Dynamics of Pure States and Linear Response for Binary Operators

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We study static and dynamical expectation values for a class of pure states. This class mimics non-equilibrium density matrices via the concept of quantum typicality and allows for a controlled preparation of expectation values close to or far away from their equilibrium values at arbitrary temperatures. While these pure states do not require specific types of observables, we investigate so-called binary operators such as local fermionic occupation numbers or local energy densities in the isotropic Heisenberg spin-1/2 chain. For these two examples, we use numerical forward-propagation methods in real and imaginary time to demonstrate the accuracy of the pure-state approach within and outside the linear-response regime. At high temperatures, our numerical results show that the dynamics in all regimes is generated by a single correlation function. These numerical results are in excellent agreement with our analytical predictions for binary operators.

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Introduction. Statistical physics provides an universal concept for the calculation of equilibrium properties of many-body quantum systems. This surprisingly simple and remarkably successful concept is to properly choose one of the textbook statistical ensembles. Furthermore, various analytical and numerical methods are available to carry out the actual calculation for a specific physical model, see e.g. [1–3]. Out of equilibrium, however, such an universal concept is absent. This absence is not least related to the diversity of non-equilibrium situations. On the one hand, there can be driving by time-dependent protocols [4–6] and by heat baths or particle reservoirs at unequal temperatures or chemical potentials [7–9]. In strictly isolated situations, on the other hand, a variety of initial states can be prepared. These initial states can be mixed or pure, entangled or non-entangled, and close to or far away from equilibrium.

Quantum many-body systems in strict isolation have experienced an upsurge of interest in recent years, also due to the advent of cold atomic gases [10], the discovery of many-body localized phases [11], and the invention of powerful numerical techniques such as density matrix renormalization group [2]. In particular, understanding the existence of equilibration and thermalization has seen substantial progress [12, 13] by as fascinating concepts as eigenstate thermalization [14–16] and typicality of pure states [17–30]. However, much less is known on the route to equilibrium as such [31, 32]. A widely used approach to the full time-dependent relaxation process is linear response theory (LRT) [33]. While this highly developed theory predicts the dynamics of expectation values on the basis of correlation functions, the calculation of these correlation functions can be a challenge in practice, see e.g. [34–38]. In addition to this practical issue, LRT as such has limitations and requires, e.g., that the initial state is (i) mixed and (ii) close to equilibrium.

In this situation, our Letter takes a fresh perspective and studies static and dynamical expectation values for a class of pure states. This class mimics non-equilibrium density matrices via the concept of quantum typicality and allows for a controlled preparation of expectation values close to or far away from their equilibrium values at arbitrary temperatures. While these pure states do not require specific types of observables, we focus on so-called binary operators. For such operators, we unveil that the dynamics in the far-from-equilibrium limit is captured by a correlation function at equilibrium. Remarkably, at high temperatures, we find that this correlation function describes the dynamics in the entire regime down to the close-to-equilibrium limit. To demonstrate the validity of these analytical results and the accuracy of the pure-state approach, we additionally perform numerical simulations for two specific examples of binary operators, i.e., local fermionic occupation numbers [33–42] and local energy densities [42–43] in the one-dimensional XXZ spin-1/2 model at the isotropic point. Our numerical simulations confirm that the high-temperature dynamics is indeed generated by a single correlation function in the entire regime between the limiting cases close to and far away from equilibrium.

Review of Linear Response. We start by considering a quantum system described by a Hamiltonian $\mathcal{H}$ which is in contact with a (weakly coupled and macroscopically large) heat bath at temperature $T = 1/\beta$. Furthermore, this quantum system is affected by a static force which gives rise to an additional potential energy described by an operator $\mathcal{O}_l$ [44–51]. (Later there will be also other operators $\mathcal{O}(\nu)$.) For such a situation, thermalization to the density matrix

$$\rho_{\text{neq}} = e^{-\beta(\mathcal{H} - \varepsilon \mathcal{O}_l)}/Z_{\text{neq}}$$

emerges, where $Z_{\text{neq}} = \text{Tr}(e^{-\beta(\mathcal{H} - \varepsilon \mathcal{O}_l)})$ is the partition function and the parameter $\varepsilon$ denotes the strength of the static force. Eventually, this force and the heat bath are both removed, i.e., there is a sudden quench. Then, $\rho_{\text{neq}}$ in Eq. (1) is no equilibrium state of the remaining...
Hamiltonian $\mathcal{H}$ such that it evolves in time according to the Schrödinger equation for this Hamiltonian.

If $\varepsilon$ is a small parameter, the exponential in Eq. (1) can be expanded according to

$$
\rho_{\text{neq}} = \rho_{\text{eq}} \left( 1 + \varepsilon \int_0^\beta \mathrm{d} \beta' \ e^{\beta' \mathcal{H}} \Delta \mathcal{O}_l \ e^{-\beta' \mathcal{H}} + \varepsilon^2 \ldots \right),
$$

where $\mathcal{O}_l = \mathcal{O}_l - \langle \mathcal{O}_l \rangle_{\text{eq}}$ and $\langle \mathcal{O}_l \rangle_{\text{eq}} = \text{Tr} \{ \rho_{\text{eq}} \mathcal{O}_l \}$ denotes the equilibrium expectation value with $\rho_{\text{eq}} = e^{-\beta \mathcal{H}} / Z_{\text{eq}}$ and $Z_{\text{eq}} = \text{Tr} \{ e^{-\beta \mathcal{H}} \}$. Hence, for small values of $\varepsilon$, the static expectation value $\langle \mathcal{O}_l \rangle_{\text{neq}} = \text{Tr} \{ \rho_{\text{neq}} \mathcal{O}_l \}$ of some operator $\mathcal{O}_l$ can be written as

$$
\langle \mathcal{O}_l \rangle_{\text{neq}} = \langle \mathcal{O}_l \rangle_{\text{eq}} + \varepsilon \chi_{l,l'},
$$

where the isothermal susceptibility may be written as a Kubo scalar product $\chi_{l,l'} = \beta (\Delta \mathcal{O}_l, \mathcal{O}_l')$. Note that the expansion in Eq. (2) is known to converge because all expressions are analytical and the operators involved have bounded spectra. In particular, in the limit $\varepsilon \rightarrow 0$, one naturally finds $\rho_{\text{neq}} \rightarrow \rho_{\text{eq}}$. Equation (3) reflects the central statement of LRT, i.e., for small values of $\varepsilon$ the response is linear in $\varepsilon$. However, when $\varepsilon$ is increased to large values, higher-order terms are expected to become non-negligible.

In fact, in the limit $\varepsilon \rightarrow \infty$, the density matrix $\rho_{\text{neq}}$ in Eq. (1) acts as a projector on the eigenstates of $\mathcal{O}_l$ with the largest eigenvalue $\mathcal{O}_{l,\text{max}}$. Thus, the expectation value $\langle \mathcal{O}_l \rangle_{\text{neq}}$ reads

$$
\lim_{\varepsilon \rightarrow \infty} \langle \mathcal{O}_l \rangle_{\text{neq}} = \mathcal{O}_{l,\text{max}}.
$$

In particular, comparing Eqs. (3) and (4) suggests that LRT has to break down for a perturbation of strength $\varepsilon \mathcal{O} = (\mathcal{O}_{l,\text{max}} - \langle \mathcal{O}_l \rangle_{\text{eq}}) / \chi_{l,l'}$.

**Classes of Initial States.** In this Letter, we discuss two different classes of pure initial states. With the first class, we intend to mimic the non-equilibrium density matrix in Eq. (1). To this end, we exploit the concept of quantum typicality (QT) [1, 2]. This concept states that a single pure state can have the same properties as the ensemble density matrix. Precisely, the main idea is to replace the trace $\text{Tr} \{ \rho_{\text{neq}} \mathcal{O}_l \}$ by the scalar product $\langle \phi | \rho_{\text{neq}} \mathcal{O}_l | \phi \rangle$, where the pure state $| \phi \rangle$ is drawn at random according to the unitary invariant Haar measure [21, 22]. By the use of this replacement, the expectation value $\langle \mathcal{O}_l \rangle_{\text{neq}}$ can be written as

$$
\langle \mathcal{O}_l \rangle_{\text{neq}} = \langle \psi_{\text{neq}} | \mathcal{O}_l | \psi_{\text{neq}} \rangle + f(|\phi\rangle) \quad (5)
$$

with the non-equilibrium pure state

$$
| \psi_{\text{neq}} \rangle = (\rho_{\text{neq}})^{1/2} | \phi \rangle / (|\langle \phi | \phi \rangle|^{1/2}.
$$

The statistical error in Eq. (5) scales as $f(|\phi\rangle) \propto 1/d_{\text{eff}}^{1/2}$, where $d_{\text{eff}} = Z_{\text{neq}}/e^{-\beta E_{\text{neq}}}$ is the effective dimension of the Hilbert space and $E_{\text{neq}}$ denotes the energy of the ground state. Thus, as the size of a many-body quantum system is increased, $f(|\phi\rangle)$ vanishes exponentially fast and can be neglected for medium system sizes already [37–40]. Hence, Eq. (5) for small $\varepsilon$ also hold for the pure state $|\psi_{\text{neq}}\rangle$.

Next, let us introduce the second class of pure initial states. As before, the intention of this class is to mimic a non-equilibrium density matrix. It reads

$$
\rho_{\text{P}} = \mathcal{P} / \text{Tr} \{ \mathcal{P} \}, \quad \mathcal{P} = \mathcal{O}_l - \mathcal{O}_{l,\text{min}},
$$

where $\mathcal{O}_{l,\text{min}}$ denotes the smallest eigenvalue of $\mathcal{O}_l$. By construction, the operator $\mathcal{P}$ is Hermitian and only has non-negative eigenvalues. For such $\mathcal{P}$, we can write [50]

$$
\langle \mathcal{O}_l \rangle_{\mathcal{P}} = \langle \psi_{\mathcal{P}} | \mathcal{O}_l | \psi_{\mathcal{P}} \rangle + g(|\phi\rangle) \quad (8)
$$

with the non-equilibrium pure state

$$
| \psi_{\mathcal{P}} \rangle = (\rho_{\mathcal{P}})^{1/2} | \phi \rangle / (|\langle \phi | \phi \rangle|^{1/2}.
$$

Once again, the statistical error $g(|\phi\rangle)$ can be considered negligibly small.

**Dynamics.** Up to this point, we have only considered static expectation values. However, the QT relations in Eq. (5) and Eq. (8) hold for finite times $t > 0$ also, i.e.,

$$
\langle \mathcal{O}_l \rangle_{\text{neq,P}} \rightarrow \langle \mathcal{O}_l(t) \rangle_{\text{neq,P}} \quad \text{and} \quad |\psi_{\text{neq,P}}\rangle \rightarrow |\psi_{\text{neq,P}(t)}\rangle
$$

in these relations. In other words, dynamical expectation values of density matrices and pure states are the same as well [50].

Now, we continue with discussing the dynamics of the second class in detail. After a short calculation, we find the equation [40, 50]

$$
\langle \psi_{\mathcal{P}(t)} | \mathcal{O}_l | \psi_{\mathcal{P}(t)} \rangle = C_{l,l'}^0(t) \quad (10)
$$

with $C_{l,l'}^0(t) = \lim_{\beta \rightarrow 0} C_{l,l'}(t)$ and

$$
C_{l,l'}(t) = \frac{c_1 + c_2 (\langle \mathcal{O}_l \mathcal{O}_l'(t) \rangle_{\text{eq}} - \langle \mathcal{O}_{l,\text{min}} \mathcal{O}_l'(t) \rangle_{\text{eq}})}{c_3 + c_2 (\langle \mathcal{O}_l \rangle_{\text{eq}} - \langle \mathcal{O}_{l,\text{min}} \rangle_{\text{eq}})}.
$$

where $c_1 = c_3 = 0$ and $c_2 = 1$ (for the moment). This equation plays a central role in the Letter at hand. It connects the expectation value of a non-equilibrium pure state to an equilibrium correlation function, evaluated in the high-temperature limit $\beta \rightarrow 0$. This connection is also remarkable since it requires (i) no small parameter and (ii) no specific operators.

It is further instructive to establish a relation between the time evolution of $|\psi_{\text{neq}}\rangle$ and $|\psi_{\mathcal{P}}\rangle$. In fact, we are able to derive such a relation if we restrict ourselves to binary operators $\mathcal{P}$, where all eigenvalues are either 0 or 1. Then, $\mathcal{P}^2 = \mathcal{P}$ and $\mathcal{P}$ describes a projection. Binary operators are, e.g., local fermionic occupation numbers [39, 40] and local energy densities [42, 43] in the isotropic Heisenberg spin-1/2 chain. (These two examples will be considered in our numerical simulations.)
As discussed in the context of Eq. (4), \( \rho_{\text{neq}} \) in Eq. (1) also acts as a projector in the limit \( \varepsilon \to \infty \). Hence, we find \( \lim_{\varepsilon \to \infty} \rho_{\text{neq}} = \rho_{\text{eq}} \propto \mathcal{P} e^{-\beta H} \mathcal{P} \) and

\[
\lim_{\varepsilon \to \infty} \langle \psi_{\text{neq}}(t) | O_{l'} | \psi_{\text{neq}}(t) \rangle = \hat{C}_{l,l'}(t) \tag{12}
\]

for finite temperatures \( \beta \), where the correlation function \( \hat{C}_{l,l'}(t) \) is defined analogously to \( C_{l,l'}(t) \) in Eq. (11) with \( c_1 = c_3 = 0 \) and \( c_2 = 1 \) (again), but here the ensemble averages are performed w.r.t. the density matrix \( \rho_{\text{eq}} \). In certain cases, \( \hat{C}_{l,l'}(t) = \text{Re} C_{l,l'}(t) \).

An intriguing picture occurs in the high-temperature limit \( \beta \to 0 \). Here, we can write \( \rho_{\text{neq}} \propto e^{\beta \varepsilon O_1} \). A Taylor expansion of this exponential and the property \( \mathcal{P}^i = \mathcal{P} \) then yield \( \rho_{\text{neq}} \propto 1 + (e^{\beta \varepsilon} - 1) \mathcal{P} \). As a consequence, the time-dependent expectation value \( \langle \psi_{\text{neq}}(t) | O_{l'} | \psi_{\text{neq}}(t) \rangle \) for any \( \varepsilon \) is given by \( C_{l,l'}(t) \) and

\[
c_1 = \langle O_{l'} \rangle_{\text{eq}}, \quad c_2 = e^{\beta \varepsilon} - 1, \quad c_3 = 1. \tag{13}
\]

Therefore, at high temperatures, the dynamics for all \( \varepsilon \) is generated by the correlation function \( \langle O_l O_{l'}(t) \rangle_{\text{eq}} \). (This prediction will be confirmed numerically.) In particular, for small \( \varepsilon \), \( C_{l,l'}(t) \) can be linearized and then becomes \( C_{l,l'}(t) = \langle O_{l'} \rangle_{\text{eq}} + \varepsilon \chi_{l,l'}(t) \) with the usual dynamical susceptibility \( \chi_{l,l'}(t) = \beta \langle [O_{l'} O_l](t) \rangle_{\text{eq}} - \langle O_{l'} \rangle_{\text{eq}} \langle O_l \rangle_{\text{eq}} \), as expected from LRT. It is worth pointing out that such a dynamical independence of \( \varepsilon \) can hardly be expected at low temperatures. There, \( \chi_{l,l'}(t) \) is not just given by \( \langle O_l O_{l'}(t) \rangle_{\text{eq}} \).

**Pure-State Propagation.** Time-dependent expectation values of the form \( \langle O_l(t) \rangle_{\text{neq}} = \text{Tr} \{ \rho_{\text{neq}}(t) O_l \} \) can be calculated exactly, if the eigenstates and eigenvalues of the Hamiltonians \( \mathcal{H} - \varepsilon O_l \) and \( \mathcal{H} \) are obtained from the exact diagonalization of finite systems. But, in addition to the main limitation set by the exponential growth of many-body Hilbert spaces, this procedure is also costly since it requires to perform the exact diagonalization of two operators. Therefore, we proceed differently and rely on the QT relation in Eq. (5). Then, we do not need to deal with density matrices and can consider pure states instead. While a forward propagation w.r.t. \( \mathcal{H} - \varepsilon O_l \) in imaginary time \( \beta \) allows us to prepare \( | \psi_{\text{neq}}(0) \rangle \), another forward propagation w.r.t. \( \mathcal{H} \) in real time \( t \) allows us to calculate \( | \psi_{\text{neq}}(t) \rangle \). These propagations can be done by iteratively solving the Schrödinger equation (in real and imaginary time) by a fourth-order Runge-Kutta scheme with a small time step \( \delta t \). This scheme does not require exact diagonalization and, due to the fact that few-body operators are relatively sparse, also the matrix-vector multiplications can be implemented in a very memory-efficient way. Hence, in comparison to exact diagonalization, we can treat systems with much larger Hilbert spaces. Note that also more sophisticated schemes can be applied such as Trotter decompositions or Chebyshev polynomials. However, for the purposes of this Letter, Runge-Kutta will be sufficient.

**Application to Models.** Next, we turn to our numerical simulations and study, as an example, non-equilibrium dynamics in the XXZ spin-1/2 chain. The Hamiltonian of this chain reads (with periodic boundary conditions)

\[
\mathcal{H} = \sum_{l=1}^{L} h_l, \tag{14}
\]

where \( S_{l,x,y,z} \) are spin-1/2 operators at site \( l \), \( L \) is the number of sites, \( J = 1 \) is the antiferromagnetic exchange coupling constant, and \( \Delta \) is the anisotropy. By the use of the Jordan-Wigner transformation, this Hamiltonian can be also mapped onto a one-dimensional model of spinless fermions with interactions between nearest neighbors. In this picture, the operator \( n_l = S_{l,z}^+ + 1/2 \) becomes a local fermionic occupation number. Because such an operator has only the two eigenvalues 0 and 1, the choice \( O_l = n_l \) implies \( \mathcal{P} = n_l \) as well. We prepare the initial states using this choice and then measure \( O_l = n_{l'} \), with \( l = l' \) or \( l \neq l' \). Note that the reference state \( | \phi \rangle \), occurring in Eqs. (16) and (19), is realized as \( | \phi \rangle = \sum_{\mathbf{k}} c_{\mathbf{k}} | \varphi_{\mathbf{k}} \rangle \), where \( | \varphi_{\mathbf{k}} \rangle \) is the Ising basis and the real and imaginary part of the complex coefficients \( c_{\mathbf{k}} \) are drawn at random according to a Gaussian distribution with zero mean.
prediction in Eq. (3). In Fig. (a) we show $\langle n_{l'=l}(t)\rangle_{\text{neq}}$ for a wide range $\varepsilon \leq 500$, high temperatures $\beta = 0.01$, 0.02, 0.05, and 0.1, as well as anisotropy $\Delta = 1$. At $\varepsilon = 0$, we have $\langle n_{l'=l}\rangle_{\text{neq}} = \langle n_{l'=l}\rangle_{\text{eq}} = 1/2$. As $\varepsilon$ increases, we observe a linear growth of $\langle n_{l'=l}\rangle_{\text{neq}}$ with $\varepsilon$. As depicted in Fig. (b), this linear growth is very well described by the LRT prediction in Eq. (3) and $\chi_{l,l'=l} = \beta/4$. For large $\varepsilon$, $\langle n_{l'=l}\rangle_{\text{neq}}$ eventually saturates at the constant value $\langle n_{l'=l}\rangle_{\text{eq}} = 1$. This saturation is expected due to Eq. (4) and the maximum eigenvalue $n_{l,\text{max}} = 1$. Lower temperatures $\beta = 1$ and 2 are calculated in Fig. (c) as well. While the linear regime decreases as $\beta$ increases, the saturation value is unaffected. In Fig. (d) we also depict $\langle n_{l\neq l'}\rangle_{\text{neq}}$ with different sites $l' \neq l$. In this case, $\langle n_{l\neq l'}\rangle_{\text{neq}} \approx \langle n_{l\neq l'}\rangle_{\text{eq}} = 1/2$ holds for all $\varepsilon$ and $\beta$ shown here, as expected from Eq. (3) and $\chi_{l,l'\neq l} \approx 0$. In the Figs. (a)-(d), the QT relation in Eq. (3) is additionally confirmed by a direct comparison with data from exact diagonalization. Even though statistical errors increase as $\beta$ increases, these errors are still negligible for all $\beta$ considered. [Note the narrow scale of the vertical axis in Fig. (d)]. Overall, the numerical results in Figs. (a)-(d) confirm our analytical predictions. In particular, static LRT breaks down for sufficiently large $\varepsilon$.

Next, we turn to dynamical expectation values, with the focus on a high temperature $\beta = 0.01$ [50]. In Fig. (a) we depict $\langle n_{l'=l}(t)\rangle_{\text{neq}}$ for perturbations $\varepsilon = 100$, 200, and 300, as resulting from the QT relation [50]. Further, we depict $\langle n_{l'=l}(t)\rangle_{\text{P}}$, as resulting from the QT relation [50]. While we observe that all curves shown differ from each other, this observation is not surprising because, as illustrated in Fig. (1) the initial values $\langle n_{l'=l}\rangle_{\text{neq}}$ depend on $\varepsilon$. In view of this fact, we try a data collapse using the simple map [50]

$$M(\langle n_{l'=l}(t)\rangle_{\text{neq}}) = a \langle n_{l'=l}(t)\rangle_{\text{neq}} + b$$  \hspace{1cm} (15)

with time-independent coefficients $a$ and $b$. Due to our discussion in the context of Eqs. (3) and (14), this linear map is reasonable for small and large $\varepsilon$. And indeed, as shown in Fig. (b), the rescaled curves lie on top of each other for all values of $\varepsilon$. This finding is a main result of our Letter and clearly confirms our analytical prediction in Eq. (13) that the dynamical behavior at high temperatures is generated by a single equilibrium correlation function, at least for binary operators.

The local fermionic occupation numbers $n_l$ considered so far appear in various physical models, not just in the Heisenberg model or in one dimension. To demonstrate, however, that our results are not restricted to such $n_l$, we extend our analysis to other operators and consider the local energy density $h_l$ in Eq. (14). This local energy density is a spin dimer. For anisotropy $\Delta = 1$, this dimer features a triplet state ($|↑↑\rangle$ with energy $E_t = 1/4$ and a singlet ground state ($|\downarrow\downarrow\rangle$) with energy $E_s = -3/4$. Hence, the choice $\Omega_l = h_l$ leads to the projector $\mathcal{P} = h_l + 3/4$. We redo the calculation in Figs. (a) and (b) for this choice and summarize the corresponding results in Figs. (c) and (d). As before, the time-dependent expectation values $\langle h_{l'=l}(t)\rangle_{\text{neq}}$ for different perturbations $\varepsilon$ lie on top of each other after a simple rescaling of the form given in Eq. (15). Therefore, our results are clearly valid for a larger class of binary operators.

**Conclusion.** To summarize, we have studied static and dynamical expectation values for a class of pure states, which imitates non-equilibrium density matrices via the concept of quantum typicality and allows for a controlled preparation of expectation values close to and far away from their equilibrium values at finite temperatures. We have particularly discussed binary operators and specific examples for such operators. For these examples, we have numerically demonstrated the accuracy of the pure-state approach for weak and strong perturbations. As a main result, our numerical results at high temperatures have unveiled that the time evolution for any perturbation strength is given by a single correlation function. These numerical results have been in excellent agreement with analytical predictions for binary operators.

Promising future directions of research include the analysis of non-binary operators and low temperatures as well as the application of the pure-state approach to specific questions in many-body quantum systems.
SUPPLEMENTAL MATERIAL

Typicality Relations

Here, we provide details on the calculation leading to Eq. (11) in the main text. To this end, we start with the r.h.s. of this equation, i.e.,

\[ C_{l,l'}^0(t) = \frac{\langle O_l|O_l(t)|\rho_{\text{eq}} - O_{l,\text{min}}\langle O_l|\rho_{\text{eq}}}{\langle O_l|O_l(t) - O_{l,\text{min}}\rangle} \]  

(S1)

Since \( \langle \cdot \rangle_{\rho_{\text{eq}}} \propto \text{Tr}\{\cdot\} \), \( \text{Tr}\{O_l(t)\} \), and \( O_{l,\text{min}} \) is a scalar, this expression can be written as

\[ C_{l,l'}^0(t) = \frac{\text{Tr}\{O_l|O_l(t) - O_{l,\text{min}}\langle O_l|\rho\}{\text{Tr}\{O_l - O_{l,\text{min}}\}} \]  

(S2)

or, more compact, as

\[ C_{l,l'}^0(t) = \frac{\text{Tr}\{(O_l - O_{l,\text{min}})O_l(t)\}}{\text{Tr}\{O_l - O_{l,\text{min}}\}} \]  

(S3)

According to the definition of \( P \) and \( \rho_P \) in Eq. (5), we can rewrite this expression as

\[ C_{l,l'}^0(t) = \frac{\text{Tr}\{P|O_l(t)\}}{\text{Tr}\{P\}} = \text{Tr}\{\rho_P|O_l(t)\} \]  

(S4)

which is the dynamical expectation value \( \langle O_l(t)\rangle_P \). By the use of \( \rho_P = (\rho_P)^{1/2}(\rho_P)^{1/2} \) and a cyclic permutation in the trace, we get

\[ C_{l,l'}^0(t) = \text{Tr}\{(\rho_P)^{1/2}O_l(t)(\rho_P)^{1/2}\} \]  

(S5)

Now, by replacing the trace by a scalar product with a single pure state \( \langle \phi \rangle \) drawn at random (according to the unitary invariant Haar measure), we find

\[ C_{l,l'}^0(t) = \frac{\langle \phi |(\rho_P)^{1/2}O_l(t)(\rho_P)^{1/2}\rangle |\phi \rangle}{\langle \phi |\phi \rangle} + g(|\phi \rangle) \]  

(S6)

where the statistical error \( g(|\phi \rangle) \) is negligibly small and will be skipped for clarity. Since \( (\rho_P)^{1/2} \) is a Hermitian operator, this expression is identical to

\[ C_{l,l'}^0(t) = \frac{(\rho_P)^{1/2}O_l(t)(\rho_P)^{1/2}\langle \phi |\phi \rangle}{\langle \phi |\phi \rangle} \]  

(S7)

Therefore, using the definition of \( |\psi_P \rangle \) in Eq. (9), we can also write

\[ C_{l,l'}^0(t) = \langle \psi_P|O_l(t)|\psi_P \rangle = \langle \psi_P(t)|O_l|\psi_P(t) \rangle \]  

(S8)

Comparing Eqs. (S4) and (S8) finally yields Eq. (10) in the main text.

In the above steps from Eqs. (S4) to (S8) we have also shown the relation

\[ \langle O_l(t)\rangle_P = \langle \psi_P(t)|O_l|\psi_P(t) \rangle \]  

(S9)

i.e., the time-dependent version of Eq. 3 in the main part of this Letter. Replacing \( \rho_P \) by \( \rho_{\text{neq}} \) and repeating these steps further leads to the relation

\[ \langle O_l(t)\rangle_{\text{neq}} = \langle \psi_{\text{neq}}(t)|O_l|\psi_{\text{neq}}(t) \rangle \]  

(S10)

i.e., the time-dependent version of Eq. 3 in the main text.

Action of Operators

To evaluate the typicality relations in practice, we need to know the action of the operators \( (\rho_{\text{neq}})^{1/2} \) and \( (\rho_P)^{1/2} \) on the pure state \( |\phi \rangle \). Since

\[ (\rho_{\text{neq}})^{1/2} \propto e^{-\beta(H - C_O)/2} \]  

(S11)

is still an exponential, we can perform the action of this operator by iteratively solving the Schrödinger equation in imaginary time \( \beta \). For

\[ (\rho_P)^{1/2} \propto P^{1/2} \]  

(S12)

the situation can become more complicated. If we deal with binary operators such as the two cases \( P = n_1 \) and \( P = h + 3/4 \) considered in the main text, the projection property \( P^{1/2} = P \) does not lead to an additional layer of complexity. However, for other non-binary operators, we need to know the eigenvalues and eigenvectors of these operators to perform the action of the square root. Of course, this information requires exact diagonalization, which we want to avoid due to the restriction to small matrix dimensions. Note that for local operators acting only on a small part of the whole many-body quantum system, exact diagonalization might still be feasible.

In a certain sense, it is possible to circumvent exact diagonalization for such cases as well. To this end, we repeat the steps from Eqs. (S4) to (S8) but do not use the decomposition \( \rho_P = (\rho_P)^{1/2}(\rho_P)^{1/2} \). Doing so, we get the expression

\[ C_{l,l'}^0(t) = \frac{\langle \phi |O_l(t)|\rho_P \phi \rangle}{\langle \phi |\phi \rangle} \]  

(S13)

Introducing the definition \( |\phi_P \rangle = \rho_P |\phi \rangle \), this expression can be rewritten as

\[ C_{l,l'}^0(t) = \frac{\langle \psi_P(t)|O_l|\phi_P(t) \rangle}{\langle \phi_P |\phi_P \rangle} \]  

(S14)

Thus, the action of square-root type can be avoided by the use of two pure states \( |\phi \rangle \) and \( |\phi_P \rangle \). This approach can be easily generalized to obtain correlation functions at arbitrary \( \beta \) and does not involve a small parameter \( \varepsilon \), see Refs. [37, 38] for details.
Now, particle-hole symmetry of the Hamiltonian leads to the relation
\[
\langle n_l n'_l(t) \rangle_{\text{eq}} = \langle [1 - n_l][1 - n'_l(t)][1 - n_l] \rangle_{\text{eq}} .
\] (S17)

Multiplying out the brackets on the r.h.s. of this relation, using \( \langle n'_l(t) \rangle_{\text{eq}} = \langle n'_l \rangle_{\text{eq}}, \langle n_l \rangle_{\text{eq}} = \langle n_l \rangle_{\text{eq}} = 1/2 \) as well as \( (n_l)^2 = n_l \), and rearranging a bit yields
\[
2\langle n_l n'_l(t) \rangle_{\text{eq}} = \langle n_l n'_l(t) \rangle_{\text{eq}} + \langle n'_l(t) n_l \rangle_{\text{eq}}
\] (S18)
and, since \( \langle n_l(t) \rangle_{\text{eq}} = \langle n_l(n_l(t)) \rangle_{\text{eq}} \),
\[
\langle n_l n'_l(t) \rangle_{\text{eq}} = \text{Re} \langle n_l n'_l(t) \rangle_{\text{eq}} .
\] (S19)

Thus, as a consequence of this identity, we can rewrite the correlation function \( \tilde{C}_{l,l'}(t) \) in Eq. (S16) as
\[
\tilde{C}_{l,l'}(t) = \text{Re} \left( \frac{\langle n_l n'_l(t) \rangle_{\text{eq}}}{\langle n_l \rangle_{\text{eq}}} \right) .
\] (S20)

Comparing this equation to Eq. (11) in the main part of our Letter and taking into account \( n_{l,\min} = 0 \), we find \( \tilde{C}_{l,l'}(t) = \text{Re} C_{l,l'}(t) \).

Linear Map

The time-independent coefficients of the linear map in Eq. (15) follow from two conditions. The first condition is about the initial value, i.e.,
\[
a \langle n_{l=1}(t = 0) \rangle_{\text{eq}} + b = c_0 .
\] (S21)

The second condition is about the long-time value, i.e.,
\[
a \langle n_{l=1}(t \to \infty) \rangle_{\text{eq}} + b = c_\infty .
\] (S22)

We choose \( c_0 = n_{l,max} \) and \( c_\infty = \langle n_{l=1} \rangle_{\text{eq}} \) and get the parameters
\[
a = \frac{n_{l,max} - \langle n_{l=1} \rangle_{\text{eq}}}{\langle n_{l=1} \rangle_{\text{eq}} - \langle n_{l=1} \rangle_{\text{eq}}} \quad \text{and} \quad b = (1 - a)\langle n_{l=1} \rangle_{\text{eq}} .
\] Other choices are also possible, of course.

Other Exchange Anisotropies

In our Letter, we have focused on the spin-1/2 XXZ chain for the isotropic case \( \Delta = 1 \). Here, we additionally present results for anisotropic cases, e.g., \( \Delta = 1.5 \). For this anisotropy \( \Delta \neq 1 \), \( P = n_l \) does not change and still is a binary operator. Thus, the analytical prediction for large \( \varepsilon \) in Eq. (12) remains valid and also the numerical simulations can be performed in exactly the same way as done before. However, \( P = h_l - h_{l,\min} \) changes and, in particular, becomes a non-binary operator with more

Lower Temperatures

In the main part of this Letter, we have calculated the time-dependent expectation values \( \langle n_{l=1}(t) \rangle_{\text{eq}} \) and \( \langle h_{l=1}(t) \rangle_{\text{eq}} \) for a high temperature \( \beta = 0.01 \). For this temperature, we have demonstrated that the curves for different perturbation strengths \( \varepsilon \) lie on top of each other after the simple linear map in Eq. (15). Clearly, such a dynamical independence of \( \varepsilon \) can hardly be expected at low temperatures. However, it may occur over a wider range of high temperatures \( \beta > 0.01 \). Thus, we redo the calculation for \( \langle n_{l=1}(t) \rangle_{\text{eq}} \) in Figs. 2 (a) and (b) for the lower temperature \( \beta = 1 \) and depict the corresponding results in Figs. S1 (a) and (b). For comparison, we also show the correlation function \( \text{Re} \langle n_l n_{l'}(t) \rangle_{\text{eq}} \), which is obtained from the previously mentioned approach based on two pure states. While the data collapse is certainly not as good as before, it is still convincing.

Particle-Hole Symmetry

As stated in the main text, the correlation functions \( \tilde{C}_{l,l'}(t) \) and \( C_{l,l'}(t) \) are, in certain cases, related to each other by \( \tilde{C}_{l,l'}(t) = \text{Re} (C_{l,l'}(t)) \). Such a case are the local fermionic occupation numbers \( n_l \) in the XXZ spin-1/2 chain. Here, the density matrix \( \rho_{\text{eq}} \propto P e^{-\beta H} P \) is given by
\[
\tilde{\rho}_{\text{eq}} = \frac{n_l e^{-\beta H} n_l}{\text{Tr}(n_l e^{-\beta H} n_l)}
\] (S15)
and, using \( (n_l)^2 = n_l \) in the denominator, we can write the correlation function \( \tilde{C}_{l,l'}(t) = \text{Tr}(\tilde{\rho}_{\text{eq}} n_{l'}(t)) \) as
\[
\tilde{C}_{l,l'}(t) = \frac{\langle n_l n_{l'}(t) n_l \rangle_{\text{eq}}}{\langle n_l \rangle_{\text{eq}}} .
\] (S16)
than two eigenvalues. The fact that $P$ is not a projector any further has two important consequences. First, this fact implies $\lim_{\varepsilon \to \infty} \rho_{\text{neq}} \neq P$ such that Eq. (12) does not need to hold. In other words, there is no immediate relation between the dynamics of $|\psi_{\text{neq}}\rangle$ for large $\varepsilon$ and the dynamics of $|\psi_P\rangle$. Therefore, we know only that the latter dynamics is generated by the correlation function in Eq. (11). Second, in order to construct $|\psi_P\rangle$, we have to apply $P^{1/2}$ to the pure state $|\phi\rangle$ in Eq. (4). Clearly, this square-root operation we can only carry out in the diagonal matrix representation of $P$. Hence, the exact diagonalization of $P$ is required. Since $P = h_l - h_{l_{\text{min}}}$ is a local operator acting on two neighboring sites only, this procedure is possible also for large systems.

In Fig. S2 we redo the calculation in Fig. 2 in the main part of this Letter for the anisotropy $\Delta = 1.5$ while the other parameters are unchanged. Once again, the curves for the time-dependent expectation values $\langle n(t)\rangle_{\text{neq}}$ in Fig. S2(a) and $\langle h(t)\rangle_{\text{neq}}$ in Fig. S2(c) depend both on the perturbation strength $\varepsilon$ but lie on top of each other after the simple linear map in Eq. (14) used before, see Figs. S2(b) and (d). This finding is remarkable especially in the case of the local energy density. It unveils that also the dynamical behavior of non-binary observables can be generated by a single correlation function, at least in the limit of high temperatures.

Error Analysis

Eventually, let us further comment on the accuracy of our pure-state approach, i.e., of the typicality relations in Eqs. (4) and (5) of the main text. While the comparison with exact diagonalization in Fig. 1 has illustrated this accuracy already for static expectation values, there is another convenient way to demonstrate the smallness of statistical errors. This way is the comparison of results for two or even more instances of the reference state $|\phi\rangle$ in Eqs. (4) and (5). Recall that a single instance of this pure state is $|\phi\rangle = \sum_k c_k |\varphi_k\rangle$, where the real and imaginary part of the complex coefficients $c_k$ are drawn at random according to a Gaussian distribution with zero mean and $|\varphi_k\rangle$ is the Ising basis.

In Fig. S3(a) we exemplarily compare the dynamical expectation values $\langle n(t)\rangle_{\text{neq}}$ for two different random realizations $|\phi_1\rangle$ and $|\phi_2\rangle$. For both realizations, we use the same perturbation $\varepsilon = 300$, temperature $\beta = 0.01$, and system size $L = 16$. Since the two curves coincide almost perfectly, we can conclude that statistical errors are indeed very small, even for chains with only $L = 16$ sites. Because these errors decrease exponentially fast as the number of sites increases, our calculations for larger system sizes $L = 28$ in the main text can be considered as practically exact.

Finally, we compare in Fig. S3(b) the time evolution of the expectation value $\langle n(t)\rangle_{\text{neq}}$ for the same set of parameters but two different Runge-Kutta time steps $\delta t = 0.01$ and $0.1$. As the curves do not differ for these
two choices, the time step \( \delta t = 0.01 \) chosen throughout our Letter is certainly small enough to ensure negligibly small numerical errors.

**Finite-Size Effects**

While it is evident from Fig. 1 that finite-size effects are negligibly small for static expectation values, let us also comment briefly on finite-size effects for dynamical expectation values. To this end, we compare in Fig. S4 numerical data for two different system sizes \( L = 24 \) and \( L = 28 \). Apparently, for \( \langle n_{\tau=\ell}(t) \rangle_\rho \) in Fig. S4 (a), both curves coincide with each other, at least for all times \( t \leq 20 \) depicted. (Data from exact diagonalization can be found for small \( L = 16 < 28 \) in \[39\].) For \( \langle h_{\tau=\ell}(t) \rangle_\rho \) in Fig. S4 (b), one can see minor deviations at times \( t \sim 20 \).

However, we should stress that such finite-size effects do not affect the conclusions in the main text. In fact, all relations discussed do not require the convergence to the thermodynamic limit.

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