

Temperature and conditions for thermalization after canonical quenches

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(Received 25 June 2025; revised 18 September 2025; accepted 27 October 2025; published 12 November 2025)

We consider quenches of a quantum system that is prepared in a canonical equilibrium state of one Hamiltonian and then evolves unitarily in time under a different Hamiltonian. Technically, our main result is a systematic expansion of the pre- and postquench canonical ensembles in the quench strength. We first demonstrate how this can be used to predict the system's temperature after the quench from equilibrium properties at the prequench temperature. For a thermalizing postquench system, it furthermore allows us to calculate equilibrium observable expectation values. Finally, in the presence of additional conserved quantities besides the Hamiltonian, we obtain a hierarchy of necessary conditions for thermalization towards the (postquench) canonical ensemble. At first order, these thermalization conditions have a nice geometric interpretation in operator space with the canonical covariance as a semi-inner product: The quench operator (difference between post- and prequench Hamiltonians) and the conserved quantity must be orthogonal in the orthogonal complement of the postquench Hamiltonian. We illustrate the results numerically for a variety of setups involving integrable and nonintegrable models.

DOI: [10.1103/bp6q-ydvv](https://doi.org/10.1103/bp6q-ydvv)

I. INTRODUCTION

If left alone, generic systems of our everyday experience tend towards thermal equilibrium, a state that is characterized by macroscopically homogeneous and stationary observable properties. Through thermodynamic ensembles, these equilibrium properties can be predicted from a few macroscopic parameters, such as the temperature, number of particles, and volume of the system. Understanding this macroscopically ubiquitous phenomenon based on the fundamental laws of quantum mechanics that describe the system's microscopic constituents has been of significant research interest in recent years [1–4].

A common way to prepare such a system out of equilibrium is a so-called quench: We start with a system in equilibrium and perform a fast, virtually instantaneous change of some of its parameters, such as suddenly moving a piston or switching an external field. This manipulation typically changes the system's energy and temperature, but it is not straightforward to predict the latter, in particular.

After the quench, the system usually relaxes towards a new (quasi)stationary state. Generically, expectation values of physical observables at sufficiently late times can be characterized by one of the standard thermodynamic ensembles (microcanonical, canonical,...) and we say that the system *thermalizes*. However, situations where this paradigm is seemingly violated and the long-time behavior retains some

memory of the initial conditions [5–7] have been of considerable interest recently, too. Mechanisms that can result in absence of thermalization include integrability [8,9], many-body localization [10–12], many-body scars [13–15], and Hilbert-space fragmentation [14,15]. It is widely agreed that conserved quantities, inherent or emergent, play a major role in understanding thermalization or its absence [8–16]. In other words, they need to be taken into account properly to characterize the system's equilibrium properties correctly. Then again, the number of independent conserved quantities of any quantum system equals its Hilbert-space dimension (take, e.g., the projectors onto energy eigenstates), which is exponentially large in the system's degrees of freedom. However, there are no known, physically realistic setups in which such an exponentially large number of conservation laws is necessary to predict the long-term behavior of a many-body system. This raises the question of which conserved quantities are relevant, meaning that they need to be considered to describe the system's equilibrium properties, and which are not. There is a variety of qualitative and quantitative criteria that assess the importance of conserved quantities for thermalization, such as locality [17,18], overlap with observables of interest [19], Mazur bounds [20–23], the quench action [24], quasiparticle excitations [25], and commutant algebras [23,26], for example. Nevertheless, a comprehensive understanding of this issue is still missing (and, to avoid misunderstandings, will not be provided here, either). A related problem is to find potentially relevant and physically meaningful (e.g., local or quasilocal) conserved quantities [27–31].

The present work contributes to the ongoing efforts to understand thermalization and the role of conserved quantities during this process. We focus on quenches from canonical equilibrium states and address the following three questions, in particular: (i) Assuming that the system thermalizes, what are its temperature and equilibrium properties after the

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quench? (ii) If the postquench system has additional conserved quantities besides the Hamiltonian, what are necessary conditions for thermalization towards the canonical ensemble? (iii) Under what circumstances must a conserved quantity be accounted for explicitly (e.g., through a generalized Gibbs ensemble [9,32,33]) to reproduce the system's equilibrium properties? Our (partial) answers to these questions will be based on a systematic expansion of postquench properties like the temperature and observable expectation values in the quench strength.

II. SETUP

We focus on isolated quantum systems that evolve unitarily in time. Before the quench, the system of interest is described by the prequench Hamiltonian $\tilde{H}$ and finds itself in thermal equilibrium, which we model by an initial state in the form of the canonical ensemble (or Gibbs state) [34] at the prequench inverse temperature $\tilde{\beta}$,

$$\tilde{\rho}_{\tilde{\beta}} := \tilde{Z}_{\tilde{\beta}}^{-1} e^{-\tilde{\beta}\tilde{H}} \quad \text{with} \quad \tilde{Z}_{\tilde{\beta}} := \text{tr}(e^{-\tilde{\beta}\tilde{H}}). \quad (1)$$

Note that thanks to dynamical typicality [35–37], all of the following conclusions equally apply to large classes of pure initial states with equilibrium-like properties. Furthermore, other thermodynamic ensembles (e.g., microcanonical) are also expected to result in similar conclusions, at least for systems with short-range interactions, as ensembles are known to be equivalent under rather general conditions [38–42], though exceptions exist (see, e.g., Refs. [43–46]).

After the quench, the system is described by the postquench Hamiltonian,

$$H := \tilde{H} + gV. \quad (2)$$

We call V the *quench operator* and g the (dimensionless) *quench strength*. In the absence of further (relevant) conserved quantities besides H , a generic isolated system is expected to thermalize, meaning that its long-term properties are characterized by the canonical ensemble of H ,

$$\rho_{\beta} := Z_{\beta}^{-1} e^{-\beta H} \quad \text{with} \quad Z_{\beta} := \text{tr}(e^{-\beta H}), \quad (3)$$

where the postquench inverse temperature β is fixed by the condition

$$\langle H \rangle_{\tilde{\rho}_{\tilde{\beta}}} = \langle H \rangle_{\rho_{\beta}}. \quad (4)$$

Here $\langle A \rangle_{\rho} := \text{tr}(\rho A)$ denotes the expectation value of the observable A in the state ρ .

The question of whether and when the system indeed thermalizes towards such a canonical state provides the overarching context of the present study. However, we will not address the related question of equilibration, i.e., whether the long-term behavior becomes macroscopically stationary, such that physically realistic observables do not change noticeably over time (apart from technically unavoidable, but extremely rare quantum revival effects). This can be shown to happen very generally under relatively weak assumptions [47–50] and will be tacitly taken for granted in the following. Likewise, we will not be concerned with timescales or any other dynamical properties of the relaxation process.

Methodologically, the main idea is to expand the postquench inverse temperature β and equilibrium expectation values $\langle A \rangle_{\rho_{\beta}}$ of an observable A in powers of g .

III. POSTQUENCH TEMPERATURE AND EXPECTATION VALUES

Our first main result is a perturbative calculation of the system temperature and further equilibrium properties after the quench. To this end, we solve Eq. (4) for the postquench inverse temperature β . The goal is to predict β for arbitrary quench strengths g from properties of the postquench system at the known prequench temperature $\tilde{\beta}$.

Our starting point is a formal expansion of β in the quench strength g ,

$$\beta = \sum_{n=0}^{\infty} \beta_n g^n. \quad (5)$$

At zeroth order ($g = 0$, no quench), we evidently have

$$\beta_0 = \tilde{\beta} \quad (6)$$

because $H = \tilde{H}$ in (4), i.e., the zeroth-order postquench temperature is the prequench temperature. The corrections β_n for $n \geq 1$ can be obtained recursively in two steps.

First, we express expectation values $\langle A \rangle_{\rho_{\beta}}$ of an arbitrary observable A in the postquench ensemble at the unknown temperature β in terms of canonical expectation values at the known prequench temperature $\tilde{\beta} = \beta_0$. To this end, we formally write $e^{-(\beta - \beta_0)H}$ as a power series in g using a multinomial expansion. This result can then be exploited, on the one hand, to calculate $\text{tr}[e^{-\beta H} A]$ as a series in g with coefficients involving factors of $\text{tr}[e^{-\beta_0 H} H^k A]$. On the other hand, it can be used to represent the ratio of partition functions Z_{β_0}/Z_{β} as a geometric series in g . Multiplying these two expressions and sorting by powers of g , we obtain the desired expansion of $\langle A \rangle_{\rho_{\beta}}$ in terms of combinations of $\langle H^k A \rangle_{\rho_{\beta_0}}$. To order g^2 , it reads

$$\begin{aligned} \langle A \rangle_{\rho_{\beta}} &= \langle A \rangle - g\beta_1 \text{cov}(H, A) \\ &\quad - g^2 \left[(\beta_2 + \beta_1^2 \langle H \rangle) \text{cov}(H, A) - \frac{\beta_1^2}{2} \text{cov}(H^2, A) \right] \\ &\quad + \dots, \end{aligned} \quad (7)$$

where

$$\langle A \rangle := \langle A \rangle_{\rho_{\beta_0}} = Z_{\beta_0}^{-1} \text{tr}(e^{-\beta_0 H} A) \quad (8)$$

denotes expectation values of the postquench ensemble at the prequench reference temperature β_0 , and

$$\text{cov}(A, B) := \langle AB \rangle - \langle A \rangle \langle B \rangle \quad (9)$$

is the corresponding covariance. In other words, we suppress the canonical ensemble in the notation for expectation values and covariances if it corresponds to the postquench system at the prequench temperature; in all other cases, the state will still be indicated explicitly as a subscript of the expectation-value brackets. Equation (7) and the full expansion beyond second order are derived in detail in Appendix A; see Eq. (A12) for the final result.

Second, we express expectation values $\langle A \rangle_{\tilde{\rho}_{\tilde{\beta}}}$ in the prequench ensemble in terms of postquench ensemble expectation values and correlation functions. In this case, we expand $e^{-\tilde{\beta}H} = e^{-\tilde{\beta}(H-gV)}$ in g , resulting in an imaginary-time Dyson series. Similarly as in the previous step, we can adopt this result to calculate series expansions of $\text{tr}[e^{-\tilde{\beta}H}A]$ and $Z_{\tilde{\beta}}/\tilde{Z}_{\tilde{\beta}}$, combine the expressions, and sort by powers of g to find the expansion of $\langle A \rangle_{\tilde{\rho}_{\tilde{\beta}}}$. To order g^2 , we obtain

$$\langle A \rangle_{\tilde{\rho}_{\tilde{\beta}}} = \langle A \rangle + g \text{cov}(\Phi_1, A) + g^2 [\text{cov}(\Phi_2, A) - \langle \Phi_1 \rangle \text{cov}(\Phi_1, A)] + \dots, \quad (10)$$

where

$$\Phi_n := \int_0^{\tilde{\beta}} d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \dots \int_0^{\lambda_{n-1}} d\lambda_n V(\lambda_1) \dots V(\lambda_n) \quad (11)$$

is the n th-order coefficient of the time-ordered exponential of the imaginary-time evolved quench operator $V(\lambda) := e^{\lambda H} V e^{-\lambda H}$. The derivation of Eq. (10) can be found in Appendix B with the full expansion given in Eq. (B11). It should be noted that Eq. (10) is effectively also a high-temperature (small- $\tilde{\beta}$) expansion because of the expanded exponential.

To extract the coefficients β_n of the temperature series (5), we substitute $A = H$ and, according to Eq. (4), compare Eqs. (7) and (10) order by order in g . For the first-order correction, we obtain

$$\beta_1 = -\beta_0 \frac{\text{cov}(H, V)}{\text{var}(H)}, \quad (12)$$

exploiting that $\text{cov}(\Phi_1, H) = \beta_0 \text{cov}(H, V)$. Here, $\text{var}(H) := \text{cov}(H, H)$ denotes the canonical ensemble variance at the prequench temperature. Equation (12) coincides with the postquench temperature correction derived in Ref. [50] via linear response theory.

At second order, we find

$$\beta_2 = \frac{\frac{\beta_1^2}{2} \text{cov}(H^2, H) - \text{cov}(H, \Phi_2)}{\text{var}(H)} - \beta_1(\beta_1 \langle H \rangle + \beta_0 \langle V \rangle). \quad (13)$$

Note that $\text{cov}(H, \Phi_2)$ can be simplified slightly by writing it as a single integral,

$$\text{cov}(H, \Phi_2) = \int_0^{\beta_0} d\lambda \lambda \langle V(\lambda)[H - \langle H \rangle]V \rangle. \quad (14)$$

Higher-order corrections β_n can be calculated recursively in principle; see Appendix C and particularly Eq. (C2) for an explicit formula. Due to the high-temperature character of the expansion (10), the temperature prediction via Eqs. (12), (13), and (C2) is expected to work better for smaller values of $\tilde{\beta} = \beta_0$, too.

In summary, Eqs. (12), (13), and (C2) describe a systematic way to estimate the temperature after a canonical quench from equilibrium properties of the system at the prequench temperature, with increasing precision as higher orders of the expansion are taken into account. Provided that the system thermalizes after the quench, the combination of Eq. (7) [see also Eq. (A12)] with Eqs. (6), (12), (13) [and (C2) for higher orders] additionally offers a systematic way to calculate postquench equilibrium expectation values of arbitrary

observables A order by order in the quench strength. In other words, it allows us to predict general equilibrium properties after the quench from equilibrium properties at the prequench temperature.

IV. NECESSARY CONDITIONS FOR THERMALIZATION

Next, we assume that there is a physical observable Q (e.g., a sum of local and few-body operators) that commutes with the postquench Hamiltonian, $[H, Q] = 0$, so Q is an additional local conserved quantity of the postquench system besides H itself. Since Q is conserved, the system's long-term properties will be described correctly by the postquench canonical ensemble (3) only if

$$\langle Q \rangle_{\tilde{\rho}_{\tilde{\beta}}} = \langle Q \rangle_{\rho_{\beta}}, \quad (15)$$

i.e., only if the initial expectation value of Q coincides with its canonical expectation value. Note that this is trivially fulfilled if $\tilde{\beta} = 0$ (and thus $\beta = 0$). We therefore assume $\tilde{\beta} > 0$ from now on; similar conclusions can be drawn for $\tilde{\beta} < 0$.

Our second main result is a sequence of conditions on the postquench expectation values and correlation functions that are necessary for the system to thermalize towards the canonical ensemble (3): Using the perturbative expansions (7) and (10), we conclude that Eq. (15) must be satisfied at each order in the quench strength g . Consequently, if any of the resulting conditions is violated, then the system will fail to thermalize since Q itself is a trivial example of a nonthermalizing, physical observable.

From a different viewpoint, we may conclude that the conserved quantity Q is *relevant* in a given setup and needs to be considered to characterize the system's equilibrium properties. Instead of the canonical ensemble (3), one thus needs to adopt a generalized Gibbs ensemble that explicitly accounts for Q .

At first order, the necessary condition for thermalization obtained this way is

$$\text{cov}(Q, V) \text{var}(H) = \text{cov}(H, Q) \text{cov}(H, V). \quad (16)$$

This condition has an interesting geometric interpretation. The canonical covariance $\text{cov}(A, B) = \text{tr}(\rho_{\beta_0} AB) - \text{tr}(\rho_{\beta_0} A) \text{tr}(\rho_{\beta_0} B)$ defines an inner-product-like structure on the space of self-adjoint operators as it is linear in both arguments, positive semidefinite, and positive-definite modulo the real numbers; cf. Appendix D for details. However, it is generally not symmetric in its arguments, even though it is for all terms occurring in Eq. (16) since both H and Q commute with ρ_{β_0} .

For an arbitrary observable A , we can define its projection onto the orthogonal complement of the postquench Hamiltonian H as

$$A^{\perp} := A - \frac{\text{cov}(H, A)}{\text{var}(H)} H. \quad (17)$$

The first-order thermalization condition can then be rewritten as

$$\text{cov}(Q^{\perp}, V^{\perp}) = 0. \quad (18)$$

To observe thermalization to the canonical postquench ensemble, it is thus necessary that the quench operator be orthogonal

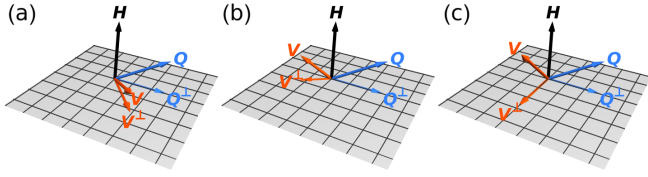


FIG. 1. Geometric interpretation of the first-order thermalization condition (18) [see also Eq. (16)]. (a) No special relationship between H , Q , and V ; the condition is violated. (b) V is orthogonal to Q [with respect to $\text{cov}(\cdot, \cdot)$], but the respective projections $V^\perp$ and $Q^\perp$ onto the orthogonal complement of H are not orthogonal to each other; the condition is violated. (c) The projections $V^\perp$ and $Q^\perp$ are orthogonal (and V and Q may or may not be orthogonal to each other); the condition is satisfied.

to additional conserved quantities in the orthogonal complement of the postquench Hamiltonian. This is illustrated in Fig. 1.

At second order, the condition (15) requires

$$\begin{aligned} \text{cov}(Q, \Phi_2) - \beta_0^2 \langle V \rangle \text{cov}(Q, V) \\ = \frac{\beta_1^2}{2} \text{cov}(H^2, Q) - (\beta_2 + \beta_1^2 \langle H \rangle) \text{cov}(H, Q). \end{aligned} \quad (19)$$

In addition to time-independent canonical expectation values, this condition also incorporates information from imaginary-time correlation functions via $\text{cov}(Q, \Phi_2) = \int_0^{\beta_0} d\lambda \langle V(\lambda) [Q - \langle Q \rangle] V \rangle$.

Higher-order conditions can be obtained from the full series expansions of $\langle Q \rangle_{\rho_\beta}$ and $\langle Q \rangle_{\tilde{\rho}_\beta}$ given in Eqs. (A12) and (B11) in the Appendixes, respectively.

It should be noted that strictly speaking, the conditions (16) and (19), etc., can only be expected to hold exactly in the thermodynamic limit. A finite system will generally exhibit deviations in the same way that deviations between time-averaged and thermal expectation values of general physical observables are expected. However, compared to the natural scale of fluctuations [e.g., $\text{var}(Q)$], these deviations should become negligibly small as the system size is increased.

Coming back to the question of what constitutes a relevant conserved quantity, we inspect the special case $V = Q$, i.e., a quench in the conserved quantity itself. In this case, the first-order condition (18) becomes

$$\text{var}(Q^\perp) = 0. \quad (20)$$

Assuming that this holds and recalling the geometric interpretation of the canonical covariance as (essentially) an inner product, Eq. (20) means that the “norm” of $Q^\perp$ vanishes and thus H and Q are collinear. More precisely (see also Appendix D), we can conclude that H and Q agree up to rescaling and shifting by a constant. This contradicts the (implicit) assumption that Q is an independent conserved quantity. Put differently, the first-order condition is violated for quenches in a conserved quantity.

The physical upshot is that any conserved quantity that can act as a quench operator is *relevant*: In a scenario where the quench operator coincides (or overlaps) with the conserved quantity, the latter must be taken into account to predict the system’s equilibrium properties after the quench. In principle,

this can be done by restricting the Hilbert space to states within a symmetry sector or a macroscopically small window of Q values compatible with the initial condition (micro-canonical approach), or by including a Lagrange parameter (generalized inverse temperature) conjugate to Q (generalized Gibbs ensemble/grand-canonical approach).

Nevertheless, it may still happen that such a generally relevant conserved quantity is irrelevant in a particular setup (i.e., a particular pair of Hamiltonian H and quench operator V) because its expectation value happens to be unchanged by the quench such that Eq. (15) holds to all orders in g .

V. EXAMPLES

We numerically explore the temperature expansion (5) and the expansions of expectation values (7) and (10) in a variety of setups. In particular, we focus on the thermalization conditions (16) and (19) for conserved quantities and various “geometric” configurations of the operators H , V , and Q with respect to the canonical-ensemble covariance as summarized in Table I.

A. Ising model

We begin with two setups where the postquench Hamiltonian $H = H_1$ is the transverse-field Ising model,

$$H_1 := - \sum_{j=1}^L (\sigma_j^x \sigma_{j+1}^x + h \sigma_j^z), \quad (21)$$

with periodic boundary conditions and $h = \frac{1}{2}$. Here σ_j^v ($v = x, y, z$) denotes a Pauli operator acting on lattice site j . This model is integrable and exhibits two families of local integrals of motion (LIOM) [2,8,17],

$$Q_n^+ := - \sum_j [\tau_{j,n}^{xx} + \tau_{j,n-2}^{yy} - h(\tau_{j,n-1}^{xx} + \tau_{j,n-1}^{yy})], \quad (22)$$

$$Q_n^- := - \sum_j (\tau_{j,n}^{xy} - \tau_{j,n}^{yx}), \quad (23)$$

where $\tau_{j,n}^{\mu\nu} := \sigma_j^\mu [\prod_{k=1}^{n-1} \sigma_{j+k}^z] \sigma_{j+n}^\nu$ for $n \geq 1$, $\tau_{j,0}^{yy} := -\sigma_j^z$, and $\tau_{j,0}^{xx} \equiv \tau_{j,-1}^{yy} := 0$. Note that $Q_1^+ = H_1$.

Since the relations derived in Secs. III and IV do not depend explicitly on the system size, we content ourselves with a relatively small value of $L = 10$ and use exact diagonalization for all numerical results in the following.

We first consider quenches in the external field. The quench operator $V = M^z$ is the total z magnetization,

$$M^z := \sum_j \sigma_j^z, \quad (24)$$

and the prequench Hamiltonian $\tilde{H} = H - gV$ is thus of the same form as (21), but with $h = \frac{1}{2} + g$.

To illustrate how Eq. (5) can be used to predict the temperature after the quench, we show in Fig. 2(a) the postquench temperature β against the prequench temperature $\tilde{\beta}$ for different strengths g along with the zeroth-, first-, and second-order approximations [cf. Eqs. (6), (12), and (13)]. As expected, the approximations work best for smaller quench strengths and higher temperatures (small β), and the prediction improves as

TABLE I. Geometric relations between the operators H , V , and Q in the examples from Sec. V. A tick ($\checkmark$) in an “ $A \perp B$ ” column indicates that $\text{cov}(A, B) = 0$ for all β_0 [cf. below Eq. (7)]; $Q^\perp \perp V^\perp$ is the first-order thermalization condition (16), see also Fig. 1; and $\langle Q \rangle_{\tilde{\rho}_\beta} = \langle Q \rangle_{\rho_\beta}$ is the full condition (15).

H	V	Q	$H \perp V$	$H \perp Q$	$Q^\perp \perp V^\perp$	$\langle Q \rangle_{\tilde{\rho}_\beta} = \langle Q \rangle_{\rho_\beta}$	plot
H_1	M^z	Q_n^+	—	—	—	—	Fig. 2
		Q_n^-	—	$\checkmark$	$\checkmark$	$\checkmark$	
		J^z	$\checkmark$	—	$\checkmark$	—	Fig. 3
H_2	W	Q_n^+	$\checkmark$	$\checkmark$	—	—	Fig. 3
		Q_n^-	$\checkmark$	$\checkmark$	—	—	Fig. 4
		M^z	—	$\checkmark$	—	—	Fig. 5(a)
H_3	M^x	M^z	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	Figs. 5(b)–5(d)
		M^x	$\checkmark$	—	$\checkmark$	—	

higher orders are included. Qualitatively, we observe that the quench cools the system at high initial temperature (small $\tilde{\beta}$), i.e., $\beta \geq \tilde{\beta}$, whereas it heats the system if starting from a low-temperature state (large $\tilde{\beta}$). This trend is reflected correctly in the first- and second-order approximations.

Let us now turn to the behavior of the LIOM and focus on Q_n^+ from (22) first. In Fig. 2(b), we plot the expectation values $\langle Q_n^+ \rangle_{\tilde{\rho}_\beta}$ for $n = 2, 3, 4$ in the prequench canonical ensemble

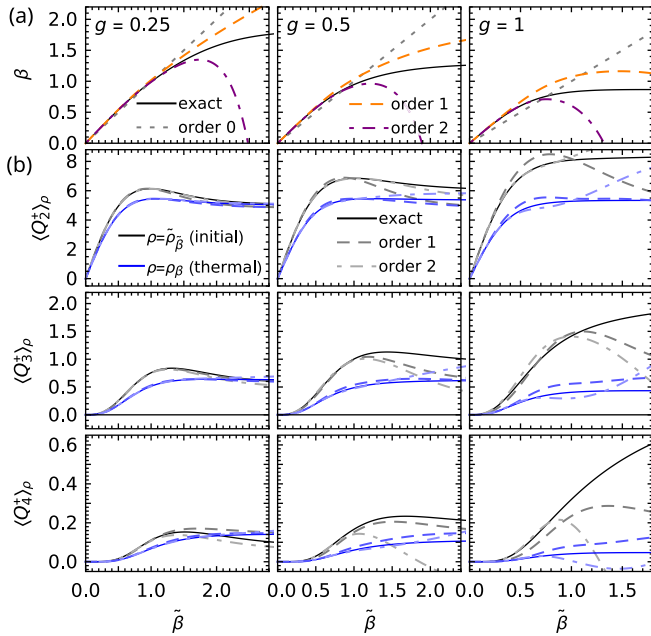


FIG. 2. (a) Postquench inverse temperature β and (b) LIOM expectation values $\langle Q_n^+ \rangle_\rho$ as a function of the prequench inverse temperature $\tilde{\beta}$ for canonical quenches in the transverse-field Ising model (21). Postquench: $h = \frac{1}{2}$; prequench: $h = \frac{1}{2} + g$, $g = 0.25$ (left), 0.5 (middle), and 1 (right). Solid lines are exact values; dotted, dashed, and dotted-dashed lines correspond, respectively, to the zeroth-, first-, and second-order approximations in the quench strength g . In (b), gray-shaded lines (with different dashings to indicate different approximation orders; see above) correspond to the initial value $\langle Q_n^+ \rangle_{\tilde{\rho}_\beta}$, while blue-shaded lines (with different dashings) correspond to the (thermal) expectation value $\langle Q_n^+ \rangle_{\rho_\beta}$ of the postquench ensemble, where $\beta = \beta(\tilde{\beta})$ is the respective postquench temperature [as shown in panel (a)]. Note that the different line dashings may be hard to distinguish in the regimes where they overlap, indicating good agreement of approximations and exact values.

as black solid lines along with the first- and second-order approximations according to Eq. (10) as gray dashed and dotted-dashed lines, respectively. Since $\tilde{\rho}_\beta$ is the initial state and the Q_n^+ are conserved, these are the actual expectation values assumed by the system after the quench. We compare them to the expectation values $\langle Q_n^+ \rangle_{\rho_\beta}$ of the postquench canonical ensemble at the postquench inverse temperature β [which itself depends on $\tilde{\beta}$ as shown in Fig. 2(a)]. Those $\langle Q_n^+ \rangle_{\rho_\beta}$ are depicted as blue solid lines in Fig. 2(b) along with their first- and second-order approximations according to Eq. (7) as blue dashed and dotted-dashed lines, respectively. They represent the values expected for a system that thermalizes in the conventional sense, meaning that its long-time properties are macroscopically indistinguishable from those of the canonical Gibbs ensemble. Hence, the necessary thermalization condition (15) is satisfied if the black and blue lines coincide.

The results in Fig. 2(b) demonstrate that the first- and second-order approximations reproduce the true expectation values in the pre- and postquench canonical ensembles as expected for sufficiently small g and $\tilde{\beta}$, and the same conclusion can be drawn from all further numerical examples below.

In the present setup, we observe that the thermalization conditions are generally violated for the Q_n^+ . In line with Ref. [17], the violation decreases in absolute terms as n increases, i.e., the “more local” conserved quantities with smaller n are more strongly violated and thus more important when setting up a generalized Gibbs ensemble to capture the system’s equilibrium properties. The thermalization conditions are already violated at first order, as can be seen by comparing the gray and blue dashed lines. Hence the simple condition (16) [or (18)] is sufficient to conclude that the system will fail to thermalize to the canonical ensemble. Geometrically, this is an instance of the scenario sketched in Fig. 1(a), where none of the operators H , Q , V , $Q^\perp$, $V^\perp$ are pairwise orthogonal with respect to the postquench canonical covariance $\text{cov}(\cdot, \cdot)$.

The situation is manifestly different for the second set of LIOM, the Q_n^- from (23). Contrary to the Q_n^+ , those are currentlike observables; e.g., $Q_1^- = -J^z$ is the nearest-neighbor hopping current of the z magnetization,

$$J^z := \frac{1}{2i} \sum_j (\sigma_j^- \sigma_{j+1}^+ - \sigma_j^+ \sigma_{j+1}^-) \quad (25)$$

with $\sigma_j^\pm := \sigma_j^x \pm i\sigma_j^y$.

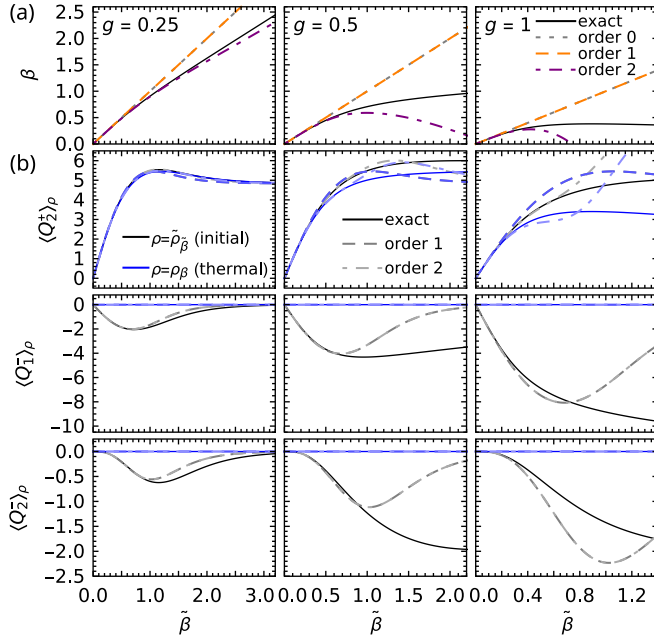


FIG. 3. (a) Postquench inverse temperature β and (b) LIOM expectation values $\langle Q_n^\pm \rangle_\rho$ as a function of the prequench inverse temperature $\tilde{\beta}$ for canonical quenches to the transverse-field Ising model $H = H_1$ from (21) with $h = \frac{1}{2}$. Prequench: $\tilde{H} = H_1 - gJ^z$ with $g = 0.25$ (left), 0.5 (middle), and 1 (right). Line styles and colors as indicated in the legends and the same as in Fig. 2.

Denoting by K the (antiunitary and self-inverse) operator defined by complex conjugation in the product basis, we observe that $KH_1K^{-1} = H_1$ and $KQ_n^-K^{-1} = -Q_n^-$, from which we can conclude that $\text{tr}[f(H_1)Q_n^-] = 0$ for an arbitrary function $f(x)$. (The latter relation can also be understood straightforwardly from the “diagonal” representations of H_1 and Q_n^- in terms of Bogoliubov operators [17].) It follows that $\langle Q_n^- \rangle_{\tilde{\rho}_\beta} = \langle Q_n^- \rangle_{\rho_\beta} = 0$ (hence they are not shown explicitly in Fig. 2). Consequently, the condition (15) is satisfied (at all orders in g) and the Q_n^- are irrelevant in this scenario. At first order, the geometric interpretation is a special case of Fig. 1(c) with $Q = Q^\perp$.

We contrast this with a second scenario where the quench operator $V = J^z$ is the spin current from (25). Temperatures and LIOM expectation values for various quench strengths are shown in Fig. 3. In contrast to the previous case, the quench now always heats up the system ($\beta \leq \tilde{\beta}$). Furthermore, the first-order correction (12) of the inverse temperature vanishes because $\text{cov}(H, V) = 0$, such that the gray dotted and orange dashed lines in Fig. 3(a) agree. However, the second-order term (13) yields a finite correction.

The Q_n^- now generally violate the first-order thermalization condition (16) as illustrated for Q_1^- and Q_2^- in Fig. 3(b) [51]. Geometrically, this can be regarded as a special case of the situation in Fig. 1(a) with $Q = Q^\perp$ and $V = V^\perp$ (and $Q = -V$ for Q_1^-). Interestingly, the second-order corrections to the expectation values in (7) and (10) vanish (such that the dashed and dotted-dashed lines coincide); hence, the second-order condition (19) is fulfilled. By contrast (and as exemplified for Q_2^+), the Q_n^+ all satisfy the first-order condition (16) in this setup because $\text{cov}(Q_n^+, V) = \text{cov}(H, V) = 0$ [see above;

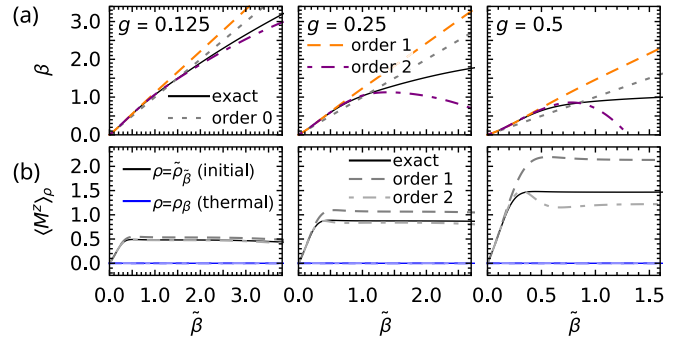


FIG. 4. (a) Postquench inverse temperature β and (b) z -magnetization expectation values $\langle M^z \rangle_\rho$ as a function of the prequench inverse temperature $\tilde{\beta}$ for canonical quenches in the non-integrable XXZ model. Postquench Hamiltonian $H = H_2$ from (26), quench operator $V = W$ from (27), and strengths $g = 0.125$ (left), 0.25 (middle), and 0.5 (right). Line styles and colors as indicated in the legends and the same as in Fig. 2.

special case of Fig. 1(c) with $V = V^\perp$], but violate the second-order condition (19). Overall, all LIOM of the transverse-field Ising model are thus relevant in this scenario, and even though this cannot be detected at first order alone, it becomes apparent at second order in the quench strength.

B. Nonintegrable XXZ model

Our second set of examples involves a variant of the XXZ model with nearest- and next-nearest-neighbor couplings. For the postquench system, we first choose $H = H_2$, where

$$H_2 := - \sum_{j=1}^L \sum_{n=1}^2 (\sigma_j^x \sigma_{j+n}^x + \sigma_j^y \sigma_{j+n}^y + \Delta \sigma_j^z \sigma_{j+n}^z) \quad (26)$$

with $\Delta = \frac{1}{2}$. This model is provably nonintegrable in the sense that the number of local conserved quantities is finite in the thermodynamic limit [52]. The only (known) local conserved quantity besides H is the total z magnetization, $Q = M^z$ from (24).

First, we inspect quenches from a system with Hamiltonian $\tilde{H} = H_2 - gW$, where

$$W := \sum_j (\sigma_j^x \sigma_{j+3}^x + \sigma_j^y \sigma_{j+3}^y + \sigma_j^z), \quad (27)$$

i.e., a model with additional third-nearest neighbor x and y couplings and a magnetic field applied in the z direction.

In this case, H and Q are orthogonal to each other [$\text{cov}(H_2, M^z) = 0$], but $V = W$ is not orthogonal to either of H or Q . This results in finite corrections to the postquench temperature and violations of the thermalization conditions at both first and second order, visualized in Fig. 4. Consequently, a generalized Gibbs ensemble that takes into account the conserved z magnetization is necessary to describe the system's equilibrium properties correctly.

Next, we prepare the system before the quench in an equilibrium state with an additional magnetic field in the x direction instead. The quench operator $V = M^x$ is thus the x

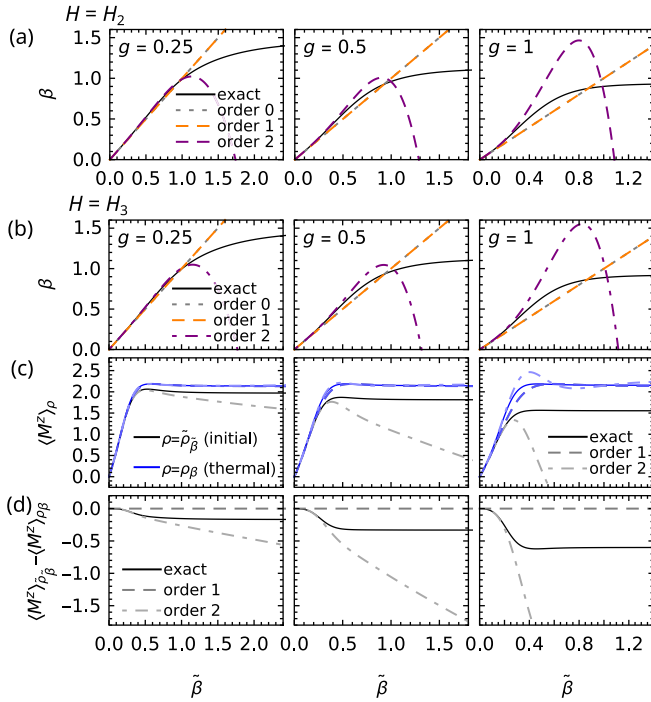


FIG. 5. (a) Postquench inverse temperature β as a function of the prequench inverse temperature $\tilde{\beta}$ for canonical quenches in the nonintegrable XXZ model with postquench Hamiltonian $H = H_2$ from (26), quench operator $V = M^x$ from (28), and quench strengths $g = 0.25$ (left), 0.5 (middle), and 1 (right). (b) Same relationship between pre- and postquench temperatures, but for the postquench Hamiltonian $H = H_3$ from (29). (c) z -magnetization expectation values $\langle M^z \rangle_\rho$ for the initial ($\tilde{\rho}_\beta$) and thermal (ρ_β) states, and (d) their difference, for the scenario with postquench Hamiltonian $H = H_3$. Line styles and colors as indicated in the legends and the same as in Fig. 2.

magnetization

$$M^x := \sum_j \sigma_j^x. \quad (28)$$

Since both $H = H_2$ and $V = M^x$ are spin-flip symmetric in the z direction (they commute with $F^z = \prod_{j=1}^L \sigma_j^z$), we have $\text{tr}[f(H, V)Q] = 0$ for an arbitrary function $f(x, y)$; hence, $\text{cov}(H, Q) = \text{cov}(Q, V) = 0$. Furthermore, H is also spin-flip symmetric in the x direction (commutes with $F^x = \prod_{j=1}^L \sigma_j^x$), such that $\text{cov}(H, V) = 0$. In conclusion, H , V , and Q are all mutually orthogonal to each other with respect to the canonical-ensemble covariance; cf. Fig. 1(c) with $V = V^\perp$ and $Q = Q^\perp$. Hence, the first-order correction of the postquench temperature vanishes as shown in Fig. 5(a) (but the second order provides a nontrivial correction).

On the other hand, the spin-flip symmetry also implies that the z magnetization vanishes in both the pre- and postquench canonical ensembles, $\langle M^z \rangle_{\tilde{\rho}_\beta} = \langle M^z \rangle_{\rho_\beta} = 0$, such that the thermalization condition (15) is satisfied to all orders. The canonical ensemble without reference to the conserved z magnetization thus reproduces the equilibrium properties of the postquench system.

Interestingly, this changes if we add the same, constant magnetic field to both the pre- and postquench Hamiltonians,

i.e., we consider $H = H_3$ with

$$H_3 := H_2 - hM^z \quad (29)$$

and the same quench operator $V = M^x$. Since H still commutes with F^x , $\text{cov}(H, V) = 0$ continues to hold. Likewise, we still have $\text{cov}(Q, V) = 0$, but H and Q are no longer orthogonal in general. This means that the first-order temperature correction still vanishes, and in fact, the relationship between the pre- and postquench temperatures is essentially unaffected by the additional magnetic field, as can be seen by comparing Figs. 5(a) and 5(b). The expectation values of the conserved z magnetization, however, are affected and now generally differ in the pre- and postquench ensembles, even though the additional field h is the same in both $H = H_3 = H_2 - hM^z$ and $\tilde{H} = H_3 - gM^x = H_2 - hM^z - gM^x$. Despite the quench operator being orthogonal to both H and M^z , the nontrivial equilibrium z magnetization induced by the field h depends on the field strength g in the x direction. The corresponding expectation values of M^z are shown in Fig. 5(c) along with their difference $\langle M^z \rangle_{\tilde{\rho}_\beta} - \langle M^z \rangle_{\rho_\beta}$ in Fig. 5(d). The first-order thermalization condition (16) fails to capture this qualitative change between the $H = H_2$ and $H = H_3$ scenarios [the dashed curve in Fig. 5(d) indicates zero violation for all $\tilde{\beta}$], but the second-order condition (19) indicates a violation (the dotted-dashed line in Fig. 5(d) shows a nonzero deviation).

VI. DISCUSSION AND CONCLUSIONS

Thanks to their experimental practicability, quenches from finite-temperature thermal equilibrium states have been of significant interest to understand the relaxation behavior of many-body systems theoretically (see, e.g., Refs. [53–60] and references therein). Considering such quenches of a quantum system from a canonical equilibrium state, we derived systematic expansions in the quench strength to relate equilibrium properties of the postquench system to equilibrium properties at its prequench temperature. The key physical insights are (i) an estimate of the postquench temperature [Eqs. (5), (12), (13), and (C2)]; (ii) a prediction of postquench equilibrium observable expectation values in thermalizing systems [Eqs. (7) and (A12)]; (iii) a hierarchy of necessary conditions for the system to thermalize to the canonical ensemble after the quench in the presence of additional conserved quantities [Eqs. (16), (19), (A12), and (B11)].

At sufficiently high temperatures and small quench strengths, low-order truncations of the expansions (i) and (ii) offer a simple and reliable way to approximate the postquench temperature and, for a thermalizing system, expected late-time values of observables. This was demonstrated numerically for various scenarios in Figs. 2–5 (see also the summary in Table I). Note that the opposite low-temperature regime and specifically quenches from the ground state of a prequench Hamiltonian, another frequently studied setup [8, 61], are not directly accessible quantitatively (unless one goes to very high orders in the expansion or very small quench amplitudes), but qualitative results like the thermalization conditions (iii) remain useful as they must be satisfied at all orders.

The thermalization conditions (iii) were obtained by comparing the pre- and postquench expectation values of

(physically observable) conserved quantities at each order in the quench strength. They can be seen as kinematic constraints and can be tested solely in terms of equilibrium properties, namely canonical-ensemble averages of the postquench system at the prequench temperature. They do not depend on or require access to any dynamical properties such as time-dependent or time-averaged expectation values. Likewise, they do not involve concepts like quantum chaos, ergodicity, or eigenstate thermalization [62–64]. Then again, they are only necessary conditions, suitable for detecting the absence of thermalization, but not for guaranteeing its presence.

An interesting complementary approach by Chiba and Shimizu [50] identified a sufficient condition for thermalization at first order in the quench strength. In particular, they showed that time-averaged expectation values of arbitrary (sums of) local observables coincide with their thermal, canonical expectation values to first order in g if and only if they do so for the quench operator V in our context. For a conserved quantity, this agreement between time-averaged and thermal expectation values boils down to Eq. (15).

Importantly, however, we observed [see Figs. 5(b)–5(d)] that the system may appear to thermalize at first order, in the sense that the necessary condition (16) holds, but is revealed to violate higher-order conditions.

Another main physical insight follows from the observation that the first-order thermalization condition is explicitly violated if the quench operator is a conserved quantity of the postquench system: This offers an operational answer to the question of what constitutes a potentially relevant conserved quantity, namely any observable that commutes with the Hamiltonian and is a legitimate quench operator. In other words, any conserved quantity for which there is an experimentally accessible conjugate control parameter will be relevant (at least) in an associated experiment where that parameter is quenched.

An otherwise commonly adopted characterization of relevant conserved quantities in theory is (sums of) local or quasilocal operators [1,2,8]. However, there may be other types of conserved quantities (e.g., momentum) that are controllable and potentially relevant [65–67]. A closely related question is what constitutes a “physical observable,” such that one generically expects its long-time expectation values to approach the values predicted by a pertinent thermodynamic ensemble. How this class is chosen clearly affects what kinds of conserved quantities need to be admitted when defining an equilibrium ensemble.

Finally, we remark that the approach adopted here can be employed more generally to expand a generalized Gibbs ensemble in all Lagrange parameters (generalized inverse temperatures). The contributions to these parameters at every order in the quench strength can then be calculated recursively by solving a linear system whose coefficients depend on lower-order parameters as well as expectation values and correlation functions of a postquench ensemble at the prequench parameter values. Furthermore, given the commonly expected and often provable equivalence of thermodynamic ensembles [38–42], it is expected that similar thermalization conditions can be formulated in the microcanonical picture, where relevant conserved quantities are constrained by restricting the Hilbert space instead of fixing mean values through Lagrange

multipliers. In case of a finite number of additional discrete and mutually commuting local conserved quantities, one may alternatively break down the analysis into symmetry subsectors and use the “one-parameter” canonical ensemble as adopted in this work in every subsector.

ACKNOWLEDGMENT

I am grateful to Peter Reimann for numerous inspiring discussions on this and related topics.

DATA AVAILABILITY

Source data for all the figures are available at Ref. [68]. The source code underlying the numerical calculations will be shared upon reasonable request.

APPENDIX A: CANONICAL ENSEMBLES AT DIFFERENT TEMPERATURES

In this section, we derive a perturbative expansion that relates canonical expectation values of an observable A at two different inverse temperatures β and β_0 . We think of β_0 as the prequench and β as the postquench temperature.

Our starting point is the expansion (5) for $\beta - \beta_0 = \sum_{n=1}^{\infty} \beta_n g^n$, which we substitute into the canonical exponential,

$$e^{-(\beta-\beta_0)H} = \sum_{n=0}^{\infty} \frac{(-H)^n}{n!} \left[\sum_{k=1}^{\infty} \beta_k g^k \right]^n. \quad (\text{A1})$$

Expanding the multinomial, we obtain

$$e^{-(\beta-\beta_0)H} = \sum_{n=0}^{\infty} \frac{(-H)^n}{n!} \sum_{\alpha: |\alpha|=n} \frac{n!}{\alpha!} \prod_{k=1}^{\infty} (\beta_k g^k)^{\alpha_k}, \quad (\text{A2})$$

where the inner sum is over all multi-indices $\alpha = (\alpha_1, \alpha_2, \dots)$ with $\alpha_k \in \mathbb{N}_0$ (non-negative integers) and length $|\alpha| := \sum_{k=1}^{\infty} \alpha_k = n$. The factorial of a multi-index is defined as $\alpha! := \prod_{k=1}^{\infty} \alpha_k!$. Since the double sum in (A2) effectively generates all multi-indices, we can write the relation more compactly as

$$e^{-(\beta-\beta_0)H} = \sum_{\alpha} \frac{(-H)^{|\alpha|}}{\alpha!} \prod_{k=1}^{\infty} (\beta_k g^k)^{\alpha_k}. \quad (\text{A3})$$

Next, we introduce the set of integer partitions

$$\mathcal{P}(n) := \left\{ (\alpha_1, \alpha_2, \dots) \in \mathbb{N}_0^{\infty} : \sum_{k=1}^n k \alpha_k = n \right\} \quad (\text{A4})$$

with $\mathcal{P}(0) := \{\emptyset\}$ by convention (the one-element set containing only the empty set). Note that, given $\alpha \in \mathcal{P}(n)$, α_k is necessarily zero whenever $k > n$; hence, we also write the elements of $\mathcal{P}(n)$ as finite n -tuples. These elements of $\mathcal{P}(n)$ encode all possible ways of writing n as a sum of positive integers. For example, $\mathcal{P}(3)$ consists of $(3, 0, 0)$, $(1, 1, 0)$, and $(0, 0, 1)$, representing the partitions $1 + 1 + 1$, $1 + 2$, and 3 , respectively.

We can now decompose the sum over all multi-indices in (A3) into integer partitions, which effectively sorts the

exponential by powers of g ,

$$e^{-(\beta-\beta_0)H} = \sum_{n=0}^{\infty} g^n \sum_{\alpha \in \mathcal{P}(n)} \frac{(-\beta)^\alpha}{\alpha!} H^{|\alpha|} \quad (\text{A5})$$

with $\beta := (\beta_1, \beta_2, \dots)$ and the shorthand notation

$$\beta^\alpha := \prod_{k=1}^{\infty} \beta_k^{\alpha_k}. \quad (\text{A6})$$

Turning to the partition function Z_β [cf. Eq. (1)], we multiply (A5) by $e^{-\beta_0 H}$ and take the trace,

$$Z_\beta = \sum_{n=0}^{\infty} g^n \sum_{\alpha \in \mathcal{P}(n)} \frac{(-\beta)^\alpha}{\alpha!} \text{tr}(e^{-\beta_0 H} H^{|\alpha|}). \quad (\text{A7})$$

Dividing by Z_{β_0} , we can rewrite this in terms of expectation values of the postquench ensemble at the prequench (or zeroth-order postquench) temperature,

$$\frac{Z_\beta}{Z_{\beta_0}} = 1 + \sum_{n=1}^{\infty} g^n z_n(\beta) \quad (\text{A8})$$

with

$$z_n(\beta) := \sum_{\alpha \in \mathcal{P}(n)} \frac{(-\beta)^\alpha}{\alpha!} \langle H^{|\alpha|} \rangle_{\rho_{\beta_0}}. \quad (\text{A9})$$

To keep the notation compact, we will usually suppress the dependence of z_n on β in the following.

To calculate expectation values in the canonical ensemble, we need the reciprocal of (A8). Using the geometric series expansion and following the same steps that led from (A1) to (A5), we obtain

$$\frac{Z_{\beta_0}}{Z_\beta} = \sum_{n=0}^{\infty} (-1)^n \left[\sum_{k=1}^{\infty} g^k z_k \right]^n = \sum_{n=0}^{\infty} g^n \sum_{\alpha \in \mathcal{P}(n)} \frac{|\alpha|! (-z)^\alpha}{\alpha!}, \quad (\text{A10})$$

where $\mathbf{z} := (z_1, z_2, \dots)$. Combining Eqs. (A5) and (A10), we find that the canonical expectation value of an observable A can be written as

$$\begin{aligned} \langle A \rangle_{\rho_\beta} &= \left[\sum_{m=0}^{\infty} g^m \sum_{\mu \in \mathcal{P}(m)} \frac{|\mu|! (-z)^\mu}{\mu!} \right] \\ &\times \left[\sum_{n=0}^{\infty} g^n \sum_{\nu \in \mathcal{P}(n)} \frac{(-\beta)^\nu}{\nu!} \langle H^{|\nu|} A \rangle_{\rho_{\beta_0}} \right]. \end{aligned} \quad (\text{A11})$$

Collecting powers of g , we arrive at

$$\langle A \rangle_{\rho_\beta} = \sum_{n=0}^{\infty} g^n \sum_{k=0}^n \sum_{\mu \in \mathcal{P}(n-k)} \frac{|\mu|! (-z)^\mu}{\mu!} \sum_{\nu \in \mathcal{P}(k)} \frac{(-\beta)^\nu}{\nu!} \langle H^{|\nu|} A \rangle_{\rho_{\beta_0}}. \quad (\text{A12})$$

Hence, we have expressed expectation values at inverse temperature β in terms of expectation values at inverse temperature β_0 , where the two temperatures are related through the perturbative expansion (5).

APPENDIX B: CANONICAL ENSEMBLES OF DIFFERENT HAMILTONIANS

In this section, we express the canonical expectation values of an observable A with respect to a Hamiltonian $\tilde{H}$ in terms of canonical expectation values of a different Hamiltonian H . We think of $\tilde{H}$ as the prequench Hamiltonian and $H = \tilde{H} + gV$ as the postquench Hamiltonian.

The idea is to expand the exponential $e^{-\tilde{\beta}\tilde{H}} = e^{-\tilde{\beta}(H-gV)}$ in the quench strength g . To this end, we define the operator

$$\Phi(\tilde{\beta}) := e^{\tilde{\beta}H} e^{-\tilde{\beta}(H-gV)} \quad (\text{B1})$$

and observe that it satisfies the integral relation

$$\Phi(\tilde{\beta}) = 1 + g \int_0^{\tilde{\beta}} d\lambda e^{\lambda H} V e^{-\lambda H} \Phi(\lambda), \quad (\text{B2})$$

as can be verified straightforwardly by differentiating with respect to $\tilde{\beta}$ and observing $\Phi(0) = 1$ [69]. With the definitions

$$\Phi_0(\tilde{\beta}) := 1, \quad (\text{B3})$$

$$\Phi_n(\tilde{\beta}) := \int_0^{\tilde{\beta}} d\lambda V(\lambda) \Phi_{n-1}(\lambda) \quad (\text{B4})$$

$$= \int_0^{\tilde{\beta}} d\lambda_1 \int_0^{\lambda_1} d\lambda_2 \cdots \int_0^{\lambda_{n-1}} d\lambda_n V(\lambda_1) \cdots V(\lambda_n), \quad (\text{B5})$$

$$V(\lambda) := e^{\lambda H} V e^{-\lambda H}, \quad (\text{B6})$$

we thus obtain a perturbative expansion of $\Phi(\tilde{\beta}) = \sum_{n=0}^{\infty} \Phi_n(\tilde{\beta}) g^n$ in g .

The partition function $\tilde{Z}_{\tilde{\beta}} := \text{tr}(e^{-\tilde{\beta}\tilde{H}})$ of the prequench Hamiltonian $\tilde{H}$ can thus be written as

$$\tilde{Z}_{\tilde{\beta}} = \text{tr} e^{-\tilde{\beta}H} + \sum_{n=1}^{\infty} g^n \text{tr}[e^{-\tilde{\beta}H} \Phi_n(\tilde{\beta})]. \quad (\text{B7})$$

Identifying $Z_{\tilde{\beta}} := \text{tr} e^{-\tilde{\beta}H}$ as the partition function of the postquench Hamiltonian H at inverse temperature $\tilde{\beta}$, we can then express $\tilde{Z}_{\tilde{\beta}}$ in terms of correlation functions in the postquench canonical ensemble,

$$\frac{\tilde{Z}_{\tilde{\beta}}}{Z_{\tilde{\beta}}} = 1 + \sum_{n=1}^{\infty} g^n \langle \Phi_n(\tilde{\beta}) \rangle_{\rho_{\tilde{\beta}}}. \quad (\text{B8})$$

To obtain the reciprocal of this relation, we apply the geometric series expansion once again [cf. above Eq. (A10)] and find

$$\frac{Z_{\tilde{\beta}}}{\tilde{Z}_{\tilde{\beta}}} = \sum_{n=0}^{\infty} g^n \sum_{\alpha \in \mathcal{P}(n)} \frac{|\alpha|!}{\alpha!} \prod_{k=1}^n \langle -\Phi_k(\tilde{\beta}) \rangle_{\rho_{\tilde{\beta}}}^{\alpha_k}. \quad (\text{B9})$$

To calculate expectation values in the prequench canonical ensemble in terms of postquench expectation values and correlation functions, we observe that

$$\text{tr}(e^{-\tilde{\beta}\tilde{H}} A) = \text{tr}[e^{-\tilde{\beta}H} \Phi(\tilde{\beta}) A] = \sum_{n=0}^{\infty} g^n \text{tr}[e^{-\tilde{\beta}H} \Phi_n(\tilde{\beta}) A]. \quad (\text{B10})$$

Combining Eqs. (B9) and (B10) and collecting powers of g [cf. Eqs. (A11) and (A12)], we obtain

$$\langle A \rangle_{\tilde{\rho}_{\tilde{\beta}}} = \sum_{n=0}^{\infty} g^n \sum_{k=0}^n \langle \Phi_k(\tilde{\beta}) A \rangle_{\rho_{\tilde{\beta}}} \sum_{\mu \in \mathcal{P}(n-k)} \frac{|\mu|!}{\mu!} \prod_{j=1}^{n-k} (-\Phi_j(\tilde{\beta}))_{\rho_{\tilde{\beta}}}^{\mu_j}. \quad (\text{B11})$$

Thus, we have expanded prequench canonical expectation values into a perturbation series in the quench strength g , which involves postquench canonical expectation values and imaginary-time correlation functions.

APPENDIX C: POSTQUENCH TEMPERATURE

If the system is prepared in the canonical ensemble $\tilde{\rho}_{\tilde{\beta}}$ of the prequench Hamiltonian $\tilde{H}$ at inverse temperature $\tilde{\beta}$, its inverse temperature β after a quench to the Hamiltonian H is determined by the condition (4), $\langle H \rangle_{\tilde{\rho}_{\tilde{\beta}}} = \langle H \rangle_{\rho_{\beta}}$. In other words, the energy $\langle H \rangle_{\tilde{\rho}_{\tilde{\beta}}}$ of the initial state has to equal the energy $\langle H \rangle_{\rho_{\beta}}$ in the postquench canonical ensemble. Using Eqs. (A12) and (B11), we can thus calculate the postquench temperature order by order in the quench amplitude g .

At zeroth order ($g = 0$), we find that $\langle H \rangle_{\tilde{\rho}_{\tilde{\beta}}} = \langle H \rangle_{\rho_{\tilde{\beta}}}$ and $\langle H \rangle_{\rho_{\beta}} = \langle H \rangle_{\rho_{\tilde{\beta}}}$. Consequently,

$$\beta_0 = \tilde{\beta}, \quad (\text{C1})$$

i.e., the zeroth-order approximation of the postquench temperature is the prequench temperature as expected.

In the following, we will use the shorthand notation introduced below Eq. (7), $\langle A \rangle := \langle A \rangle_{\rho_{\beta_0}} \equiv \langle A \rangle_{\rho_{\tilde{\beta}}}$ for postquench canonical expectation values at the prequench temperature as well as $\text{cov}(A, B) := \langle AB \rangle - \langle A \rangle \langle B \rangle$ and $\text{var}(A) := \text{cov}(A, A)$. Furthermore, we define $\Phi := (\Phi_1(\beta_0), \Phi_2(\beta_0), \dots)$ and recall the notation from (A6) for “sequences to the power of multi-indices.”

Comparing Eqs. (A12) and (B11) at order n , we find that β_n can be calculated recursively as follows:

$$\begin{aligned} \beta_n \text{var}(H) = & -\text{cov}(\Phi_n(\beta_0), H) + \sum_{\mu \in \mathcal{P}'(n)} \frac{1}{\mu!} \{ |\mu|! \langle H \rangle [(-z)^{\mu} \\ & - \langle -\Phi \rangle^{\mu}] + \text{cov}(H^{|\mu|}, H) (-\beta)^{\mu} \} \\ & + \sum_{k=1}^{n-1} \sum_{\mu \in \mathcal{P}(n-k)} \frac{|\mu|! (-z)^{\mu}}{\mu!} \sum_{\nu \in \mathcal{P}(k)} \frac{(-\beta)^{\nu} \langle H^{|\nu|+1} \rangle}{\nu!}, \end{aligned} \quad (\text{C2})$$

where $\mathcal{P}'(n)$ denotes the set of all integer partitions of n except $(0, \dots, 0, 1) (\equiv n)$. The first-order correction (12) follows by observing that the sums on the right-hand side of Eq. (C2) are empty if $n = 1$ and

$$\text{cov}(\Phi_1(\beta_0), H) = \beta_0 \text{cov}(H, V). \quad (\text{C3})$$

The second-order correction (13) is obtained by using $\mathcal{P}(0) = \{\emptyset\}$, $\mathcal{P}(1) = \{(1)\}$, $\mathcal{P}(2) = \{(2, 0), (0, 1)\}$, and $\mathcal{P}'(2) = \{(2, 0)\}$.

APPENDIX D: PROPERTIES OF THE CANONICAL COVARIANCE

For completeness, we collect a few properties of the canonical covariance

$$\text{cov}(A, B) := \text{tr}(\rho_{\beta_0} AB) - \text{tr}(\rho_{\beta_0} A) \text{tr}(\rho_{\beta_0} B) \quad (\text{D1})$$

that establish its similarity to an inner product on $\mathcal{L}_H(\mathcal{H})$, the vector space of self-adjoint operators on the underlying Hilbert space $\mathcal{H}$.

Bilinearity. Let $A, A_1, A_2, B, B_1, B_2 \in \mathcal{L}_H(\mathcal{H})$, and $\lambda_1, \lambda_2 \in \mathbb{R}$. Then,

$$\text{cov}(\lambda_1 A_1 + \lambda_2 A_2, B) = \lambda_1 \text{cov}(A_1, B) + \lambda_2 \text{cov}(A_2, B) \quad (\text{D2})$$

and

$$\text{cov}(A, \lambda_1 B_1 + \lambda_2 B_2) = \lambda_1 \text{cov}(A, B_1) + \lambda_2 \text{cov}(A, B_2). \quad (\text{D3})$$

Positive definiteness. Let $A \in \mathcal{L}_H(\mathcal{H})$. We observe that

$$\begin{aligned} \text{cov}(A, A) &= Z_{\beta_0}^{-1} \text{tr}[e^{-\beta_0 H} (A - \langle A \rangle)^2] \\ &= Z_{\beta_0}^{-1} \|e^{-\beta_0 H/2} (A - \langle A \rangle)\|_{\text{F}}^2, \end{aligned} \quad (\text{D4})$$

where $\|X\|_{\text{F}} := \sqrt{\text{tr}(X^\dagger X)}$ denotes the Frobenius norm of the (not necessarily self-adjoint) operator X . Hence $\text{cov}(A, A) \geq 0$, which establishes that the canonical covariance is positive semidefinite. Furthermore, Eq. (D4) implies that $\text{cov}(A, A) = 0$ if and only if $e^{-\beta_0 H/2} (A - \langle A \rangle) = 0$. Since $e^{-\beta_0 H/2}$ is a positive operator, the latter condition is equivalent to $A = \langle A \rangle$. Hence, the canonical covariance is positive definite on $\mathcal{L}_H(\mathcal{H})/\mathbb{R}$, i.e., on the quotient space of self-adjoint operators modulo the real numbers.

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