Dynamics and relation to coherence of many-body entropy and statistical relaxation in ultracold parabolically trapped bosons

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Abstract

We study the quantum many-body dynamics in the entropy production of \( N = 10 \) interacting identical bosons in an external harmonic trap. We use the multiconfigurational time-dependent Hartree for bosons or MCTDHB, an essentially exact many-body theory, for the solution of the time-dependent Schrödinger equation. We introduce new and genuinely many-body measures for the entropy production that relate to the time-dependent many-body basis set used in MCTDHB. With these measures, we demonstrate the transition from regular or quasi-periodic to irregular or chaotic dynamics in the time-evolution of quantum information (Shannon) entropy, number of principal basis components and inverse participation ratio for various repulsive interaction strengths on a many-body level. The many-body Shannon information entropy approaches the value of \( \ln(0.48 D) \), where \( D \) is the number of time-dependent many-body states employed in the MCTDHB computations for larger interaction strength, as predicted by the Gaussian orthogonal ensemble (GOE) of random matrices. This is a clear signature of statistical relaxation, here demonstrated for the first time with a genuine many-body entropy measure. We find a fundamental connection between the production of entropy, the build-up of correlations and the loss of coherence.

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I. INTRODUCTION

The onset of thermalization in an isolated quantum system of a finite number of interacting particles is one of the important issues considered in theoretical physics in recent days. Experimental progress with various quantum systems formed of interacting particles has further corroborated this interest. These experiments reveal that the question how entropy is produced in a quantum system is one of the basic outstanding problems of many-body physics. A necessary condition for thermalization is the statistical relaxation of a system including the fluctuations of its observables to some kind of equilibrium. In isolated dynamical quantum systems of interacting particles, the emergence of statistical relaxation relates to chaos in the energy spectra. Statistical relaxation is the emergence of statistical behavior from microscopic dynamics. An important aspect of the onset of thermalization in isolated dynamical quantum systems is interparticle interactions. Recently, it was proposed that the eigenstates’ statistics contain crucial information about the relation of chaotic dynamical behavior to the onset of thermalization. In earlier studies in this direction the eigenstate thermalization hypothesis (ETH) was tested using a basis set relating to non-interacting particles and a large spread was found with these measures. Calculations have been done for 1D spin-$\frac{1}{2}$ systems with nearest-neighbor and next-nearest-neighbor coupling as well as for gapped systems of hard-core bosons. The onset of chaos and relaxation in such isolated systems of interacting spins has been studied by the energy shell approach. Increasing the perturbation strength results in a transition to chaos. Manifestation of classical chaos in the statistics of quantum energy levels and the confirmation of random matrix fluctuation in molecular spectra has also been established before.

In the present work we consider many-body quantum dynamics of ten bosons confined in a one-dimensional (1D) harmonic trap that interact with a contact interaction potential. The 1D regime is easily achieved in optical and magnetic traps with tight transverse confinement when the radial degrees of freedom are frozen. Quantum many-body effects are more important in reduced dimensional and interacting systems as the competition between statistical properties and quantum fluctuations is enhanced. Experimentally, 1D harmonically trapped quantum degenerate systems have been realized which makes the study of quantum many-body dynamics of the ultracold Bose gas in 1D especially interesting. The
motivation of our present work is as follows: We use the multiconfigurational time-dependent
Hartree method for bosons (MCTDHB)\cite{27, 29, 30} to obtain highly accurate results for the
ongoing many-body dynamics and monitor the production of entropy throughout these
dynamics using genuine many-body measures.

This is in contrast to most previous calculations where the wave function is expanded
on a non-interacting basis and exclusively one-body measures were employed to follow the
production of entropy. We study the production of entropy as the spreading of the expansion coefficients \(\{C^{|\vec{n};t}\}\) for different \(\mathrm{time-dependent}\) many-body basis states \(\{\vec{n};t\}\) for
different inter-particle interaction strengths. It is important to stress, that the many-body
entropy measure is minimized by quantum states which can be described by effective one-
body (mean-field) theories such as the Gross-Pitaevskii equation. We expect a dynamical
transition from regular (quasi periodic) to irregular (chaotic) dynamics with the increase of
the inter-particle interaction strength. It is known that the Hamiltonian of the bosons in
the 1D regime is given by the Lieb-Linger model where the two-body interaction is assumed
to be mediated by a contact interaction potential\cite{31}. In the limit of \(n/g \rightarrow 0\) ( where \(n\) is
the particle density, \(g\) is the inter-atomic coupling strength ) fermionization occurs. When
\(n/g \rightarrow \infty\) limit corresponds to the mean-field approximation of weakly interacting bosons and
should exhibit regular dynamics. In the Tonks-Girardeau (TG) regime, the density of the
interacting bosons becomes identical to that of non-interacting fermions. In the crossover
between the two regions, near \(n/g \simeq 1\), the mean-field approach breaks down, correlations
become crucial and many-body features will be exhibited in the quantum dynamics and
the entropy measures. Thus the study of many-body dynamics by MCTDHB and study of
the crossover from the regular to (quantum) irregular dynamics is highly interesting. One
important question is how the entropy of an isolated quantum system increases with time
at the transition point, especially for the defined many-body measures. The Shannon en-
tropy \(S(t)\) of the system is an ideal measure as it is directly related to the vanishing of
interference fringes when the external confinement is removed and the bosons are allowed
to expand ballistically, as shown in Ref.\cite{32} for a Shannon entropy defined using a non-
interacting basis set. The Shannon entropy \(S(t)\) also allows one to accurately measure the
effective number of many-body states involved in the dynamics which is calculated through
the so-called number of principal components, \(N_{pc}(t) = \exp[S(t)]\). Let us note here that the
number of significant coefficients in an MCTDHB treatment also shows directly the num-
ber of contributing many-body states, since MCTDHB uses a time-adaptive variationally optimized many-body basis set. The MCTDHB basis is time-dependent and follows the dynamics and therefore the number of principal components is exponentially smaller than in a treatment with a time-independent basis set. We also measure the delocalization of the coefficients’ distribution for larger interaction and through the inverse participation ratio defined as $I_{\text{ipr}}(t) = \sum_{\tilde{n}} \left| |C_{\tilde{n}}(t)|^4 \right|^{-1}$. These quantities basically measure how spread out the wave function $\Psi(t)$ is in the employed time-dependent many-body basis $|\tilde{n}; t\rangle$. In the literature, quite often $N_{\text{pc}}$ is referred as Shannon or information entropy and $I_{\text{ipr}}$ as the number of principal components [33]. We aim to analyze the emergence of statistical relaxation measured by genuine many-body properties of the interacting trapped ultracold bosons which are related to the time-dependent many-body basis. To do so, we employ the essentially-exact MCTDHB method. By gradually increasing the strength of the interaction we move the system further and further away from integrability. The analysis of the above mentioned time-dependent statistical properties will show the intensified production of entropy in the dynamics of the wave function $\Psi(t)$ when the interaction strength is increased. In such a system, the eigenstate thermalization hypothesis (ETH) states that thermalization occurs at the level of individual eigenstates of the Hamiltonian and the criterion for this thermalization is the statistical relaxation of system observables and averages for large interaction strength [19, 22, 34–36]. In the present work we study the interaction quench dynamics by calculating the time-evolution of the Shannon entropy (information entropy). We calculate the information entropy $S^{\text{info}}(t)$ using the time-dependent expansion coefficients of the time-dependent many-body basis set as well as the occupational entropy $S^{\text{occu}}(t)$ (see also Ref. [37]) from the natural orbital occupation numbers, i.e., the eigenvalues of the reduced one-body density matrix. $S^{\text{info}}(t)$ and $S^{\text{occu}}(t)$ behave in a similar way, a linear increase followed by saturation, i.e. there is statistical relaxation [21, 22]. Also $S^{\text{info}}(t)$ approaches the value $ln(0.48D)$ predicted by the GOE random matrix ensemble [33, 38, 39]. This will be discussed in detail in Section III. The saturation of $S^{\text{info}}(t)$ close to the GOE value $S_{\text{GOE}} \simeq ln(0.48D)$ is a main aspect of statistical relaxation.

To complement the dynamics of the different defined entropies, the number of principal components $N_{\text{pc}}(t)$, and the inverse participation ratio $I_{\text{ipr}}(t)$ with another point of view, we compute the correlation function and coherence [40]. We point out how the dynamics in entropy relate to the dynamics in coherence, correlations, and occupation numbers. The
fringe visibility in interference experiments is determined by the first order correlation function \( g^{(1)}(\vec{r}', \vec{r}; t) \). In the Young double slit experiment the maximal fringe visibility of the interference pattern corresponds to \(|g^{(1)}(\vec{r}', \vec{r}; t)| = 1\). However, the interaction between the particles will modify this maximal fringe visibility in the interference pattern. Our numerical results also reveal that \(|g^{(1)}(\vec{r}', \vec{r}; t)|\) is close to unity for very small interaction which shows that the state of the system is close to being coherent. However, \(|g^{(1)}(\vec{r}', \vec{r}; t)|\) is close to zero for larger interaction which indicates that the interacting bosons are anti-correlated, and therefore incoherent. The entropy measures introduced, related to many-body quantities, i.e. \( S^{\text{inf}}(t) \) and \( S^{\text{occu}}(t) \), exactly measure this departure from coherence.

This paper is organized as follows. In Sec. II we give a brief introduction to the numerical many-body method, MCTDHB, that we use [27, 29, 30]. Sec. III considers our results on the different entropy measures for various interaction strengths and Sec. IV considers how the observation in Sec. III conciles with the observation of (de-)coherence. Sec V concludes the summarizes the work.

II. METHODOLOGY

The evolution of \( N \) interacting bosons is governed by the time-dependent many-body Schrödinger equation (TDSE):

\[
\hat{H} \psi = i \frac{\partial \psi}{\partial t}.
\]

The total Hamiltonian is

\[
\hat{H}(x_1, x_2, ..., x_N) = \sum_{i=1}^{N} \hat{h}(x_i) + \Theta(t) \sum_{i<j=1}^{N} \hat{W}(x_i - x_j)
\]

where \( \hat{h}(x) = \hat{T}(x) + \hat{V}(x) \) is the one body Hamiltonian in the external trapping potential \( V \) and the kinetic energy \( T = \frac{1}{2} \frac{\partial^2}{\partial x^2} \), \( \hat{W}(x_i - x_j) \) is the two-body interaction, and \( \Theta(t) \) is the Heaviside function. In the method we use to solve the time-dependent many-boson Schrödinger equation, [11], with the Hamiltonian, (2), MCTDHB, the ansatz for the many-body wave function is taken as a time-dependently weighted linear combination of time-dependent permanents

\[
|\psi(t)\rangle = \sum_{\vec{n}} C_\vec{n}(t) |\vec{n}; t\rangle; |\vec{n}; t\rangle = \sum_{\vec{n}} C_\vec{n}(t) \prod_{i=1}^{M} \left( \frac{\hat{b}_i^\dagger(t)}{\sqrt{n_i!}} \right) |\text{vac}\rangle
\]
Here, the summation runs over all possible configurations $|\vec{n}; t\rangle$, $\hat{b}_i^\dagger(t)$ creates a boson in the $i$th single-particle state $\phi_i(x, t)$, and $|\text{vac}\rangle$ denotes the vacuum. It is important to stress that in the ansatz, Eq. (3), both, the expansion coefficients and the orbitals, $\{\phi_i(x, t)\}_{i=1}^{M}$, that build up the permanents $|\vec{n}; t\rangle$ are time-dependent fully variationally optimized quantities. MCTDHB has been established as the presently most efficient way to solve the time-dependent many-body problem of interacting bosons accurately and for a wide set of problems [41]. In MCTDHB(M), the vectors $\vec{n} = (n_1, ..., n_M)$ represent the occupations of the orbitals in a single configuration and preserve the total number of particles, $n_1 + ... + n_M = N$, $M$ is the number of one particle functions that build up the permanents. The method’s efficiency lies in the variationally optimized, time-adaptive basis that makes the sampled Hilbert space dynamically follow the motion of the many-body dynamics. In the limit of $M \to \infty$, the set of permanents $\{|\vec{n}; t\rangle\}$ spans the complete $N$-boson Hilbert space and thus expansion in Eq.(3) is exact. In practice, we have to limit the size of the Hilbert space in the computation. Since the permanents are time-dependent, one can use a much shorter expansion than if only the expansion coefficients are taken to be time-dependent. This leads to a significant computational advantage. The expansion coefficients $\{C_{\vec{n}}(t)\}$ and orbitals comprising the permanents are independent variational parameters. To solve the TDSE, Eq. (1) for the wave function $\Psi(t)$, one needs to determine the evolution of the coefficients and orbitals in time. Their equations of motion are derived by the requirement of the stationarity of the action functional with respect to the variations of the time-dependent coefficients and the set of time-dependent orbitals. The obtained equations form a coupled set of nonlinear integro-differential equations [29] that we solve simultaneously with the recently developed recursive MCTDHB (R-MCTDHB) package [27]. In order to calculate eigenstates of the Hamiltonian $\hat{H}$ (Eq.(2)), one uses the so-called improved relaxation method. By propagating a given initial guess in imaginary time, excitations are damped exponentially and the system relaxes to the ground state. Thus, besides time-evolutions, one can also study eigenstates. It should be noted that in the widespread time-dependent Gross-Pitaevskii (TDGP) theory, the many-body wave function is given by a single permanent $|n_1 = N; t\rangle$ i.e., all particles reside in one orbital and there is consequently only a single coefficient. MCTDHB(M) boils down to the TDGP theory for $M = 1$. 

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III. NUMERICAL RESULTS ON THE PRODUCTION OF ENTROPY IN INTER-
ACTION QUENCH DYNAMICS

For our present calculation we work in one dimension. We consider $N = 10$ repulsively
interacting bosons in an external harmonic trap. When contact interactions $W(x_i - x_j) =
\lambda_0 \delta(x_i - x_j)$ are considered the dimensionless Hamiltonian has the form

$$H = \sum_{i=1}^{N} \left( -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} + V(x_i) \right) + \lambda_0 \sum_{i<j}^{N} \delta(x_i - x_j). \quad (4)$$

As an external potential we choose an harmonic trap $V(x_i) = \frac{1}{2} x_i^2$. $\lambda_0$ is the strength
of the dimensionless interparticle interaction which we vary in our investigation. In the
computation we restrict the number of orbitals to $M = 6$, yielding a total of $N_{\text{conf}} = 3003$
permanents. A key aspect of many-body quantum chaos is how the many-body wave function
spreads with an increase in interparticle interaction. Thus, depending on the strength of
the interaction, the number of contributing components will vary from a small to a very
large number. Here, the isolated systems with finite range interaction strongly differ from
the random matrices. In full random matrices, the eigenstates are completely extended
irrespective of the number or choice of basis states. However, for isolated systems with finite
range interactions only a fraction of the coefficients $C_{\vec{n}}$ is non-zero.

In Fig. 1, we plot $|C_{\vec{n}}(t)|^2$ as a function of the lexicographical index of expansion basis
states for interaction parameter $\lambda_0 = 0.5$ for the times $t = 0.2, 0.5, 1.0, \text{ and } 2.0$. It should
be noted here that the coefficients relate to a genuine many-body basis. The vectors in this
basis are not eigenstates of the Hamiltonian. However, a one-to-one correspondence exists:
Every eigenstate of the interacting problem can be represented as a pattern, i.e., a limited
number of significantly contributing configurations weighted by their respective coefficients.
Initially, at $t = 0$, only a single coefficient is nonzero. As depicted in Fig. 1a)-d), the number
of significant coefficients grows with time due to the interparticle interactions. For smaller
interactions, we expect that the number of significantly contributing coefficients $C_{\vec{n}(t)}$ is only
a small portion of the available basis states for $M = 6$, since the spreading of the coefficients’
distribution is driven by the repulsion of the particles. If the number of nonzero elements of
$\{C_{\vec{n}}\}$ is a small portion of $N_{\text{conf}} = 3003$, we describe the state as localized. With increasing
time, the distribution of contributing or non-negligible coefficients spreads. We may say that
for such small interaction the state is very close to the mean-field description for which only
a single coefficient would contribute. In Fig. 2, we plot the coefficients $C_{\vec{n}}(t)$ as in Fig. 1, but for larger interaction ($\lambda_0 = 10.0$). We observe a substantial spreading of the coefficients of the wave function as compared to the case of weaker interactions depicted in Fig. 1. Since the contributing coefficients spread almost the whole available space, we refer to such a state as delocalized.

The degree of complexity of individual states and global properties of eigenstates can be further characterized by the number of principal components $N_{pc}(t)$, and the inverse participation ratio, $I_{ipr}(t)$, that are defined as

$$S^{info}(t) = -\sum_{\vec{n}} |C_{\vec{n}}(t)|^2 \ln |C_{\vec{n}}(t)|^2,$$

$$N_{pc}(t) = \exp[S^{info}(t)],$$

$$I_{ipr}(t) = \frac{1}{\sum_{\vec{n}} |C_{\vec{n}}(t)|^4}.$$

The Shannon information entropy $S^{info}(t)$ actually allows to estimate the effective number of many-body states which are involved in the dynamics, whereas $N_{pc}(t)$ and $I_{ipr}(t)$ are the measures which quantify the average number of basis states that make up the wave function. In Fig. 3, we plot $N_{pc}(t)$ and $I_{ipr}(t)$ for smaller interaction $\lambda_0 = 0.5$, and in Fig. 4 for larger interactions $\lambda_0 = 10.0$. For smaller interactions, when the system is made of weakly interacting bosons, the inter-atomic correlation is small, and large fluctuations are expected. This is because in the limit of localized states, there are few contributing components with large overlaps. Whereas for larger interactions, fluctuations should follow the GOE of random matrices [38, 39, 42] and a curve with smaller fluctuations is expected as shown in Fig. 4. For such large interactions, the number of principal components becomes large and the fluctuations in the values of the overlaps also decrease. In contrast to the time-dependence for smaller interactions the increase of the number of principal components $N_{pc}(t)$ is very different from $N_{pc}(t)$ defined by the entropy and for $I_{ipr}(t)$ determined by the inverse participation ratio for larger interactions. It increases exponentially fast before saturation. The characteristic time for this saturation is $\tau = 0.8$.

The quench dynamics of the system and the time-evolution of Shannon entropy therein are also a nice tool to observe the emergence of statistical relaxation and to verify ETH for a generic non-integrable system. The occupational entropy is defined as follows:
\[ S^{\text{occu}}(t) = - \sum_i \bar{n}_i(t) \ln \bar{n}_i(t). \] (8)

\( S^{\text{occu}}(t) \) is obtained using the relative occupancies of different single particle states, \( \bar{n}_i(t) = \frac{n_i(t)}{N} \). The \( n_i(t) \) are termed natural occupation numbers and are the eigenvalues of the reduced one-body density matrix of the system\ref{45}. Numerical data calculated from Eq. (5) and (8) is shown in Fig. 5 for various interaction strengths. We observe that the Shannon entropy increases for very small values of \( t \) before saturating. For smaller interactions \( S^{\text{info}}(t) \) almost increases linearly before saturation, however it saturates at the value \( S^{\text{info}} \simeq 3.2 \) which is far below the expected value of \( S_{\text{GOE}} \). Hence, there is no signature of chaos as the wave function is localized. Whereas for larger interaction \( S^{\text{info}}(t) \) shows very quick saturation. It is to be noted that for our present calculation with 10 bosons in 6 orbitals the value of \( D = 3003 \). This yields the value of \( S_{\text{GOE}} = \ln(0.48D) = 7.273 \). Whereas for large interaction strength with \( \lambda_0 = 10.0 \), it is close to 6.49 and with \( \lambda_0 = 15.0 \), saturation occurs at 7.17, which are slightly smaller than the GOE value because the interaction strength is finite. As discussed in the Ref.\ref{43}, in interacting particle systems, due to the operation of embedded Gaussian orthogonal ensemble (EGOE) of random matrices (they are appropriate for systems with lower body rank operators such as the one plus two-body Hamiltonian used in the present study), \( S^{\text{info}} \) will be close to but not same as the GOE value. At larger time the saturation is maintained as shown in Fig. 6, it clearly demonstrates the existence of statistical relaxation. The big difference of the characteristic time scale on which the saturation is happening as shown in the inset of Fig. 6 for various interaction strengths is of importance. Although we get the signature of statistical relaxation for stronger interaction, we are unable to prove whether chaos is an essential criterion for the emergence of statistical relaxation. Our observation of the broadening of the coefficients’ distribution for larger interactions is sufficient to show statistical relaxation. For a final conclusion on the importance of chaos to the production of many-body entropies further studies are needed, especially with a larger number of coefficients, in order to assess if the wave-function indeed would completely explore also larger Hilbert spaces.

In the Fig. 5 we plot the calculated value of \( S^{\text{occu}}(t) \) for various inter-particle interactions. At \( t = 0 \), when all bosons are in the lowest single particle orbital, \( n_1 = N \) and \( n_i = 0 \) for \( i = 2, 3, \ldots M \). Then \( \bar{n}_1 = 1 \) and all others are zero. Therefore \( S^{\text{occu}} = -\ln(1) = 0 \). This
implies that when all bosons are in the lowest orbital, entropy is zero and the system is fully ordered. However, at later time, all bosons start to distribute themselves in all $M$ orbitals. For larger interaction strengths, when the eigenstates are fully delocalized, all bosons are on average roughly equally distributed in the $M$ orbitals and this is the situation corresponding to the GOE. Then $n_i = \frac{N}{M}$ for all $i$ giving $\bar{n}_i = \frac{1}{M}$ for all $i$. Therefore $S^\text{occu} = -\sum_{i=1}^{M} \left(\frac{1}{M}\right) \ln\left(\frac{1}{M}\right) = \ln(M)$. In our present calculations with $M = 6$ and $N = 10$, $S^\text{occu}_{\text{GOE}} = \ln(M) = \ln(6) = 1.79$. In Fig. 5 we also observe that $S^\text{occu}$ quickly saturates to the value of 1.76 which is close to but a little smaller than the GOE value. This is again due to the interaction being strong but finite.

IV. RELATION OF CORRELATIONS AND ENTROPY PRODUCTION

An important conjecture which we would like to put forward, is that the dynamics in entropy are strongly related to the dynamics in coherence. The coefficients are the time-dependent occupations in the time-dependent many-body basis we employ by using MCT-DHB. Let us briefly elaborate on the extreme cases of the minimal and maximal spread of Shannon entropy $S^\text{info}(t)$ that we can get with this measure.

The minimal spread, i.e. the minimal entropy we get in our many-body entropy when for instance only the first configuration contributes to the wave function. In this case only a single coefficient is 1 (or $N$, subject to normalization). This is a very special case concerning a many-boson system – the following statements apply to it 1) The Gross-Pitaevskii equation fully describes it. 2) It is fully coherent, i.e., the first order correlation function $|g^{(1)}(\vec{x}', \vec{x}; t)|$ of such a state is exactly 1 for all space. 3) It is the most ordered state that one can have for a many-boson system. The state in Fig. 1a) is close to this case.

Let’s come now to the case of maximal spread of the coefficients. In this case the maximal many-body entropy is reached and that corresponds to a state for which all coefficients are equal, see Eq. (10) below. The following statements apply to it. 1) The state is maximally disordered. 2) The state is incoherent, i.e., the first order correlation function $|g^{(1)}(\vec{x}', \vec{x}; t)|$ of such a state is close to 0 for all space. 3) The TDGP equation is the farthest from applicability. In other words, the Hilbert space occupied by the wave function is maximally large in this case and thus far bigger than what can be covered by a TDGP product or even multi-orbital mean-field ansatzes [44]. As is easily seen, the number of coefficients and
many-body basis states in our expansion is determined by the number of orbitals used. This
means that the maximal entropy that can be supported in a computation with MCTDHB
is limited by the number $M$ of orbitals chosen. Indeed, $S^{info}(t) \equiv S^{info}(n_1, ..., n_M; t)$ can
be shown to have a maximum where the coefficients are all equal. For this purpose we
define the coefficients as a function $f$ dependent on the occupations $n_1, ..., n_M$ and time $t$.
Consequently, we obtain for $S^{info}(t)$

$$S^{info}(n_1, ..., n_M; t) = \sum \hat{n} [f(n_1, ..., n_M; t) \ln (f(n_1, ..., n_M; t))] , \tag{9}$$

and its derivative,

$$\frac{\partial S^{info}(\vec{n}; t)}{\partial \vec{n}} = \sum \vec{n} \left[ \sum_i \left[ \frac{\partial f(n_1, ..., n_M; t)}{\partial n_i} \ln (f(n_1, ..., n_M; t)) \right] + \sum_i \left[ \frac{\partial f(n_1, ..., n_M; t)}{\partial n_i} \right] \right]. \tag{10}$$

In order for this derivative to vanish, the partial derivative of $f$ with respect to all $n_i, i = 1, ..., M$ has to be identically $0$, i.e., $\frac{\partial f(n_1, ..., n_M; t)}{\partial n_i} = 0, \quad \forall i = 1, ..., M$. This can only
hold for a constant $f$ and this, in turn, corresponds to a uniform distribution of coefficients
{$C_{\vec{n}}(t)$}. It is worthwhile to note here that one could also use the many-body entropy
to judge the accuracy of an MCTDHB computation: When it is close to the maximally
supported entropy, probably the results are no longer exact and one should think about
including more orbitals in the description.

For a given wave function $\Psi(x_1, x_2, ..., x_N, t)$ of $N$ identical spin-less bosons with spatial
coordinates $x_i$, the $p$th order reduced density matrix is defined as \[45\]

$$\rho^{(p)}(x_1, ..., x_p|x'_1, ..., x'_p; t) = \frac{N!}{(N-p)!} \int \Psi(x_1, ..., x_p, x_{p+1}, ..., x_N; t) \times \Psi(x'_1, ..., x'_p, x_{p+1}, ..., x_N; t) \, dx_{p+1}...dx_N \tag{11}$$

The normalized $p$th order correlation function at time $t$ is then defined as

$$g^{(p)}(x'_1, ..., x'_p, x_1, ..., x_p; t) = \frac{\rho^{(p)}(x_1, ..., x_p|x'_1, ..., x'_p; t)}{\sqrt{\prod_{i=1}^{p} \rho^{(1)}(x_i|x_i; t) \rho^{(1)}(x'_i|x'_i; t)}} \tag{12}$$

The normalized $p$th order correlation function $g^{(p)}$ measures the degree of $p$th order coherence. $|g^{(p)}(x_1, ..., x_p, x_1, ..., x_p; t)| > 1$ means the detection probability at the positions $x_1, ..., x_p$
are correlated whereas \( |g^{(p)}(x_1, \ldots x_p, x_1 \ldots x_p; t)| < 1 \) means the detection probabilities at \( x_1, \ldots x_p \) are anti-correlated. As pointed out earlier \( |g^{(1)}(x'_1, x_1; t)| = 1 \) corresponds to maximal fringe visibility of the interference pattern in interference experiments. However switching on the interaction between the particles will modify the observed interference pattern. Thus, our earlier observation of transition from localization to delocalization of the spread of the contributing coefficients for larger interactions, is directly related with the measurement of degree of coherence: For larger interactions with time, the wave function occupies more single particle states than with a smaller interaction. This has two consequences: 1) The coefficients’ spread and entropy grow with the interparticle interaction strength and 2) the coherence is lost since the correlation functions tend to zero for the case that the wave function departs from being captured by a single particle product state. This can for instance be observed experimentally by studying the interference fringes in a ballistic expansion[32].

For one-dimensional systems, the reduced one-body density matrix is calculated as

\[
\rho^{(1)}(x_1|x'_1; t) = N \int \psi^*(x'_1, x_2, \ldots, x_N; t)\psi(x_1, x_2, \ldots, x_N; t) dx_2 dx_3 \ldots dx_N
\]  

(13)

The dynamics of the first order correlation function \( g^{(1)}(x'_1, x_1, t) \) is defined as

\[
|g^{(1)}(x'_1, x_1, t)|^2 = \frac{\rho^{(1)}(x_1|x'_1; t)}{\rho(x_1, t)\rho(x'_1, t)}
\]  

(14)

where \( \rho(x, t) \) is the diagonal part of the one-body density matrix. The normalized first-order correlation function \( |g^{(1)}(x'_1, x_1, t)|^2 \) is a complex function of two spatial variables. In our present calculation in one spatial dimension, \( |g^{(1)}(x'_1, x_1, t)|^2 \) can hence be represented by a two-dimensional plot which measures the degree of first-order coherence. In Fig. 6, we plot the absolute value square of the normalized first order correlation function \( |g^{(1)}(x'_1, x_1; t)|^2 \) of the many-body solution for various times and strong as well as weak interactions. Note, that we restrict the plotted region, avoiding the regions of space where the density is essentially zero. We plot the correlation function only in regions where the density is larger than 1% of the maximal value of the density in the entire space. For small interaction, \( \lambda_0 = 0.5 \), \( |g^{(1)}(x'_1, x_1; t)|^2 \) is very close to one all through the space. Thus, the system is close to first-order coherent. With increasing interactions, as the wave function gradually becomes delocalized in Hilbert space, the coherence is gradually lost and at \( \lambda_0 = 10.0 \), \( |g^{(1)}(x'_1, x'_1; t)|^2 \) is close to zero which shows anti-correlation and the almost complete loss of coherence.
We conclude that the production of entropy goes hand in hand with a stronger loss of coherence. That is, the larger the disorder (measured by the entropy) in a quantum mechanical system actually is, the less it can be described by a product of a single complex valued function. This means that effective single-particle models (such as the TDGP) can generally not adequately describe processes in which the entropy is increasing with time. Further, it hence stands to reason, if thermalization could at all be captured by mean-field methods.

V. CONCLUSION

We studied many-body entropy production, statistical relaxation and coherence of trapped interacting bosons by an essentially exact many-body method (MCTDHB), going beyond commonly applied mean-field approaches like the TDGP theory. The full time-dependent solution of the many-body problem with MCTDHB allowed us to compute various new many-body entropy measures, the number of principal components, inverse participation ratio and relate these quantities to the loss of coherence in the dynamics. For larger interactions these measures unambiguously prove the existence of irregular dynamics and statistical relaxation. All the measures are in mutual agreement.

For larger interparticle interaction strengths, the states’ coefficients delocalize more strongly and we observe a very quick saturation of the many-body entropy production to the GOE value for the size of the Hilbert space considered. This universally shows the statistical relaxation in the system. The states coefficients’ delocalization can be taken as the main aspect of the existence of statistical relaxation which is in turn the key feature of the ETH. By studying the time-dependence of the first order correlation we demonstrate a link between the dynamics of entropy and the dynamics of coherence. Our present calculation nicely exemplifies that large production in many-body entropy relates to a stronger loss of coherence. This may also be taken as another signature of the existence of statistical relaxation and allows to study it from another perspective. However, further investigations are needed to assess the generality of statistical relaxation also for larger Hilbert spaces as well as its relation to chaos and test the ETH.

It is worthwhile to note that for all the employed measures for many-body entropy production, coherent product states such as the ones obtained within TDGP theory, constitute
the cases of minimal entropy. It stands to reason that one hence needs a genuine many-body treatment like MCTDHB to tackle thermalization and test the ETH.

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FIG. 1. Time-evolution of the distribution of the magnitude of the coefficients $\{|C_n(t)|^2\}$ for weak interactions, $\lambda_0 = 0.5$. Panels a)–d) show the magnitude of the coefficients at times $t = 0.2, 0.5, 1.0, 2.0$, respectively, for weak interactions. The index $n$ is computed from the vector $\vec{n}$ using the mapping described in Ref. [28]. With increasing time, more coefficients in the expansion become significant, but the spread is far from the whole available space spanned by the $N_{\text{conf}} = 3003$ configurations. The state stays rather localized throughout the quench dynamics. The coefficients with $n > 70$ are smaller than $10^{-4}$ and not plotted therefore. All quantities are dimensionless.
FIG. 2. Time-evolution of the distribution of the magnitude of the coefficients $\{|C_n(t)|^2\}$ for stronger interactions, $\lambda_0 = 10.0$. Panels a)–d) show the magnitude of the coefficients at times $t = 0.2, 0.5, 1.0, 2.0$, respectively, for stronger interactions. The index $n$ is computed from the vector $\vec{n}$ using the mapping described in Ref. [28]. With increasing time, more coefficients in the expansion become significant; the spread is exploring almost the whole available space spanned by the $N_{\text{conf}} = 3003$ configurations. The state becomes rather delocalized throughout the quench dynamics as compared to the localized case in Fig. 1. All quantities are dimensionless.
FIG. 3. Time-evolution of the number of principal components $N_{pc}(t)$ and the inverse participation ratio $I_{ipr}(t)$ for weak interactions $\lambda_0 = 0.5$. Both $N_{pc}(t)$ (green, upper line) and $I_{ipr}(t)$ (red, lower line) exhibit the same overall behavior. As expected for weak interactions, large fluctuations emerge in both quantities due to the absence of strong correlations for weak interactions. See text for further discussion. All quantities are dimensionless.
FIG. 4. Time-evolution of the number of principal components $N_{pc}(t)$ and the inverse participation ration $I_{ipr}(t)$ for stronger interactions $\lambda_0 = 10.0$. Both $N_{pc}(t)$ (green, upper line) and $I_{ipr}(t)$ (red, lower line) exhibit the same overall behavior. The thin black dashed lines are provided to guide our eyes and to estimate the magnitude of fluctuations. As expected for stronger interactions, the fluctuations are quenched due to the presence of strong correlations for stronger interactions as compared to weak interactions, see Fig. 3. See text for further discussion. All quantities are dimensionless.
FIG. 5. Dynamics of many-body Shannon entropy $S_{\text{info}}(t)$ and $S_{\text{occu}}(t)$ for different interparticle interaction strengths. Statistical relaxation is represented in the convergence of both quantities, $S_{\text{info}}(t)$ (red, upper lines) and $S_{\text{occu}}(t)$ (green, lower lines), to the values $S_{\text{GOE}}(t)$ and $S_{\text{GOE}}(t)$ (horizontal black dashed lines), respectively, as the interaction increases from panel a)–c). Implications are discussed in the text, all quantities shown are dimensionless.
FIG. 6. Long-time-evolution of many-body Shannon entropy $S_{\text{info}}(t)$ for weak $\lambda_0 = 0.5$ and stronger $\lambda_0 = 15.0$ interactions. To verify that the saturation of the many-body entropy measures is indeed non-transient, it’s instructive to look at their time-dependence for longer times – panel a) shows $S_{\text{info}}(t)$ for $\lambda_0 = 0.5$ and panel b) for $\lambda_0 = 15.0$. The behavior for smaller times is presented in the inset. Importantly, the saturation happens on a much faster time-scale in the case of strong interaction $\lambda_0 = 15.0$ as compared to weak interactions $\lambda_0 = 0.5$. See text for details, all quantities shown are dimensionless.
Coherence in the dynamics of many-body entropy measured with the correlation function $|g^{(1)}(x' | x_1; t)|^2$ for weak $\lambda_0 = 0.5$ and strong $\lambda_0 = 10.0$ interactions. The left column depicts $|g^{(1)}|^2$ for $t = 0.1, 5.0, 10.0$ and $\lambda_0 = 0.5$, respectively. The right column shows $|g^{(1)}|^2$ for the same times but $\lambda_0 = 10.0$. Interestingly, the states with localized coefficients’ distributions (compare Fig. 1) are also closer to coherent ($|g^{(1)}|^2 \approx 1$) than the states with spread coefficients’ distributions (compare Fig. 2). In the case of spread-out coefficients, $|g^{(1)}|^2 \approx 0$ holds almost everywhere but for the diagonal $|g^{(1)}(x, x; t)|^2$. Entropy production and loss of coherence go hand in hand. See text for further discussion, all quantities shown are dimensionless.
[1] J. M. Deutsch, Phys. Rev. A 43, 2046 (1991).
[2] M. Srednicki, Phys. Rev. E 50, 888 (1994).
[3] M. Rigol, V. Dunjko, and M. Olshanii, Nature (London) 452, 854 (2008).
[4] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, Rev. Mod. Phys. 83, 863 (2011).
[5] M. Marcuzzi, J. Marino, A. Gambassi, and A. Silva, Phys. Rev. Lett. 111, 197203 (2013).
[6] Q. Zhuang and B. Wu, Phys. Rev. E 88, 062147 (2013).
[7] M. Rigol, Phys. Review Lett. 112, 170601 (2014).
[8] W. Beugeling, R. Moessner, and M. Haque, Phys. Rev. E 89, 042112 (2014).
[9] M. Rigol and L. F. Santos, Phys. Rev. A 82, 011604 (R) (2010).
[10] N. D. Chavda, V. K. B. Kota, and V. Pothbare, Phys. Letts A 376, 2972 (2012).
[11] V. K. B. Kota, A. Relano, J. Retamosa, and M. Vyas, J. Stat. Mech., P10028 (2011).
[12] M. C. Banuls, J. I. Cirac, and M. B. Hastings, Phys. Rev. Lett. 106, 050405 (2011).
[13] M. Rigol, Phys. Rev. Lett. 103, 100403 (2009).
[14] L. F. Santos and M. Rigol, Phys. Rev. E 81, 036206 (2010).
[15] V. V. Flambaum and F. M. Izrailev, Phys. Rev. E 55, R13 (1997); ibid Phys. Rev. E 56, 5144 (1997); F. Borgonovi and F. M. Izrailev, Phys. Rev. E 62, 6475 (2000).
[16] M. Greiner, O. Mandel, T. W. Hänsch, and I. Bloch, Nature (London) 419, 51 (2002).
[17] J. Simon et al., Nature (London) 449, 334 (2007).
[18] S. Trotzky et al. Nature Physics 8, 325 (2012)
[19] L. F. Santos, F. Borgonovi, and F. M. Izrailev, Phys. Rev. E 85, 036209 (2012).
[20] B. V. Chirikov, Open Sys. Information Dyn. 4, 241 (1997).
[21] C. Bartsch and P. Vidal, Eur. Phys. J. Special Topics 151, 29 (2007).
[22] L. F. Santos, F. Borgonovi, and F. M. Izrailev, Phys. Rev. Lett. 108, 094102 (2012).
[23] Th. Zimmermann, H.D. Meyer, H. Köppel, and L. S. Cederbaum Phys. Rev. A 33, 4334 (1986).
[24] Th. Zimmermann, L. S. Cederbaum, H.D. Meyer, and H. Köppel J. Phys. Chem. 91, 4446 (1987).
[25] Th. Zimmermann, H. Köppel, L. S. Cederbaum, G. Persch, and W. Demtröder, Phys. Rev. Lett. 61, 3 (1988).
[26] A. Görlitz et. al., Phys. Rev. Lett. 87, 130402 (2001); F. Schreck et. al. 87, 080403 (2001); M. Greiner et. al. Phys. Rev. Lett. 87, 160405 (2001).

[27] A. U. J. Lode and M. C. Tsatsos, The Recursive Multiconfigurational Time-Dependent Hartree for Bosons package (2014), http://ultracold.org, http://r-mctdhb.org; http://schroedinger.org.

[28] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum Phys. Rev. A 81, 022124 (2010).
[29] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. A 77, 033613 (2008).
[30] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. 100, 130401 (2008).

[31] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).

[32] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A 81, 022124 (2010).

[33] V. K. B. Kota, Embedded Random Matrix Ensembles in Quantum Physics, Lecture Notes in Physics, 884 (Springer, Heidelberg, 2014).

[34] M. Horoi, V. Zelevinsky, and B. A. Brown, Phys. Rev. Lett. 74, 5194 (1995).

[35] T. A. Brody, Rev. Mod. Phys. 53, 385 (1981).

[36] V. K. B. Kota and R. Sahu, Phys. Rev. E 66 037103 (2002).

[37] M. C. Tsatsos, and A. U. J. Lode, arXiv:1410.0414 [cond-mat.quant-gas] (2014); I. Březinová, A. U. J. Lode, A. I. Streltsov, O. E. Alon, L. S. Cederbaum, and J. Burgdörfer, Phys. Rev. A 86, 013630 (2012).

[38] F. Haake, Quantum signature of chaos (Springer, New York, 2010).

[39] M. L. Mehta, Random Matrices (Academic Press, New York, 1991).

[40] R. J. Glauber, Phys. Rev. 130, 2529 (1963).

[41] A. U. J. Lode, K. Sakmann, O. E. Alon, L. S. Cederbaum, and A. I. Streltsov, Phys. Rev. A 86, 063606 (2012); A. U. J. Lode, Tunneling Dynamics in Open Ultracold Bosonic Systems, Springer Theses (Springer, Heidelberg, 2014); K. Sakmann, Many-Body Schrödinger Dynamics of Bose-Einstein Condensates, Springer Theses (Springer, Heidelberg, 2011).

[42] O. Bohigas, M. J. Giannoni, and C. Schmit, Phys. Rev. Lett. 52, 1 (1984).

[43] V. K. B. Kota and R. Sahu, Phys. Rev. E 64, 016219 (2001).

[44] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Lett. A 362, 453 (2007).

[45] K. Sakmann, A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A 78, 023615 (2008).