Exploring Local Quantum Many-Body Relaxation by Atoms in Optical Superlattices

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We establish a setting—atoms in optical superlattices with period 2—in which one can experimentally probe signatures of the process of local relaxation and apparent thermalization in nonequilibrium dynamics without the need of addressing single sites. This opens up a way to explore the convergence of subsystems to maximum entropy states in quenched quantum many-body systems with present technology. Remarkably, the emergence of thermal states does not follow from a coupling to an environment but is a result of the complex nonequilibrium dynamics in closed systems. We explore ways of measuring the relevant signatures of thermalization in this analogue quantum simulation of a relaxation process, exploiting the possibilities offered by optical superlattices.

Is it possible to consider the relaxation of a closed quantum system to an apparently equilibrated state? In contrast to the deep understanding we have of equilibrium quantum statistical mechanics, nonequilibrium relaxation processes are far from being fully understood. Specifically, the question of how Gibbs or relaxed states emerge dynamically is a question that is receiving a lot of attention recently [1–9]. Part of the reason for the renaissance in the study of questions of nonequilibrium dynamics of quantum many-body systems stems from the fact that systems have become available that promise to make such issues amenable to experiment [10]: The states of cold atoms in optical lattices can be manipulated with a high degree of control, offering a test bed for questions of nonequilibrium dynamics.

The setting of interest in this work is the one of a sudden quench [1–9,11,12]. Starting in the ground state of a local many-body Hamiltonian, system parameters are suddenly changed such that the old state is no longer an eigenstate of the new Hamiltonian, generating a nonequilibrium situation. The dynamics of the system is then monitored in time. It has been conjectured that, in such a nonequilibrium situation, one may—in some sense—arrive at the maximum entropy state consistent with the expectation values of the constants of motion fixed by the initial state [6,13,14]. This is appealing as it parallels Jaynes's approach to equilibrium statistical mechanics. Yet, of course, if the system can be meaningfully treated as a closed quantum system, one cannot expect the entire system to relax, as an initially pure state will remain so in time [2–4]. The entire information of the initial condition is still present in the system, albeit in a very dilute fashion.

This is, however, by no means inconsistent with the expectation that the system may locally appear to be relaxed [2–5]. Locally, such a relaxation can well be true: Any subsystem may appear to be in a maximum entropy state under the constraints dictated by the constants of motion and remain so for an arbitrary amount of time. Reference [2] introduces an instance in which this local relaxation of subsystems, referred to as the local relaxation conjecture, can actually be proven rigorously to hold: When quenching a state in a Mott phase in a Bose-Hubbard system to the noninteracting deep superfluid phase, the reduced state of consecutive sites converges to a maximum entropy state consistent with the constants of motion [2]—without having to invoke a time average. The intuition is that the quench creates local excitations that travel through the lattice at a finite speed [2,7,15]. Their incommensurate influence then leads to a relaxation without environment. This intuition is corroborated in Ref. [4], where local relaxation for Gaussian initial states is shown.

Unfortunately, while many situations that give rise to local relaxation may be generated, a challenge so far unresolved is to actually probe signatures of local relaxation: Demonstrating local relaxation appears to necessitate local addressing, a requirement that poses a great experimental challenge in systems of atoms in optical lattices.

This dilemma will be resolved in this work, employing a simple yet promising idea. We will make use of a periodic setting, but we are by no means obliged to stick to period 1: The idea is that we can well make use of a period-2 setting, exploiting optical superlattices. This approach will open up a way to quantitatively explore local relaxation effects in experiment, without the need of addressing single sites at any point. To demonstrate the validity of this idea, we will make use of analytical as well as numerical methods, based on a time-dependent density-matrix renormalization-group (t-DMRG) approach. Our findings provide a simple guideline to what is to be expected in realistic experimental situations.

Proposed experimental setup.—Ultracold atoms in optical lattices provide a great deal of control over the system's parameters [10]. In particular, sudden quenches of parameters are accessible, and, on experimental time scales, systems can be treated as essentially closed. To address the

local detection problem, we propose to study local relaxation using optical superlattices [16]. We follow the setup recently realized by Bloch and co-workers [16], considering bosonic ^{87}Rb atoms in a period-2 optical superlattice geometry. This experimental setting allows for changing the relative intensity of the two optical lattices, shifting their relative position, and coupling and uncoupling double well potentials. In such double well potentials, one may introduce an alternating bias between the chemical potentials of neighboring sites. This allows for the following three steps: (I) *Periodic patterns* of atoms can now be prepared by isolating double wells and introducing a bias between odd and even sites. Further experimental techniques make sure that multiply occupancies are highly suppressed, leaving, e.g., a sequence of empty and singly occupied sites. (II) *Period-2 local* density measurements can be performed by mapping odd and even sites to different Brillouin zones: Each part of a decoupled double well has multiple bands separated by well-defined energies. Biasing the odd sites relative to the even ones by an energy in excess of the separation energy of the band-separation energy, odd-site particles are reloaded into the higher bands of the even sites, whereas the even-site particles stay in the lowest band. A time-of-flight mapping then reveals the even-site particles in the first and the odd-site particles in the higher Brillouin zones. (III) *Correlations between even and odd sites* can be measured using more sophisticated techniques [16].

Setting and initial condition.—We propose to start from a two-periodic initial state prepared by the superlattice setup, where the odd sites are occupied by exactly a single boson, all even sites being empty, such that the initial state vector is $|\psi(0)\rangle = |1, 0, 1, 0, \ldots 1, 0\rangle$ (Fig. 1). The 2a lattice is then suddenly switched off, generating a nonequilibrium situation, and the state vector will evolve $|\psi(t)\rangle = e^{-it\hat{H}/\hbar}|\psi(0)\rangle$ according to the Bose-Hubbard Hamiltonian

$$\hat{H} = -J \sum_{i=1}^{L} (\hat{b}_{i+1}^{\dagger} \hat{b}_i + \hat{b}_i^{\dagger} \hat{b}_{i+1}) + \frac{U}{2} \sum_{i=1}^{L} \hat{n}_i(\hat{n}_i - 1),$$

U and J being the interaction and hopping parameters, respectively, of the Bose-Hubbard model that can be calculated from the lattice parameters ($J = \hbar = 1$). L defines the system size, which will be taken to be even. Occupation
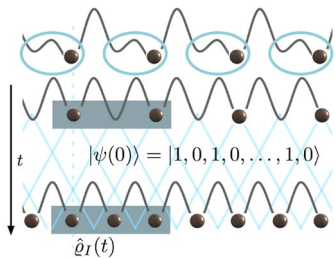

FIG. 1 (color online).   Sketch of a local relaxation starting from an initial condition of bosonic atoms being present or absent, in even and odd sites of a one-dimensional Bose-Hubbard system, achieved by imposing a superlattice to an optical lattice.

of higher order bands will not be considered, and we stay within the limit of applicability of the Bose-Hubbard model. We will now see how local relaxation manifests itself in such a periodic setting.

Signatures of local relaxation for observable quantities.—We find that quantitative signatures of local relaxation can be observed by the global measurement of the total occupation of even and odd sites (II) $\langle \hat{N}_{o,e}(t) \rangle$ and correlations between nearest neighbors (III) $\langle \hat{b}_i(t)\hat{b}_{i+1}(t) \rangle$. In a translationally invariant setting, such measurements amount to accessing local observables as $\langle \hat{N}_e(t) \rangle = \sum_{i=1}^{L/2} \langle \hat{n}_{2i}(t) \rangle = L \langle \hat{n}_{2i}(t) \rangle / 2$. The limiting cases $U = 0$ and $U = \infty$ are or can be mapped to free models. For $U = 0$, one finds in the Heisenberg picture $\hat{b}_i(t) = \sum_{j=1}^{L} V_{i-j}(t)\hat{b}_j(0)$, where $V_l(t) = \sum_{k=1}^{L} e^{-it\lambda_k} e^{2\pi ikl/L}/L$ and $\lambda_k = -2\cos(2\pi k/L)$. In the limit $U \to \infty$, the interaction manifests itself in that bosons become hard-core, rendering them solvable via the Jordan-Wigner transformation to spinless fermions.

To study the relaxation dynamics for finite U, we turn to the time-dependent variant [17] of DMRG [18], allowing us to follow the coherent time-evolution of strongly interacting quantum systems very precisely, keeping up to 5000 states in the matrix-product state calculations.

In all of the considered cases, we do find local relaxation: The intuition is that the incommensurate influences of traveling excitations [2,7] lead to a mixing in time and, hence, the emergence of properties that locally appear like ones of maximum entropy states. These excitations propagate at most with the Lieb-Robinson velocity, giving rise to an approximate locality in the lattice [15]. The situation is especially clear for $U = 0$, where relaxation is due to dephasing in the sense that freely propagating excitations lead to reduced state contributions of quickly oscillating phases that average out [2]. One can indeed prove that, for any subblock I, the system relaxes to the reduction of a maximum entropy state given the constraints of motion. This is true without time average, arbitrarily exactly to any small error in trace norm, and for an arbitrarily long time [19]. For interacting cases with $U > 0$, we would expect that, for very short times, observables evolve as in the $U = 0$ limit, with a crossover in behavior for longer times when they start interacting. We will explore to what interaction strengths the remarkably simple limiting pictures remain essentially valid and when one can identify genuinely different relaxation dynamics.

Time evolution of densities.—Signatures of nonequilibrium relaxation dynamics are specifically apparent in the observation of local densities. Local densities evolve in both exactly solvable cases $U = 0, \infty$ as

$$\langle \hat{n}_i(t) \rangle = \frac{1}{2} - \frac{(-1)^i}{2L} \sum_{k=1}^{L} e^{4it\cos(2\pi k/L)} \to \frac{1}{2} - \frac{(-1)^i}{2} J_0(4t)$$

for $L \to \infty$, where J_n denote the Bessel functions of first kind. Odd- and even-site densities relax symmetrically

about the $n = 1/2$ axis to $n = 1/2$, with an asymptotic decay in time as $t^{-1/2} + o(t^{-1/2})$; see Fig. 2.

For the interacting cases, all t-DMRG results are compatible with a relaxation of densities to $n = 1/2$. As excitations are responsible for local relaxation, on very short time scales ($t < 1$) particles have typically not interacted yet and are not quite sensitive to different values of U, giving rise to a similar behavior as for $U = 0, \infty$. The dynamics of relaxation deviates quite strongly for intermediate times, however. This is clearly exhibited in Fig. 2 (for $L = 32$). The decay behavior as estimated from the data is also shown by power-law exponents compatible with the data. We clearly see that, for very small U and $U > 4$, the limiting noninteracting cases provide a very good approximation to the interacting dynamics (one encounters a slope similar to $-1/2$, as for the limiting cases). For intermediate values of U, close to the critical point, scattering appears to be most effective, leading to a strongly enhanced damping and relaxation. Such strong deviations from the limiting behavior are expected be visible experimentally, as a signature of interaction effects.

Time evolution of correlators.—We now turn to nearest-neighbor correlator $\langle \hat{b}_{i+1}^\dagger(t)\hat{b}_i(t) \rangle$. This quantity is specifically interesting, going beyond local densities: The buildup of correlations in time starting from the uncorrelated initial state becomes apparent. In the limiting free cases, we find

$$\langle \hat{b}_{i+1}^\dagger(t)\hat{b}_i(t) \rangle = \frac{(-1)^i}{2L} \sum_{k=1}^{L} \frac{e^{4ti\cos(2\pi k/L)}}{e^{2\pi i k/L}} \longrightarrow -\frac{(-1)^i}{2i} J_1(4t).$$

The real part of the correlator is zero for all times, whereas the imaginary part relaxes to 0 with an asymptotics of $t^{-1/2}$, following a quick growth to a maximal value of about 0.28 at time $t \sim 1/2$, reflecting the buildup of corre-

lations due to particle motion with speed approximately linear in J. Figure 3 shows the real and imaginary parts of the correlators. The buildup of the imaginary part of correlations is largely independent of U, reflecting the fact that, over the distance 1 between particles at $t = 0$, few collisions have yet happened. When the interaction becomes visible, the relaxation dynamics follows quite different paths, local relaxation again being fastest around $U \approx 3$.

For all finite U, the real part converges to a finite value. Indeed, for large U the converged value is well-approximated by a U^{-1} curve (for $U > 4$). This dependence is, in fact, exactly what one would expect in the thermal or Gibbs state of the Bose-Hubbard model. This can already be seen using thermal perturbation theory,

$$\langle \hat{b}_{i+1}^\dagger \hat{b}_i \rangle = \frac{J}{U} \sum_{n,m} e^{-\beta(E_n + E_m)} n(m + 1) \frac{e^{\beta U(n-m-1)} - 1}{z^2(n - m - 1)},$$

up to $o(J/U)$, where $z = \sum_n e^{-\beta E_n}$ and $E_n = Un(n - 1)/2$ are the local energies of the unperturbed Hamiltonian. So, indeed, within the validity of perturbation theory, we do find the anticipated linear dependence on $1/U$, as seen also in DMRG simulations. This insight further corroborates the intuition that, locally, the state is indistinguishable from the situation as if the system was, globally, in a state maximizing the entropy, respecting the constraints of motion [2,4].

Entanglement dynamics.—The traveling excitations give rise to entanglement between any subsystem and the rest of the lattice [11,12], indeed to maximal entanglement given the constraints of motion. The speed of information transfer also governs the dynamics at which bipartite and long-range entanglement is being built up. The buildup of entanglement is both a resource (being ultimately responsible for local relaxation) and a burden: Linear entanglement growth as found here leads to an exponential growth in the numerical resources, limiting simulations to $t \approx 6J$.

Time scales of local relaxation.—In all quantities studied so far, one can identify three regimes in time: (a) Initially, correlations are being built up. In this regime $Jt < 1$, the dynamics is largely independent of U, as collisions have not yet become important. (b) The second time
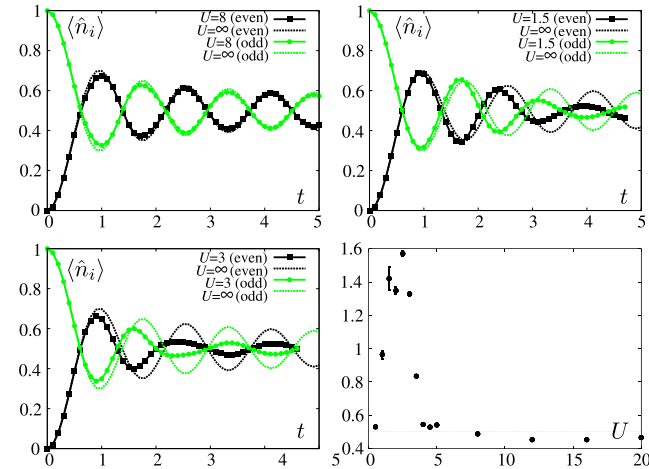

FIG. 2 (color online). Local density $\langle \hat{n}_i(t) \rangle$ vs time, showing local relaxation. Shown is the time evolution of an even and an odd site for different values of U, as well as the estimated negative exponents of asymptotic power-law decay (right lower figure). Note the strong deviation from the noninteracting limit and the strong suppression of density oscillations for $U = 3$, as well as the similarity for $U = 8$ with the limit $U = \infty$.
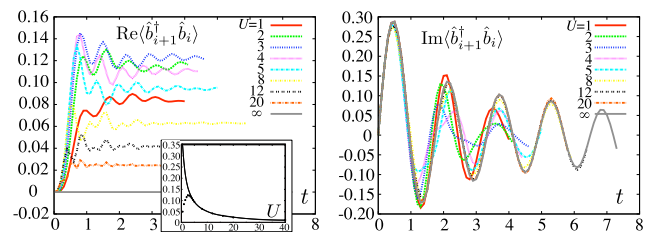

FIG. 3 (color online). Real and imaginary parts of the correlations to neighbors $\langle \hat{b}_{i+1}^\dagger(t)\hat{b}_i(t) \rangle$, for different values of U. The inset shows the equilibrated value of the real part of correlations to neighbors for large t for different values of U (with a solid line proportional to $1/U$ as a guide to the eye).

regime is the one of actual local relaxation. The fast oscillatory dynamics between neighboring sites is accompanied by slow local relaxation, resulting from the incoming excitations from farther and farther sites, broadened by dispersion. This results in relaxation, not due to decoherence but due to the dilution of information over the lattice. This information propagation is expected to happen at a finite speed related to J [15], in a "ballistic transport." In the free models, one finds a polynomial decay: The Bessel function fulfills $J_0(x) = x^{-1/2} + o(x^{-1/2})$. For finite U, numerics is consistent with polynomial decay, which for intermediate U seems to be much faster. (c) The third and very large time is the recurrence time where the finite size of the quantum system becomes visible.

The interaction strength also marks three regimes: (A) For small interactions $U < 1$, the dynamics strongly resembles the noninteracting bosonic limit. (B) For large values of U, the dynamics is very similar to the hard-core bosonic or free fermionic limit, with relaxation exponents being $\approx -1/2$. The observed local correlations proportional to $1/U$ are consistent with assuming that we locally observe a global state having maximum entropy. (C) The case of intermediate $U \sim 3$ appears to mark the crossover between the two free cases of $U = 0$ and $U = \infty$, characterized by the most efficient relaxation.

Quasimomentum distribution.—Remarkably, the quasimomentum distribution (QMD), measurable via time of flight, defined as $S(q, t) = \sum_{i,j=1}^{L} e^{iq(i-j)} \langle \hat{b}_i^\dagger(t) \hat{b}_j(t) \rangle / L$ can be shown not to relax for $U = 0$. This creates, for small U, the interesting situation that local relaxation can be probed, while at the same time signatures of the memory of the initial condition can be certified by the absence of relaxation for the QMD [20].

Effect of a harmonic confinement potential.—We find little influence on the local quantities, up to the finite-size recurrence time, which can be shortened in the presence of a realistic trap: The generated excitations no longer travel with a constant speed but are slowly reflected.

Summary.—In this work, we have introduced a setting allowing for the observation of apparent thermalization in closed quantum many-body systems, without the need of addressing single sites of a lattice system. We show how, by making use of optical superlattices, signatures of local relaxation, including relevant time scales and dependencies on interactions, can be probed. In such dynamics, local maximum entropy states—Gibbs states in the absence of further constraints—emerge without having any external heat bath: Instead, in a symmetric fashion, each system forms the effective environment of the other in complex many-body dynamics. It is the hope that ideas along the line of the present work open up a way of experimentally quantitatively simulating an instance of the fundamental physical process of thermalization.

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[19] For any $\varepsilon > 0$, $t_{rec} > 0$ there exists a system size L and a relaxation time $t_{rel} > 0$ such that the reduced state satisfies $||\hat{\varrho}_I(t) - \hat{\varrho}_{max}||_1 < \varepsilon$ for all $t \in [t_{rel}, t_{rec}]$ [2].

[20] For very long times and considerable U, one may find a relaxation in momentum space due to coupling of eigenmodes, as being corroborated by flow approaches [9].