to the ones in the proof for a single site, we find in the same sense a convergence for a block S of s sites: $\mathrm{tr}_{L\setminus S}[|\psi(N, t)\rangle\langle\psi(N, t)|] = \hat{\varrho}_S(N, t) \to \hat{\varrho}_G^{\otimes s}$. The block tends to a product of maximal entropy states, which is in contrast to the thermal state of the new Hamiltonian $\hat{H}_{\mathrm{SF}}$, which is *always* correlated for all temperatures $T > 0$ [15]. Although the system does mix and we do arrive at a state with local maximal entropy, it does *not* relax to the thermal state of the new Hamiltonian; the conserved second moments prevent this from happening.

More general situations.—An argument along the lines of the above proof can be carried out whenever the initial state has sufficiently rapidly decaying correlations (details of this argument will be presented elsewhere). We will now consider more general initial states of the form $\otimes_{i=1}^{N}|m_i\rangle$, allowing for different particle numbers at different sites—allowing, e.g., for configurations occurring in harmonic traps and periodic distributions with periodicity different from one, reminiscent of *charge density waves* or checkerboard phases. These can be realized, e.g., by superimposing a second lattice with different wavelength [12]. For these inhomogeneous initial states the second moments are no longer preserved. However, for initial states with $m_j = m$ for almost all j, we always find relaxation to a steady state as we also do for P-periodic initial configurations: Consider an initial state with $m_i = m_{i-P}$, completely determined by $m_1, \ldots, m_P$. Then, we find again that the characteristic function tends to a Gaussian: $\lim_{t\to\infty}\lim_{N\to\infty}\chi_S(\boldsymbol{\alpha}; N, t) = e^{-(\bar{m}+1/2)\boldsymbol{\alpha}^\dagger\boldsymbol{\alpha}}$, where $\bar{m} = \sum_{p=1}^{P} m_p/P$. While initially different sites are uncorrelated, correlations build up over time and finally go to zero for large times (see Fig. 2) and the local state relaxes to a direct product of the same Gaussian at each site, $\hat{\varrho}_S \to \hat{\varrho}_G^{\otimes s}$.

Higher dimensional systems.—One can prove the exponentially suppressed influence of sites outside the cone for quite general situations: consider a local but otherwise arbitrary coupling matrix $\mathcal{J}$, i.e., $\mathcal{J}_{i,j} = 0$ for $\mathrm{dist}(i, j) > l$, where the distance is now taken as the graph-theoretical distance to allow for arbitrary underlying lattices. We only need to replace $2J$ by the operator norm $\|\mathcal{J}\|$ of the general coupling matrix in the above proof. We then find exactly as before that contributions outside the causal cone, now defined by $\mathrm{dist}(i, j) > 3l\|\mathcal{J}\|t$, are exponentially suppressed. Utilizing this fact, we can also extend the argument inside the causal cone to higher dimensions: the matrix entries of $V(N, t)$ are then given by a Riemann sum approximation to a product of Bessel functions, and the same reasoning as above applies.

Spin systems.—Note finally that the developed intuition also carries over to other integrable models such as *XY spin systems* with transverse magnetic field corresponding to *fermionic systems* by virtue of a Jordan-Wigner transformation. This includes the case where we start with the system initially in $|m\rangle^{\otimes N}$, $m = 0, 1$, corresponding to the magnetized spin states $|\downarrow\rangle^{\otimes N}$, $|\uparrow\rangle^{\otimes N}$, and study time evolution under a Hamiltonian corresponding to a nonisotropic fermionic quadratic Hamiltonian. Again, one can identify regimes in which one does find a local relaxation to a steady state without invoking a time average.

Summary and discussion.—In this work, we have investigated the relaxation of Bose-Hubbard type systems and related models following a sudden quench. The intuition

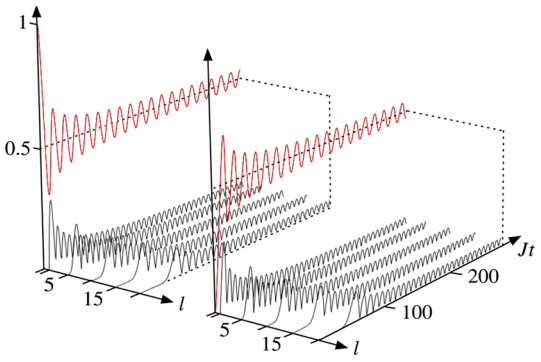

FIG. 2 (color online). Second moments $\langle \hat{b}_1^\dagger \hat{b}_{1+l} \rangle$ (left) and $\langle \hat{b}_2^\dagger \hat{b}_{2+l} \rangle$ (right), $l = 0$, 1, 5, 10, 15, 20, for an initial periodic configuration $|1, 0, 1, 0 \cdots\rangle$ on a lattice of size $N = 300$. For larger times recurrences occur (not shown), while for $N \to \infty$, one has $\lim_{t\to\infty} \langle \hat{b}_i^\dagger \hat{b}_j \rangle = \delta_{i,j}/2$.

we developed was that within a causal cone, the incommensurate influence of the propagating quasiparticles will give rise to a relaxation dynamics. We have considered a setting in which we could prove an exact local relaxation to a maximal entropy state, providing a guideline of what is expected to happen in similar cases. Indeed, the system ''looks'' perfectly relaxed, while at the same time keeping a perfect memory of the initial situation. We hence can clarify the difference between an apparent (which does happen) and an actual global (which does not happen) relaxation. The argument presented here is expected to be valid whenever the initial correlations are clustering.

Note that in the presented approach, we do not have to invoke an instance of Jaynes's principle of maximum entropy, motivated by a Bayesian argument when having incomplete prior information, to arrive at a maximum entropy final state. Instead, this local steady state is *derived* as resulting from the nonequilibrium dynamics. Our work hence also complements kinematical approaches to quantum statistical problems: when randomizing over all possible pure states of a large system [3,16], the local state of a subsystem will typically have almost maximal entropy. Here, we arrive at a similar result, but not by having to assume imperfect knowledge about the initial conditions, in a *kinematical* argument, but via a *dynamical* one, where the mixing is actually achieved through local physical dynamics in a lattice system.

A key motivation is that settings very similar to these are readily accessible in experiments using ultracold bosonic atoms in optical lattices [1]. The general guideline is that local observables will relax. Most accessible would be a situation where only second moments would have to be monitored, starting, e.g., with a checkerboard type situation of alternating occupation numbers in a Mott state (see Fig. 2), prepared using two distinct optical lattices [12]. An observation of the occupation of even sites (in the translationally invariant setting a truly local observable) as in Ref. [12] would reveal signatures of this apparent relaxation effect. The idealized case of a vanishing interaction U gives rise to a guideline for what to expect in realistic settings and also to a general principle: the local relaxation conjecture. It is our hope that the present work fosters further experiments along these lines.

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