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Fidelity and Entropy Production in Quench Dynamics of Interacting Bosons in an Optical Lattice

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Abstract: We investigate the dynamics of a few bosons in an optical lattice induced by a quantum quench of a parameter of the many-body Hamiltonian. The evolution of the many-body wave function is obtained by solving the time-dependent many-body Schrödinger equation numerically, using the multiconfigurational time-dependent Hartree method for bosons (MCTDHB). We report the time evolution of three key quantities, namely, the occupations of the natural orbitals, that is, the eigenvalues of the one-body reduced density matrix, the many-body Shannon information entropy, and the quantum fidelity for a wide range of interactions. Our key motivation is to characterize relaxation processes where various observables of an isolated and interacting quantum many-body system dynamically converge to equilibrium values via the quantum fidelity and via the production of many-body entropy. The interaction, as a parameter, can induce a phase transition in the ground state of the system from a superfluid (SF) state to a Mott-insulator (MI) state. We show that, for a quench to a weak interaction, the fidelity remains close to unity and the entropy exhibits oscillations. Whereas for a quench to strong interactions (SF to MI transition), the relaxation process is characterized by the first collapse of the quantum fidelity and entropy saturation to an equilibrium value. The dip and the non-analytic nature of quantum fidelity is a hallmark of dynamical quantum phase transitions. We quantify the characteristic time at which the quantum fidelity collapses and the entropy saturates.

1. Introduction

The non-equilibrium dynamical properties and statistical relaxation, where various observables of an isolated and interacting quantum many-body system dynamically converge to equilibrium values, have garnered immense interest in the last decade [1–4]. Recent experiments with cold atoms in optical lattices have had an enormous impact in this field [5–7] because they provide a test bed for theories, with unprecedented experimental control and perfect isolation from the surroundings. Theoretically, it is an established fact that an isolated quantum system thermalizes; the eigenstate thermalization

hypothesis (ETH) states that the thermalization of an isolated quantum system is approached when the expectation values of (few-body) observables relax to an equilibrium and approach their long-time average value given by the Gibbs ensemble [8–10]. The analysis of the time-evolution of an isolated quantum many-body system far from equilibrium is the most fundamental way to establish its thermalization. Flambaum and Izrailev investigated the time evolution of generic quantum many-body systems [11,12]. Many-body quantum dynamics of δ-interacting bosons confined in a one-dimensional ring have been studied in Reference [13]. A linear increase, followed by a saturation of the many-body information entropy, has been shown to be associated with the onset of chaos and thermalization [13]. Whereas, in some recent works [14,15], one-dimensional spin$-\frac{1}{2}$ lattices with two-body interactions have been addressed. In the quench dynamics of this model, a system which is initially in an eigenstate $|\psi(0)\rangle$ of the initial Hamiltonian $\hat{H}_I$ is suddenly quenched to a new Hamiltonian. The probability for finding the system at a time t in initial state $|\psi(0)\rangle$ is known as the survival probability or quantum fidelity and is given by $F(t) = |\langle\psi(0)|e^{-i\hat{H}t}|\psi(0)\rangle|^2$. Here $\hat{H}$ is the final Hamiltonian, that is, after a quench. This quantum fidelity, $F(t)$, measures how close the two quantum states $|\psi(0)\rangle$ and $|\psi(t)\rangle$ are. In a lattice, the power-law behavior in $F(t)$ anticipates thermalization. This anticipation is independent of integrability, level repulsion, and the presence or absence of disorder. The behavior of the quantum fidelity is solely determined by the system Hamiltonian and the initial state.

A necessary condition for thermalization is statistical relaxation of various dynamical variables to some kind of equilibrium. The Shannon information entropy is one of these basic dynamical variables to follow such a relaxation. How entropy is produced, and on which time scale it relaxes to an equilibrium value after a quench, in quantum many-body systems is a challenging question. In the present work, we consider the fundamental problem of a few bosons in an optical lattice—a pioneering experiment with many bosons was performed by Greiner et al. in 2002 [16]. A transition between a superfluid (*SF*) phase (each atom spread out over the entire lattice) and a Mott-insulator (*MI*) phase (with a fixed number of atoms in each lattice site) is observed at a critical lattice depth.

In this article, we report the relaxation dynamics of a few interacting bosons in a triple-well lattice from a general many-body perspective. We initially prepare the system in the *SF* phase and induce dynamics in the system by a quench to a different interaction strength. With the interaction strength to which we quench the system, we cover the whole range from weak to strong interactions. Here, and in the following, we use—for simplicity—the terms "phase" and "quantum phase" to discuss the quantum states in finite systems that are only finite-size precursors of the true (quantum) phases in the thermodynamic limit. We thus quench the system via changing its two-body interactions and accurately measure several dynamical variables—occupations of the different natural orbitals $n_i(t)$, the quantum fidelity $F(t)$ and the many-body information entropy $S^{info}(t)$. The motivation of our present work is two-fold. First, we provide a highly accurate quantitative measure of the fidelity in the quench dynamics of interacting bosons in optical lattices. Second, from the time-evolution of our observables, we establish a link between the fragmented many-body state, the collapse of the quantum fidelity and the saturation of the many-body information entropy to an equilibrium value.

Here, "fragmentation" and "fragmented" refers to many-body states whose one-body density matrix has more than one significant eigenvalue [17,18]; this is to be contrasted with the terms "condensation" and "condensed", which refer to many-body states that have a one-body density matrix with only one significant eigenvalue [19]. Generally, many-body states in the *MI* phase are highly fragmented (one significant eigenvalue per site in the lattice) and many-body states in the *SF* phase are condensed (only one eigenvalue).

We observe that all the three measures—the eigenvalues $n_i(t)$, the quantum fidelity $F(t)$, and the entropy $S^{info}(t)$—are in mutual agreement. For quenches to weak interactions, the many-body states start to fragment but a complete ($n_i(t) \sim \frac{1}{5}$) fragmentation (where S is the number of sites) is not achieved. The corresponding quantum fidelity remains close to unity ($F(t) \sim 1.0$) with small fluctuations, and the information entropy oscillates. We conclude that the system does not relax even in its long time dynamics. The quenched state does not reach the *MI* phase. For quenches

to strong interactions, the many-body states exhibit $\frac{1}{S}$ fragmentation, that is, the quenched state reaches the *S*-fold fragmented *MI* phase. The corresponding quantum fidelity exhibits a collapse and the many-body information entropy saturates to a maximal equilibrium value. We also define a characteristic time t_c for the quench process as the unique time at which, synchronously, the many-body states attain full fragmentation for the first time, the fidelity exhibits its first collapse and the Shannon entropy saturates. This synchronization demonstrates the system's relaxation for quenches to a strong interaction.

Below, in Section 2 we first introduce the multiconfigurational time-dependent Hartree for bosons (MCTDHB) approach, our triple-well setup, and details on the analyzed quantities of interest. In Section 3, we discuss the obtained results and in Section 4 we conclude our work.

2. Methodology

2.1. Numerical Approach

To study the time evolution of a system of *N* interacting bosons, we solve the time-dependent Schrödinger equation,

$$\hat{H}|\psi\rangle = i\hbar\frac{\partial|\psi\rangle}{\partial t}, \tag{1}$$

using the MCTDHB approach [20,21], open-source software available at http://ultracold.org. The MCTDHB and MCTDHB-based approximations [22–25] were successfully applied to study the out-of-equilibrium dynamics of bosonic systems [26–36], see Reference [37] for a review and Reference [38] for a direct comparison of MCTDHB with experimental data using so-called single-shot simulations [39–44]. In this work, we use the MCTDHB method as implemented in the MCTDH-X package [45–47].

With MCTDHB, the many-body wave function is expanded as a linear combination of time-dependent permanents, $|\vec{n};t\rangle$, and time-dependent coefficients, $C_{\vec{n}}(t)$,

$$|\psi(t)\rangle = \sum_{\vec{n}} C_{\vec{n}}(t)|\vec{n};t\rangle. \tag{2}$$

The summation runs over all possible configurations $\vec{n}$ resulting from the arrangement of *N* bosons in a set of *M* orbitals, that is, $N_{conf} = \binom{N+M-1}{N}$. Note that the permanents are time-dependent because the orbitals (i.e., single-particle functions) used to build them are time-dependent, $\{\phi_i(x,t)\}_{i=1}^{M}$. The MCTDHB approach is derived using the time-dependent variational principle to optimize both the $\{C_{\vec{n}}(t)\}$ and $\{\phi_i(x,t)\}$. The configurations, $\vec{n} = (n_1, n_2, ..., n_M)$, represent the occupation numbers of the *M* orbitals with the particle-conservation constraint $\sum_i^M n_i = N$. The number of orbitals used to describe a given system is a critical parameter, it must be sufficiently large to ensure convergence; in the limit of $M \to \infty$ Equation (2) represents an exact solution to the Schrödinger equations, Equation (1), see References [47–50] for a practical demonstration with MCTDHB. For practical computations, *M* needs to be made small enough to make the numerical calculation feasible.

In the computations of the dynamics that we discuss below, the many-body wave function shows a strong fragmentation, that is, several natural orbitals have a significant population. We tested the convergence of all presented results by systematically increasing the number of orbitals *M* until no change in the calculated quantities such as energy, relaxation time, and entropy production was observed. Additionally, we find the occupation of the least-populated orbital to be negligible. For the interaction quenches that we study, we find that $M = 9$ orbitals are sufficient to achieve convergence.

2.2. Setup

In this work, we consider a system of N interacting bosons in a one-dimensional optical lattice. Such a quasi-one-dimensional (1D) system has already been realized experimentally [51,52] using a strong transversal confinement [51–54]. The Hamiltonian of the 1D system is given by,

$$\hat{H}(\lambda) = \sum_{i=1}^{N} \left[-\frac{1}{2}\frac{\partial^2}{\partial x_i^2} + V_{OL}(x_i) \right] + \sum_{i<j} \lambda \delta(x_i - x_j). \tag{3}$$

The one-body potential, V_{OL}, represents the optical lattice, $V_{OL}(x) = V\sin^2(kx)$, x_i is the coordinate of the i-th boson, V is the lattice depth, and k the wave-number. We use periodic boundary conditions. The interaction between the particles is described by a pairwise contact interaction, $\lambda\delta(x_i - x_j)$, with the 1D interaction strength, λ, proportional to the s-wave scattering length of the atoms [55,56]. The Hamiltonian $\hat{H}$ is scaled in terms of the recoil energy $E_R = \hbar^2 k^2/2m$, where m is the mass of the atoms. We use natural units, $\hbar = m = k = 1$, and all terms are dimensionless. In the following, the unit of time and distance are $\frac{\hbar}{E_R}$ and k^{-1}, respectively.

The dynamics of the system are induced by a quantum quench, for which one parameter of the Hamiltonian—here we use λ—is instantaneously changed. Our quench protocol follows two steps: (i) The ground state of $\hat{H}(\lambda_i)$, obtained via imaginary time-propagation, is used as the initial wave function $|\psi(t=0;\lambda_i)\rangle$. (ii) The initial state evolves unitarily under the influence of a different Hamiltonian $\hat{H}(\lambda_f)$ for a time t. Such a quantum quench can be experimentally realized using the tuning of an external magnetic field to change the s-wave scattering length of the atoms via a Feshbach resonance [57,58].

2.3. Quantities of Interest

The quench dynamics of the system will be investigated using three different quantities—the eigenvalues of the reduced one-body density matrix or natural orbital occupations $n_i(t)$, the Shannon information entropy of the natural orbital occupations $S^{info}(t)$, and the quantum fidelity $F(t)$. We now define these quantities.

(a) *Shannon information entropy and natural occupations.* The Shannon information entropy that we consider is defined from the natural occupations $n_i(t)$, that is, the eigenvalues $n_i(t)$ of the reduced one-body density matrix:

$$\rho(x,x',t) = \langle \psi(t)|\hat{\psi}^\dagger(x)\hat{\psi}(x')|\psi(t)\rangle = \sum_i n_i(t)\phi_i^{(NO)*}(x',t)\phi_i^{(NO)}(x,t), \tag{4}$$

with $\hat{\psi}(x)$ [$\hat{\psi}(x)^\dagger$] the bosonic annihilation [creation] field operator [17–19], the natural orbitals $\phi_i^{(NO)}(x,t)$ being the eigenfunctions of $\rho(x,x',t)$. See Ref. [59] for their evaluation with the MCTDHB wave function. The occupation Shannon information entropy is defined as [60–62],

$$S^{info}(t) = -\sum_i^M n_i(t)\ln[n_i(t)]. \tag{5}$$

This definition of Shannon entropy has already been considered for the MCTDHB wave function [30,63–65]. If a single natural orbital is occupied, $n_1(t) = 1$, the entropy is $S^{info}(t) = 0$ at all times. It is, for instance, the case for the Gross-Pitaevskii (GP) mean-field theory, where a single orbital is considered. Thus S^{info} is also a good measure of the many-body nature of the time-evolution of the system. For a given number of orbitals M, S^{info} reaches its maximum value for identical occupations of all natural orbitals $n_i = 1/M$. Thus $S^{info}(t)$ is a good measure of the dynamical fragmentation of the system.

(b) *Fidelity.* The Fidelity, $F(t)$, measures the overlap between the time-evolving wave function $|\psi(t)\rangle$ and the initial wave function $|\psi(0)\rangle$. It reads:

$$F(t) = |\langle \psi(0)|\psi(t)\rangle|^2. \tag{6}$$

The evaluation of the fidelity from an MCTDHB wave function requires the evaluation of permanents, and thus can only be performed for a small number of particles [66]. The fidelity is the absolute value squared of the autocorrelation function, $c(t) = \langle \psi(0)|\psi(t)\rangle$. The autocorrelation function is routinely used in molecular physics [67–69] to compute many-body excitation spectra [70] with wave function based approaches for discernible degrees of freedom, such as the multiconfigurational time-dependent Hartree method [71,72]. The relation between $c(t)$ and $F(t)$ indicates that the time-evolution of $F(t)$ is highly sensitive to the many-body eigenstates and energies of the Hamiltonian that play a role in the dynamics.

3. Results

We consider $N = 3$ bosons in a 1D triple-well optical lattice with periodic boundary conditions and a lattice depth of $V = 3.0$. We use the system to study the quantum phase transition between a superfluid (*SF*) phase and a Mott-insulator (*MI*). Keeping the lattice depth constant, the phase transition occurs when the interaction strength, λ, is increased. The phase diagram of the system provides information on the static properties of the many-body state as a function of λ. The critical interaction strength, λ_c, for which this phase transition occurs is $\lambda_c \approx 0.4$ for our system; for a detailed discussion of the phase diagram, see References [73,74].

We now investigate the dynamics of the system following a quantum quench. We start from the ground state of a Hamiltonian with small interactions λ_i in the *SF* phase. We then compute the unitary evolution under the action of a new Hamiltonian at larger interactions $\lambda_f > \lambda_i$ with MCTDHB. The ground state of the Hamiltonian with interactions $\lambda_f > \lambda_c$ is in the *MI* phase. More formally, before some quenches we have $\lambda_i < \lambda_c$ and $\lambda_f > \lambda_c$. Such an evolution is also investigated in the field of dynamical quantum phase transitions [75,76].

The ground state is prepared for an interaction strength $\lambda_i = 0.05$ in Equation (3). For this interaction strength, the system is in the *SF* phase and the particles are coherently delocalized over the triple-well lattice potential. The state has a single significant occupation, $n_1(t = 0) \approx 1, n_k(t = 0) \approx 0$ for $k > 1$, and is thus well described by the mean-field GP theory. The quench increases the energy of the system from the ground state energy $E_{gs}(\lambda_i)$ to a final value $E(\lambda_f)$. We report the excitation energy of the system, $E_{ex} = E(\lambda_f) - E_{gs}(\lambda_i)$, for different quenches ($0.2 \leq \lambda_f \leq 10$) in Table 1. Note that for $\lambda_f = 0.2$, the ground state of the final Hamiltonian is also in the *SF* phase, while for the larger values considered $\lambda_f \geq 0.5$, the ground state of the final Hamiltonian is in the *MI* phase.

We now analyze the time-evolution of the system after the quench as a function of λ_f in terms of its natural occupations, see Figure 1. Before the evolution ($t = 0$), only the first natural orbital is occupied, $n_1(t = 0) \approx 1, n_k(t = 0) \approx 0$, as expected for the *SF* phase. As time evolves after the quench, the population of the first natural orbital decreases while the population of the second and third orbitals increases, the other occupation numbers ($n_{i>3}$) remain comparatively small. The dynamics are different if the interaction strength after the quench, λ_f, is across the superfluid-to-Mott-insulator transition that takes place in the ground state for $\lambda_c \approx 0.4$. When $\lambda_f = 0.2 < \lambda_c$ [Figure 1a] the populations n_2 and n_3 increase at first, but reach a first maximum (~ 0.14) at $t = 19$ and then decrease again back to almost zero. This oscillations repeat several times (not shown in Figure 1). We infer that the system attempts fragmentation but fails to reach the *MI* phase that is characterized by a threefold fragmentation ($n_1 \approx n_2 \approx n_3 \sim 1/3$).

When the quench is performed such that $\lambda_f > \lambda_c$, the threefold fragmentation occurs at first at some characteristic time t_c [Figure 1b–e and Table 1] and reappears several times almost periodically (not shown). We can thus infer that the final Hamiltonian has an *MI* ground state, from the dynamical

emergence of threefold fragmentation. The characteristic time of the emergence of fragmentation decreases when the value of λ_f increases. This decrease is likely due to the higher energy pumped into the system by the quench [Table 1].
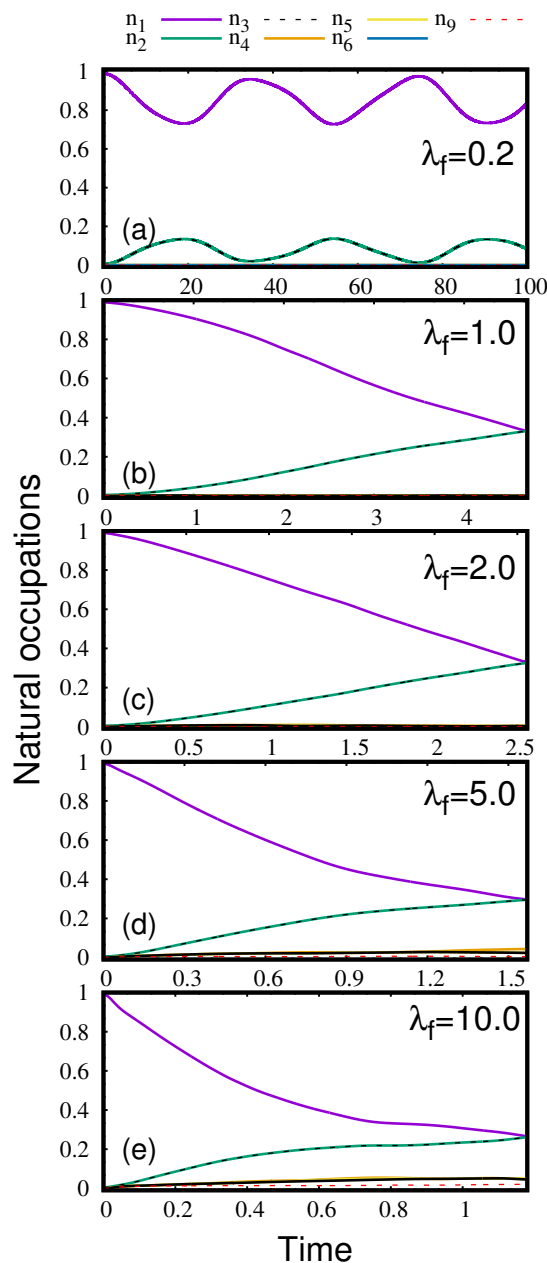

Figure 1. Time evolution of the natural occupations $n_i(t)$ for different interaction quenches (**a**) $\lambda_f = 0.2$ (small). (**b**) $\lambda_f = 1.0$. (**c**) $\lambda_f = 2.0$. (**d**) $\lambda_f = 5.0$. (**e**) $\lambda_f = 10.0$. As time increases, the occupation of the first orbital decreases and two other orbitals start to contribute. For small interactions after the quench, $\lambda_f = 0.2$, the system thus never reaches the complete fragmentation with $n_1 \approx n_2 \approx n_3 \approx \frac{1}{3}$ that characterizes the *MI* state. When λ_f increases, the state becomes threefold fragmented ($n_1 \simeq n_2 \simeq n_3 \simeq 33\%$). For larger interaction strengths, the time required to first observe threefold fragmentation is smaller.

Table 1. Values of the interaction strength of the quench λ_f, the excitation energy $E_{ex} = E(\lambda_f) - E_{gs}(\lambda_i)$ of the system and the time of the first occurrence of the *MI* state with a threefold fragmentation, t_c.

λ_f	E_{ex}	t_c
0.2	0.061	N.A.
1.0	0.263	4.70
2.0	0.667	2.56
5.0	1.878	1.57
10.0	3.898	1.18

We now turn to the Shannon information entropy defined from the natural occupations, Equation (5). Of course, the time-evolution of $S^{info}(t)$ reflects directly the dynamics of the natural occupations.

For a quench within the *SF* phase, $\lambda_f = 0.2 < \lambda_c$, the information entropy exhibits regular oscillations which resemble the collapse and revival dynamics observed in the experimental work of Reference [16], see Figure 2.
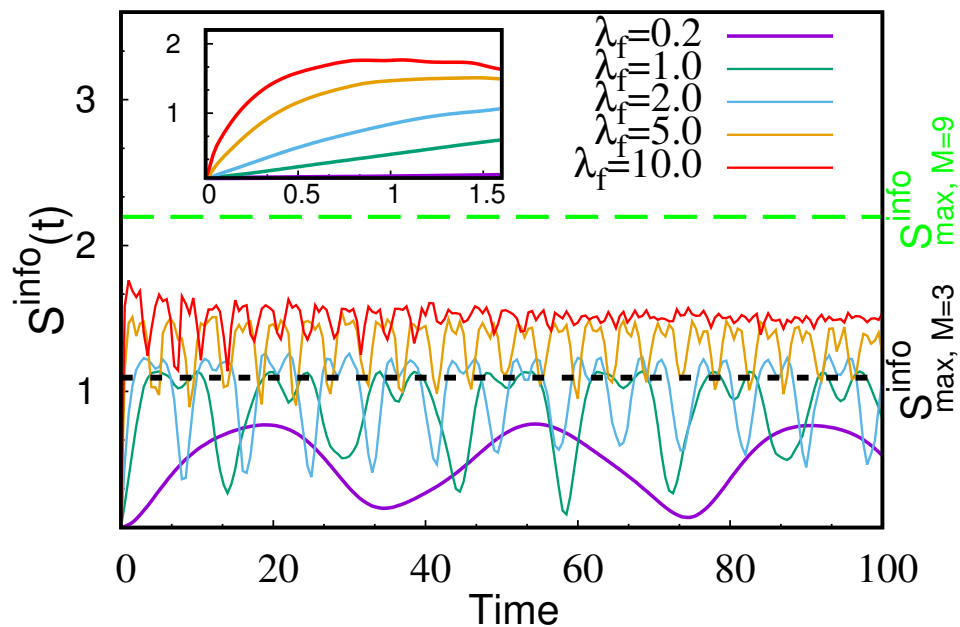
Figure 2. Plot of the Shannon information entropy $S^{info}(t)$ as a function of time. For smaller λ_f, $S^{info}(t)$ oscillates with time and does not saturate. When λ_f increases, the oscillations reduce and the system tries to attend a saturation value. At a sufficiently large value of λ_f, the oscillations vanish and the entropy saturates to a maximum entropy state. The larger the interaction strength, the smaller the time to reach the saturation value (inset). See the text for further discussion.

For quenches that cross the superfluid-to-Mott-insulator transition value λ_c, the information entropy exhibits a sharp linear increase at short time ($t \leq t_c$), inset in Figure 2. This short-time entropy production indicates that an exponentially growing number of many-body states participate in the dynamics. The production of information entropy, $S^{info}(t)$, reflects that the evolution of the system includes an *MI* state. Importantly, the first maximum of the information entropy is reached at the characteristic time determined by the natural occupations, Table 1. At longer time ($t > t_c$), the entropy exhibits oscillations in time for quenches to $\lambda_f = 1$ and 2. These oscillations indicate that the system undergoes a periodic dynamical transition between a threefold fragmented *MI* state at maximal ($S^{info}(t) \sim \ln(3) \sim 1.1$) and a condensed state with minimal entropy ($S^{info}(t) \to 0$). In the case of quenches to larger interaction strength, $\lambda_f > 5$, the occupation entropy reaches maximal values that are larger than the one expected for a threefold fragmentation [$S^{info} > \ln(3) = 1.099$]. This results from the occupations of more than three natural orbitals that can bee seen in Figure 1d,e at short times. Moreover, at longer times, we observe that the oscillations of the entropy become aperiodic and their amplitudes decrease and even disappear almost for $\lambda_f = 10$. Thus, we conclude that the entropy relaxes to some equilibrium value for the quantum quenches to large interaction strength. We note that this equilibrium value is close to the value 1.099 expected for the *MI* state and significantly smaller than the maximal entropy $S^{info}_{max} = -\sum_{i=1}^{9} \frac{1}{9} \ln(\frac{1}{9}) = 2.197$ that our $M = 9$ basis can support.

We have shown that the time-evolution of the natural occupations and the Shannon information entropy illustratively characterizes the quantum nature of the time-evolution of the quenched triple-well system. We now address the role of the many-body eigenstates involved in the dynamics by considering the time evolution of the fidelity, Equation (6), see Figure 3. The fidelity provides a measure of the magnitude of the autocorrelation function, that is, the overlap between the initial $|\psi(t = 0)\rangle$ and the time-evolved state $|\psi(t)\rangle$.

For a quench to a weak interaction strength, $\lambda_f = 0.2 < \lambda_c$ Figure 3a the fidelity remains close to unity. In this situation, the system is only weakly fragmented and thus the time-evolved wave function strongly overlaps with the initial one. For quenches to larger interaction strengths, $\lambda_f = 1$ and 2, pronounced dips in the fidelity ($F(t) < 10^{-2}$) are observed, first at the characteristic time t_c and repeatedly thereafter. At the times where $F(t)$ is small, the time-evolved wave function $|\psi(t_c)\rangle$ has a small, finite overlap with the initial state. The dips in the fidelity mark times, where the ground state of the initial Hamiltonian has almost no contribution to the time-evolved state; due to the synchronization with our observation from the natural occupations in [Figure 1], we interpret the dips as a hallmark of the dynamical transition to the *MI* state. For the quenches to the largest interaction strengths that we consider, $\lambda_f > 5$, the shape of the dips transforms into "spikes"; a non-analytical point in the fidelity function at $t = t_c$ that we term collapse point. The overlap with the initial state is strongly suppressed when the *MI* state is reached. This non-analytical behavior is reminiscent of the non-analyticity of the Loschmidt echo rate function in dynamical quantum phase transitions as described in References [75,76].
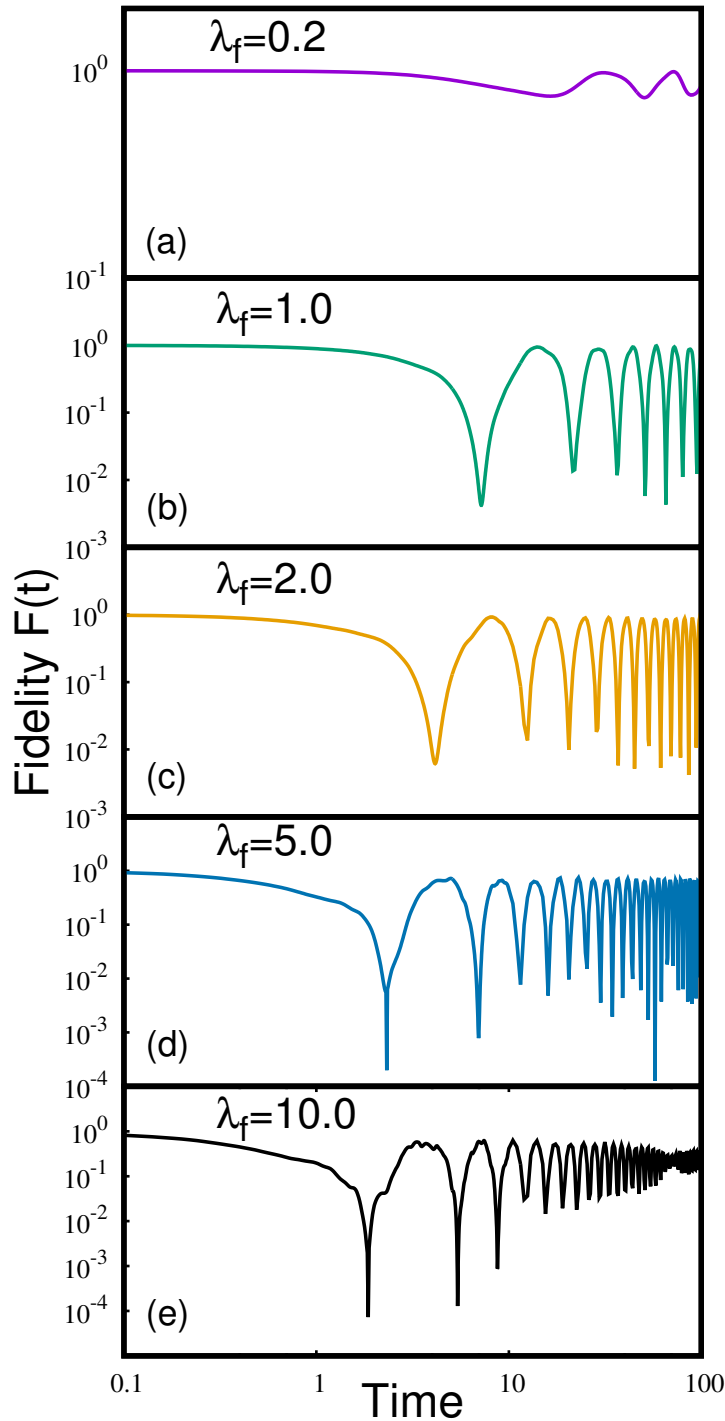
Figure 3. Quantum fidelity for different interaction quenches in logarithmic scale. For a quench to weak interactions, $\lambda_f = 0.2$, the fidelity $F(t)$ remains close to unity at all times. For stronger interaction quenches $\lambda_f = 1$ and 2, the quantum fidelity exhibits prominent but smooth dips. When the interaction is quenched to a large value, i.e., $\lambda_f \geq 5$, the dips transform into non-analytical "spikes"; the first spike in time is termed collapse point.

4. Summary and Conclusions

In this paper, we studied the quench dynamics of interacting bosons in a 1D triple-well optical lattice from a general many-body perspective utilizing the MCTDHB method to obtain highly accurate numerical solutions of the time-dependent Schrödinger equation. We described the process of

relaxation by the dynamical evolution of the three key quantities, namely the natural occupations, the Shannon information entropy, and the fidelity. We studied quantum quenches and covered the whole range of final interaction strengths from weak to strong interactions. We addressed the fundamental question of whether, and on which time-scale, the signatures of the relaxation of the system are seen. We found that quenches to weak or moderate interactions do not lead to a complete relaxation of the system. In contrast, quenches to strong interactions lead to a relaxation of the isolated quantum system solely determined by the interaction strength after the quench. Our three observables characterize this relaxation in mutual agreement—a threefold-fragmented many-body state, a saturation of the Shannon information entropy, and a collapse of the fidelity function. All three features of relaxation in the time-evolution of our observables emerge—in synchronization—for the first time at the characteristic relaxation time t_c.

We thus exhibited the features of relaxation for an isolated quantum system and its relation to a dynamical quantum phase transition characterized by a collapse point in the quantum fidelity.

Abbreviations

The following abbreviations are used in this manuscript:

SF	Superfluid
MI	Mott-insulator
GP	Gross-Pitaevskii
MCTDHB	Multiconfigurational time-dependent Hartree for bosons

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