

Quantum Hertz entropy increase in a quenched spin chain

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Abstract. The classical Hertz entropy is the logarithm of the volume of phase space bounded by the constant energy surface; its quantum counterpart, the quantum Hertz entropy, is $\hat{S} = k_B \ln \hat{N}$, where the quantum operator \hat{N} specifies the number of states with energy below a given energy eigenstate. It has been recently proved that, when an isolated quantum mechanical system is driven out of equilibrium by an external driving, the change in the expectation of its quantum Hertz entropy cannot be negative, and is null for adiabatic driving. This is in full agreement with the Clausius principle. Here we test the behavior of the expectation of the quantum Hertz entropy in the case when two identical XY spin chains initially at different temperatures are quenched into a single XY chain. We observed no quantum Hertz entropy decrease. This finding further supports the statement that the quantum Hertz entropy is a proper entropy for isolated quantum systems. We further quantify how far the quenched chain is from thermal equilibrium and the temperature of the closest equilibrium.

PACS. 05.30.Ch Quantum ensemble theory – 05.70.-a Thermodynamics – 65.40.Gr Entropy and other thermodynamical quantities

1 Introduction

The recent tremendous development in the field of nonequilibrium quantum fluctuations [1, 2], has unveiled with an unprecedented clarity that many phenomena traditionally associated exclusively with macroscopic thermodynamic behaviour may manifest themselves even at the microscopic quantum level. Notably, the Second Law of thermodynamics, in the work-free energy formulation [3],

$$\langle w \rangle \geq \Delta F, \quad (1)$$

holds down to the quantum level [4]. In Eq. (1), w is the work done on a quantum system that is initially in equilibrium with a thermal bath, when the system is perturbed by an external time dependent protocol that changes its Hamiltonian in time. The brackets indicate average over many realizations, and ΔF is the difference between the free energy of a hypothetical equilibrium state (not necessarily reached by the system) corresponding to the final Hamiltonian, and the actual initial free energy of the system. Eq. (1) follows straightforwardly from the quantum version of the Jarzynski identity [5, 6, 7, 8].

For a cyclical driving, $H(\tau) = H(0)$, $\Delta F = 0$, Eq. (1) says, in accordance with Kelvin postulate, that no energy can be extracted by the cyclic variation of a parameter from a system in contact with a single bath [4]:

$$\langle w \rangle \geq 0 \quad \text{Kelvin (cyclic, with bath)} \quad (2)$$

Given the recent theoretical and experimental advances concerning the nonequilibrium dynamics of isolated quantum systems [9], an interesting question is whether a microscopic quantum formulation of the second law in accordance with Clausius formulation, is possible as well. According to Clausius' formulation the change of entropy of a *thermally insulated* driven system, which begins and ends in equilibrium, is non-negative:

$$\Delta S \geq 0 \quad \text{Clausius (no bath)} \quad (3)$$

Answering this question is not a simple task because it amounts to singling out a quantum mechanical quantity that behaves as prescribed by the Clausius principle and goes over to the usual thermodynamic entropy in the classical/thermodynamic limit. Of course von Neumann “entropy”, $-\text{Tr} \rho \log \rho$, proves inadequate in this respect because it is invariant under the quantum unitary time evolution.

One proposal in the direction of answering the above question was put forward by Polkovnikov [10, 11], with the introduction of the so-called diagonal entropy. Another proposal, put forward by Hal Tasaki and by one of us [12, 13, 14], uses instead the Hertz entropy [15, 16, 17] see Eq. (4), or in quantum mechanics, its quantum counterpart, that is the logarithm of the “quantum number operator” \hat{N} [12, 13, 14], see Eq. (5) below. In [12, 13, 14] it was shown that the expectation of the quantum Hertz entropy behaves in accordance to the Clausius principle. Here we scrutinize whether it complies also with another property

of thermodynamic entropy, namely whether it increases in a scenario when two quantum systems initially at different temperatures are allowed to exchange energy via the sudden switch-on of an interaction. This is a scenario that has recently attracted considerable attention [18, 19], and that, given the recent advances, e.g., in ultra-cold-atom physics [20], is amenable to experimental investigations.

In our study the two interacting bodies are two isotropic XY spin chains of length $N/2$, which are initially at different temperatures, and are suddenly quenched into a single isotropic XY spin chain of length N . While the quench dynamics in spin-chains has been thoroughly studied, only few studies addressed their thermodynamics [21, 22].

In Secs. 2 and 3 we review the quantum Hertz entropy and present our model, respectively. In Secs. 4 and 5 we calculate the initial and final expectation of the quantum Hertz entropy. Results concerning the entropy change and the deviation of the final state from thermal equilibrium are presented in Sec. 6 and Sec. 7, respectively. Conclusions are drawn in Sec. 8.

2 Quantum Hertz entropy

The microcanonical entropy of a classical system is the so-called Hertz entropy [15, 16, 17, 23] presented also by Gibbs in his classic book [24], namely

$$S = k_B \ln[\Phi/h^f], \quad (4)$$

where k_B is Boltzmann constant, Φ is the phase space volume enclosed by the hyper-surface of constant energy in the system phase space of dimension $2f$ and h is Planck's constant. According to semiclassical reasoning [25], in the quantum limit, the quantity Φ/h^f gets the discrete values $n = 1, 2, \dots$.¹ The associated quantum operator is the quantum number operator \hat{N} , whose eigenvectors are the energy eigenvectors, with the integers the corresponding eigenvalues. For a driven system, the operator \hat{N} is time dependent, and its spectral decomposition reads (for non degenerate Hamiltonians) $\hat{N}(t) = \sum n \Pi_n(t)$, with $\Pi_n(t)$ the instantaneous eigenprojectors on the eigenspace spanned by the instantaneous eigenvalue $E_n(t)$ of the Hamiltonian $H(t)$. Here it is assumed that the energy eigenvalues are non-degenerate and ordered in increasing fashion: $E_1(t) < E_2(t) < \dots$. Accordingly, the quantum mechanical operator associated to the Hertz entropy is

$$\hat{S}(t) = k_B \ln \hat{N}(t). \quad (5)$$

Under the assumption that (i) the density matrix $\rho(0)$ describing the initial state of the system is diagonal in the energy eigenbasis $\rho(0) = \sum p_n \Pi_n(0)$, and (ii) the population p_n decreases with increasing energy (i.e., $p_n \leq p_m$, if $E_n(0) > E_m(0)$); it has been shown that [12, 13, 14]:

$$S(t) \geq S(0), \quad (6)$$

¹ Depending on the problem at hand, the quantization rule may prescribes a shift $\Phi/\hbar \rightarrow n + a$, which is not relevant in this context.

where

$$S(t) = \text{Tr} \hat{S}(t) \rho(t). \quad (7)$$

For adiabatic transformations the equal sign holds in Eq. (6). The quantity $S(t)$ hence behaves in accordance to the Clausius principle and goes over to the usual thermodynamic entropy in case of large classical systems at equilibrium. These facts make it a sound quantum mechanical counterpart for the thermodynamic entropy of a thermally insulated system. In the following we shall refer to S and \hat{S} as to the quantum entropy, and the quantum entropy operator, respectively. Note however that unless the system is in equilibrium at time t , the quantum entropy $S(t)$ should not be considered as the thermodynamic entropy of the system. The latter is an exclusively equilibrium property.

2.1 Remarks

We remark that unlike the Boltzmann entropy $S_B = k_B \log[\Omega/h^f]$, [$\Omega = \partial_E \Phi$ being the density of states], the Hertz entropy *is not postulated*, but rather *rationally derived* from the fundamental requirement that its differential dS exactly equals the quantity $\delta Q/T$ as calculated in the microcanonical ensemble, the so-called generalized Helmholtz theorem [16, 17]. As such, at equilibrium, the Hertz entropy has to be identified with the thermodynamic entropy. It is commonly assumed that S and S_B are equivalent [26], which is true in most cases but has important exceptions, e.g., in small systems or systems with a finite spectrum. In this latter case they can give drastically different results, notably S , a monotonically increasing function of E , gives only positive temperatures in accordance to thermodynamic fundamentals [27], whereas S_B predicts also negative ones. This is a topic of current interest as testified by recent experiments [28].

For a Gibbs ensemble of systems at canonical temperature $T_c = 1/k_B \beta$, one finds the following expression for the work dissipated, $W_{\text{diss}} = \langle w \rangle - \Delta F$, due to an external driving [29, 30, 31, 32]:

$$W_{\text{diss}} = k_B T_c D[\rho(t) | \rho^{\text{eq}}(t)] \quad (8)$$

where $D[\rho(t) | \rho^{\text{eq}}(t)] = \text{Tr} \rho(t) \log \rho(t) - \text{Tr} \rho(t) \log \rho^{\text{eq}}(t)$ is the Kullbeck-Leibler divergence between $\rho(t)$, the density matrix of the system at time t , and $\rho^{\text{eq}}(t) = e^{-\beta H(t)} / \text{Tr} e^{-\beta H(t)}$ the corresponding equilibrium density matrix. The quantity $W_{\text{diss}}/T_c = k_B D[\rho(t) | \rho^{\text{eq}}(t)]$ is often referred to as the entropy production [33]. This off-equilibrium quantity should not be confused with the change in thermodynamic entropy $\int \delta Q/T$, which involves quasi-static heat exchanges, instead. However there exist a strict connection between W_{diss} and the change in thermodynamic entropy ΔS .

Noticing that the Kullbeck-Leibler divergence is a non-negative quantity, it is apparent from Eq. (8) that $W_{\text{diss}} \geq 0$ for $T_c > 0$, $W_{\text{diss}} \leq 0$ for $T_c < 0$. This can be easily obtained also from the Jarzynski identity [1]. It says

that when one perturbs a Gibbs ensemble of thermally isolated systems characterized by a positive canonical T_c , one gets out less energy than one puts in, on average. This is the second law in the usual Kelvin formulation. Vice-versa one gets out more energy than one puts in, if the ensemble was characterized by a negative T_c .² This is well described by Ramsey's account of the early experiments on negative spin temperatures. He writes [35, see p. 27] "when a negative temperature spin system was subjected to resonance radiation more radiant energy was given off by the spin system than was absorbed." In sum, it is an experimental fact that when perturbing canonical ensembles characterized by negative T_c , the second law is inverted. Accordingly the entropy should decrease, and this is in fact the behavior of the Hertz entropy [13]: $\Delta S \geq 0$ for $T_c > 0$, $\Delta S \leq 0$ for $T_c < 0$, which shows the equivalence of Kelvin and Clausius formulations down to microscopic quantum level, and also to negative T_c 's.

One difference between the quantum Hertz entropy and the diagonal entropy [10] is that the latter would always increase, regardless of the sign of T_c of the initial canonical ensemble. Presumably the diagonal entropy does not differ much from the Hertz entropy in ordinary large systems with unbound spectrum. This question however deserves a detailed investigation that goes beyond the scope of the present contribution.

3 The Model

Our model consists of two identical isotropic XY spin chains, which are quenched at time $t = 0$ to a single XY chain of twice the length, see Fig. 1. At times $t < 0$, the system Hamiltonian is:

$$H_0 = H_L + H_R, \quad (9)$$

with:

$$H_L = -\frac{h}{2} \sum_{j=1}^{N/2} \sigma_j^z + \frac{J}{2} \sum_{j=1}^{N/2-1} [\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y], \quad (10)$$

$$H_R = -\frac{h}{2} \sum_{j=N/2+1}^N \sigma_j^z + \frac{J}{2} \sum_{j=N/2+1}^{N-1} [\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y]. \quad (11)$$

Here σ_j^α , $j = 1 \dots N$, $\alpha = x, y, z$, denotes the Pauli matrices of the j -th spin. At $t < 0$ the left (right) chain is in the Gibbs state of temperature $T_{L(R)}$, hence the total system density matrix is given by their product:

$$\rho_0 = \frac{e^{-\beta_L H_L}}{Z(\beta_L)} \otimes \frac{e^{-\beta_R H_R}}{Z(\beta_R)}, \quad (12)$$

where $Z(\beta) = \text{Tr} e^{-\beta H} = \text{Tr} e^{-\beta H}$ is the partition function, and $\beta_{L(R)} = (k_B T_{L(R)})^{-1}$, with k_B Boltzmann constant. At time $t = 0$ an interaction between spin $N/2$ and

spin $N/2 + 1$ is turned on, such that the Hamiltonian is, for $t > 0$:

$$H_1 = -\frac{h}{2} \sum_{j=1}^N \sigma_j^z + \frac{J}{2} \sum_{j=1}^{N-1} [\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y]. \quad (13)$$

The Hamiltonians H_L, H_R, H_1 all represent isotropic XY chains of different lengths. Following the standard procedures they can be put in diagonal form by means of Jordan-Wigner transformation followed by a sine transform [36, 37]. Specifically

$$H_1 = \sum_{j=1}^N \varepsilon_k b_k^\dagger b_k + \frac{Nh}{2}, \quad (14)$$

where

$$\varepsilon_k = -h - 2J \cos\left(\frac{k\pi}{N+1}\right), \quad (15)$$

$$b_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^N \sin\left(\frac{ki\pi}{N+1}\right) a_i, \quad (16)$$

$$a_j = \prod_{k=1}^{j-1} \sigma_k^z \sigma_j^-, \quad (17)$$

$$\sigma_j^\pm = \frac{1}{2} (\sigma_j^x \pm i \sigma_j^y); \quad (18)$$

We shall denote the eigenvectors and eigenvalues of H_1 as $|\mathbf{n}\rangle = |n_1, n_2, \dots, n_N\rangle$ and $E_{\mathbf{n}}$, respectively, where $n_i = 0, 1$:

$$H_1 |\mathbf{n}\rangle = E_{\mathbf{n}} |\mathbf{n}\rangle, \quad E_{\mathbf{n}} = \sum_{k=1}^N \varepsilon_k n_k + \frac{Nh}{2}. \quad (19)$$

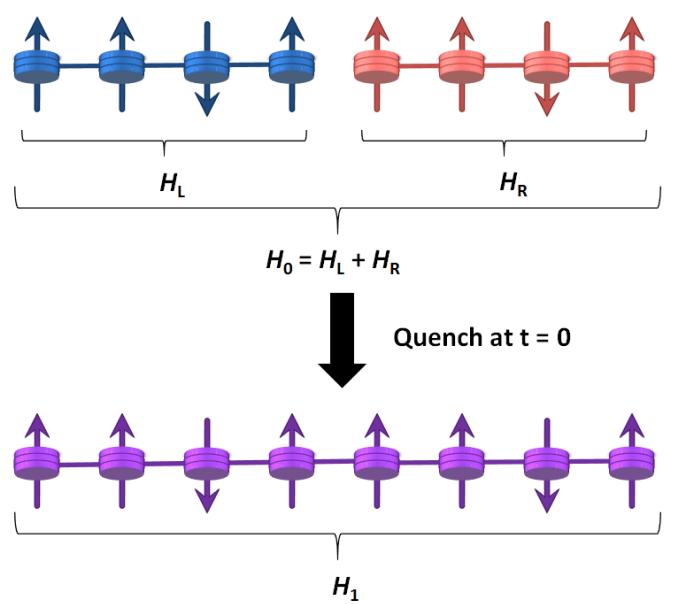


Fig. 1. Schematics of our model

² Note that "negative temperature can never exist in equilibrium states. It is however, possible to create it in certain transient processes" [34, see pag. 148].

The states $|\mathbf{n}\rangle$ are the Fock states associated to the fermionic operators b_k . For future reference we recall their properties

$$b_k^\dagger b_k |\dots n_k \dots\rangle = n_k |\dots n_k \dots\rangle \quad (20)$$

$$b_k |\dots n_k \dots\rangle = n_k (-1)^{\sum_{i=1}^{k-1} n_i} |\dots n_k - 1 \dots\rangle \quad (21)$$

$$b_k^\dagger |\dots n_k \dots\rangle = (1 - n_k) (-1)^{\sum_{i=1}^{k-1} n_i} |\dots n_k + 1 \dots\rangle \quad (22)$$

Similarly, for the L -chain:

$$H_L = \sum_{k=1}^{N/2} \varepsilon'_k b_k'^\dagger b_k' + \frac{Nh}{4}, \quad (23)$$

$$\varepsilon'_k = -h - 2J \cos\left(\frac{k\pi}{N/2 + 1}\right), \quad (24)$$

$$b_k' = \sqrt{\frac{2}{N/2 + 1}} \sum_{i=1}^{N/2} \sin\left(\frac{ki\pi}{N/2 + 1}\right) a_i. \quad (25)$$

Note that the same Jordan-Wigner operators a_i are used for the L -chain and the total chain. In defining b_k all N operators are used, while only the first $N/2$ are employed to define the primed operators b_k' . We shall denote the eigenvectors and eigenvalues of H_L as $|\mathbf{l}\rangle = |l_1, l_2, \dots, l_{N/2}\rangle$ and $E_{\mathbf{l}}$, respectively:

$$H_L |\mathbf{l}\rangle = E_{\mathbf{l}} |\mathbf{l}\rangle, \quad E_{\mathbf{l}} = \sum_{k=1}^{N/2} \varepsilon'_k l_k + \frac{Nh}{4}. \quad (26)$$

Likewise for the R -chain,

$$H_R = \sum_{k=1}^{N/2} \varepsilon'_k b_k''^\dagger b_k'' + \frac{Nh}{4}, \quad (27)$$

$$b_k'' = \sqrt{\frac{2}{N/2 + 1}} \sum_{i=1}^{N/2} \sin\left(\frac{ki\pi}{N/2 + 1}\right) a_i'' \quad (28)$$

$$a_j'' = \prod_{k=1}^{j-1} \sigma_{N/2+k}^z \sigma_{N/2+j}^- \quad (29)$$

Note two prominent facts: i) the single mode eigenenergies ε'_k are the same for the L -chain and the R -chain, because the two chains are identical. (ii) The Jordan Wigner operators a_j'' of the R -chain differ from the Jordan Wigner operators a_j of the L -chain and total chain, because the latter begin with spin 1, while the R -chain begins with spin $N/2 + 1$. We shall denote the eigenvectors and eigenvalues of H_R as $|\mathbf{r}\rangle = |r_1, r_2, \dots, r_{N/2}\rangle$ and $E_{\mathbf{r}}$, respectively:

$$H_R |\mathbf{r}\rangle = E_{\mathbf{r}} |\mathbf{r}\rangle, \quad E_{\mathbf{r}} = \sum_{k=1}^{N/2} \varepsilon'_k r_k + \frac{Nh}{4}. \quad (30)$$

4 Initial quantum Entropy

At times $t < 0$ the entropy of the two non-interacting chains is given by the sum of their individual entropies.

We proceed by calculating the quantum entropy S^β of the left chain at inverse thermal energy β . Since the two chains are identical this also gives the quantum entropy of right chain at the same inverse thermal energy β .

According to Eq. (7)

$$\begin{aligned} S^\beta &= \frac{k_B}{Z(\beta)} \text{Tr } e^{-\beta H_L} \ln \hat{L} \\ &= \frac{k_B}{Z(\beta)} \sum_{\mathbf{l}} e^{-\beta E_{\mathbf{l}}} \langle \mathbf{l} | \ln \hat{L} | \mathbf{l} \rangle \\ &= \frac{k_B}{Z(\beta)} \sum_{\mathbf{l}} e^{-\beta E_{\mathbf{l}}} \ln \lambda_{\mathbf{l}}. \end{aligned} \quad (31)$$

Here \hat{L} is the principal quantum number operator associated to the L -chain. Its eigenvectors are the Fock states $|\mathbf{l}\rangle$, and its eigenvalues are $\lambda_{\mathbf{l}}$. The eigenvalues $\lambda_{\mathbf{l}}$ are calculated in the following way. The energy eigenvalues $E_{\mathbf{l}}$ are ordered accordingly to their increasing values, so as to obtain a sequence

$$E_{\mathbf{l}_1} < E_{\mathbf{l}_2} < \dots < E_{\mathbf{l}_{2^{N/2}}}, \quad (32)$$

where $|\mathbf{l}_1\rangle$ is the ground state, $|\mathbf{l}_2\rangle$ is the first excited state, \dots $|\mathbf{l}_{2^{N/2}}\rangle$ is the state of highest energy. Then $\lambda_{\mathbf{l}_1} = 1, \lambda_{\mathbf{l}_2} = 2$, etc.

The total initial quantum entropy S_0 , is given by:

$$S_0 = S^{\beta_L} + S^{\beta_R}. \quad (33)$$

5 Final quantum entropy

Due to the assumption of sudden quench, at time $t = 0^+$ the density matrix retains the initial form in Eq. (12). The final quantum entropy S_1 is therefore given by

$$\begin{aligned} S_1 &= k_B \frac{\text{Tr } e^{-\beta_L H_L} e^{-\beta_R H_R} \ln \hat{N}}{Z(\beta_L) Z(\beta_R)} \\ &= k_B \frac{\sum_{\mathbf{n}} \langle \mathbf{n} | e^{-\beta_L H_L} e^{-\beta_R H_R} | \mathbf{n} \rangle \ln \nu_{\mathbf{n}}}{Z(\beta_L) Z(\beta_R)}. \end{aligned} \quad (34)$$

Here \hat{N} is the quantum number operator associated to the total chain, and $\nu_{\mathbf{n}}$ are its integer eigenvalues, obtained as described above for the smaller L -chain, with the difference that now one has to order the 2^N eigenvalues $E_{\mathbf{n}}$.

We next consider the basis $|\mathbf{lr}\rangle = |\mathbf{l}\rangle \otimes |\mathbf{r}\rangle$ formed by the direct product of the eigenbasis of H_L and H_R : Using the resolution of the identity $\sum_{\mathbf{l}, \mathbf{r}} |\mathbf{lr}\rangle \langle \mathbf{lr}| = \mathbb{1}$, the final quantum entropy reads:

$$S_1 = k_B \frac{\sum_{\mathbf{n}, \mathbf{l}, \mathbf{r}} P(\mathbf{n} | \mathbf{l}, \mathbf{r}) e^{-\beta_L E_{\mathbf{l}}} e^{-\beta_R E_{\mathbf{r}}} \ln \nu_{\mathbf{n}}}{Z(\beta_L) Z(\beta_R)}, \quad (35)$$

where

$$P(\mathbf{n} | \mathbf{l}, \mathbf{r}) = \langle \mathbf{n} | \mathbf{lr} \rangle \langle \mathbf{lr} | \mathbf{n} \rangle. \quad (36)$$

In order to calculate $P(\mathbf{n} | \mathbf{l}, \mathbf{r})$ we consider the basis $|\mathbf{s}\rangle = |s_1, s_2, \dots, s_N\rangle = |s_1\rangle \otimes |s_2\rangle \otimes \dots \otimes |s_N\rangle$ formed by the direct

product of the eigenstates $|s_j\rangle$ of the z component of each spin operator: $\sigma_j^z|s_j\rangle = s_j|s_j\rangle$ with $s_j = \pm$. Employing the resolution of the identity twice we obtain:

$$\begin{aligned} P(\mathbf{n}|\mathbf{l}, \mathbf{r}) &= \sum_{\mathbf{s}, \mathbf{s}'} \langle \mathbf{n} | \mathbf{s} \rangle \langle \mathbf{s} | \mathbf{l} \mathbf{r} \rangle \langle \mathbf{l} \mathbf{r} | \mathbf{s}' \rangle \langle \mathbf{s}' | \mathbf{n} \rangle \\ &= \sum_{\mathbf{s}, \mathbf{s}'} \langle \mathbf{n} | \mathbf{s} \rangle \langle \mathbf{s}' | \mathbf{n} \rangle \langle \mathbf{l} \mathbf{r} | \mathbf{s}' \rangle \langle \mathbf{s}' | \mathbf{l} \mathbf{r} \rangle. \end{aligned} \quad (37)$$

The next crucial step in the calculation consists in expressing the operators $|\mathbf{s}\rangle\langle\mathbf{s}'|$ in terms of spin rising and lowering operators. For a single spin, say spin j , we have $|+\rangle\langle+| = \sigma_j^+ \sigma_j^-$, $|-\rangle\langle-| = \sigma_j^- \sigma_j^+$, $|+\rangle\langle-| = \sigma_j^+$, $|-\rangle\langle+| = \sigma_j^-$ which can be compactly written

$$|\mathbf{s}\rangle\langle\mathbf{s}'| = \delta_{ss'}\sigma_j^s\sigma_j^{-s} + (1 - \delta_{ss'})\sigma_j^s, \quad (38)$$

where $\delta_{ss'}$ denotes the Kronecker symbol, and σ_j^\pm are given in Eq. (18). Therefore:

$$|\mathbf{s}\rangle\langle\mathbf{s}'| = \prod_j [\delta_{s_j s'_j} \sigma_j^{s_j} \sigma_j^{-s_j} + (1 - \delta_{s_j s'_j}) \sigma_j^{s_j}]. \quad (39)$$

In order to calculate $\langle \mathbf{n} | \mathbf{s} \rangle \langle \mathbf{s}' | \mathbf{n} \rangle$ we express $|\mathbf{s}\rangle\langle\mathbf{s}'|$ in terms of the fermionic operators b_k of the total system. This can be accomplished by using the inverse sine transforms:

$$a_j = \sqrt{\frac{2}{N+1}} \sum_{k=1}^N \sin\left(\frac{k j \pi}{N+1}\right) b_k, \quad (40)$$

and the following identities:

$$\sigma_j^s \sigma_j^{-s} = a_j^s a_j^{-s}, \quad (41)$$

$$\sigma_j^{-s} = \prod_{k=1}^{j-1} (2a_k^+ a_k^- - 1) a_j^{-s}, \quad (42)$$

where we set the convenient notations $a_j^+ \doteq a_j^\dagger$, $a_j^- \doteq a_j$. By plugging Eqs. (40, 41, 42) into Eq. (39), the operator $|\mathbf{s}\rangle\langle\mathbf{s}'|$ is expressed in terms of the operators b_k and b_k^\dagger . The wanted term $\langle \mathbf{n} | \mathbf{s} \rangle \langle \mathbf{s}' | \mathbf{n} \rangle$ is calculated then by using the properties (20-22) and the orthonormality condition $\langle \mathbf{n} | \mathbf{n}' \rangle = \delta_{n_1, n'_1} \delta_{n_2, n'_2} \dots \delta_{n_N, n'_N}$.

In order to calculate $\langle \mathbf{l} \mathbf{r} | \mathbf{s}' \rangle \langle \mathbf{s}' | \mathbf{l} \mathbf{r} \rangle$ we proceed by expressing $|\mathbf{s}'\rangle$ as the direct product of two subchain states $|\mathbf{s}'\rangle = |s_1 \dots s_N\rangle = |s_1 \dots s_{N/2}\rangle \otimes |s_{N/2+1} \dots s_N\rangle = |\mathbf{s}_L\rangle \otimes |\mathbf{s}_R\rangle$. Accordingly, the wanted term reduces to the product of two terms each pertaining to each subchain: $\langle \mathbf{l} \mathbf{r} | \mathbf{s}' \rangle \langle \mathbf{s}' | \mathbf{l} \mathbf{r} \rangle = \langle \mathbf{l} | \mathbf{s}'_L \rangle \langle \mathbf{s}_L | \mathbf{l} \rangle \cdot \langle \mathbf{r} | \mathbf{s}'_R \rangle \langle \mathbf{s}_R | \mathbf{r} \rangle$. The calculation of $\langle \mathbf{l} | \mathbf{s}'_L \rangle \langle \mathbf{s}_L | \mathbf{l} \rangle$ proceeds as the above calculation of $\langle \mathbf{n} | \mathbf{s} \rangle \langle \mathbf{s}' | \mathbf{n} \rangle$, with the only difference that now all quantities pertain to the smaller L -chain. Since the L and R chains are identical this automatically gives also the R -chain term $\langle \mathbf{r} | \mathbf{s}'_R \rangle \langle \mathbf{s}_R | \mathbf{r} \rangle$.

In the Appendix we provide further details on how these calculations were implemented.

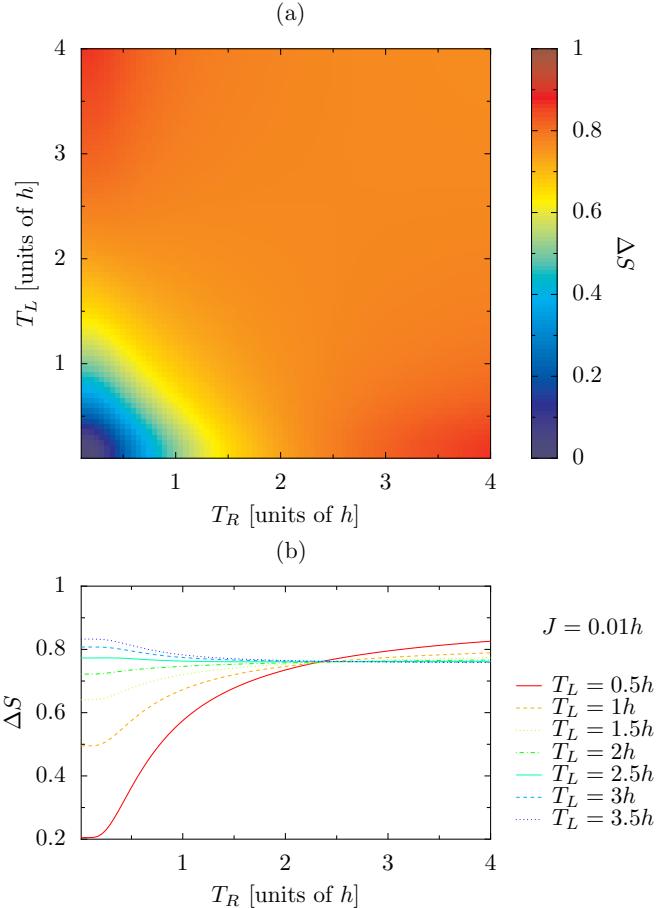


Fig. 2. (a): Entropy change, Eq. (43), as a function of T_L, T_R . (b): Entropy change, Eq. (43), as a function of T_R for various fixed T_L 's. Here $h = 1$, $J = 0.01h$ and $N = 8$.

6 Entropy change

Using the method detailed above, we have calculated the change of quantum entropy

$$\Delta S = S_1 - S_0 \quad (43)$$

caused by the sudden quench, for different values of the parameters defining our problem. These are the initial temperatures of the left and right chains, $k_B T_{L,R} = \beta_{L,R}^{-1}$, the length N of the total chain, and the interaction strength J . The field strength h was used as the unit of energy, and we adopted the convention that temperatures are measured in units of energy. In these units we have k_B , Boltzmann's constant, equal to 1.

Figure 2, top panel, shows a surface plot of the entropy change in a chain of length $N = 8$ at $J = 0.01h$, as a function of T_L and T_R . Figure 2, bottom panel, shows for the same values of $N = 8$, $J = 0.01h$, the behavior of ΔS as function of T_R for various left chain temperatures $T_L = 0.5h$ to $3.5h$. The quantum entropy change here is always positive and approaches a saturation value as T_R becomes very large. We see qualitatively different behaviors of ΔS as a function of T_R , depending on T_L . As T_L increases, ΔS changes from a monotonically increasing function of T_R to

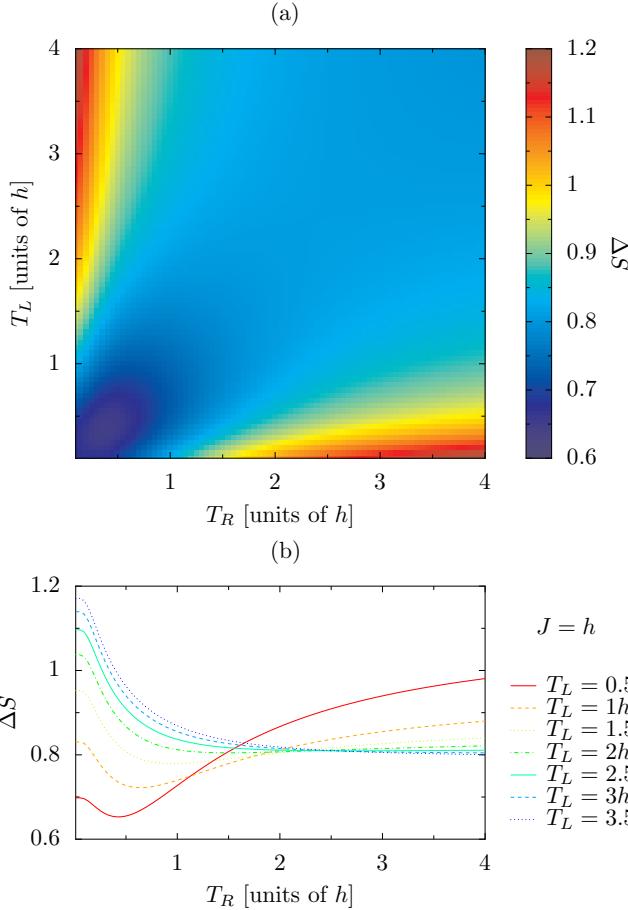


Fig. 3. (a): Entropy change, Eq. (43), as a function of T_L, T_R . (b): Entropy change, Eq. (43), as a function of T_R for various fixed T_L 's. Here $h = 1$, $J = h$ and $N = 8$.

a monotonically decreasing function of T_R . The transition occurs for T_L of the order of the width of the spectrum of H_L (which takes on the value $2.6h$ in this case).

In Fig. 3 we report the same quantities as in Fig. 2 with the only difference that now $J = h$. For this value $J = h$ the quantum entropy change, seen as a function of T_R features minima for small values of T_L and a monotonically decreasing behavior for large T_L . As with Fig. 2 the transition occurs for T_L of the order of the width of the spectrum of H_L (which is $2h$ in this case).

In both Fig. 2 and 3, we see a common feature. The values of ΔS corresponding to lower T_L is smaller than the value of ΔS corresponding to larger T_L at lower T_R , whereas it is vice-versa at larger values of T_R . We observed a similar behavior also at other values of J (e.g., for $J = 0.0001, 0.1, 2, 5$) and $N = 2, 4, 6$ for same value of all other parameters). In no case have we observed a negative change in quantum entropy.

For $T_L = T_R$, ΔS gives the entropy of mixing. In the high temperature limit $T_L = T_R \gg \Delta E$, where ΔE is the width of the spectrum, one gets $\Delta S = 2^{-N} \ln(2^N!) - 2^{-N/2+1} \ln(2^{N/2}!)$. For $N = 8$, as in Figs. 2 and 3, this gives $\Delta S \simeq 0.72$. For large N , using Stirling approximation one gets $\Delta S \simeq 1$. The mixing entropy is non-zero

because the spin chain is made of distinguishable particle (one can distinguish one spin from the other by its site label). It is however negligibly small as compared to the entropy itself, which is of order N , because it is a surface effect, and as such is of order 1.

7 Thermalization

After the quench, the system is in an out-of-equilibrium state. In order to quantify how far the system is from an equilibrium Gibbs state, one can employ one of the many metrics in the space of density matrices discussed in the literature, e.g., in reference [38]. Among them the Hilbert-Schmidt distance:

$$D_{HS}[\rho, \sigma] = \sqrt{\text{Tr}(\rho - \sigma)^2} \quad (44)$$

appears best suited to the problem at hand. The reason is that, in our problem, the Hilbert-Schmidt distance between the after-quench density matrix ρ_t and a Gibbs state

$$\rho_\beta = e^{-\beta H_1} / Z_1(\beta), \quad (45)$$

where $Z_1(\beta) = \text{Tr } e^{-\beta H_1}$, does not depend on time t . Furthermore it can be calculated by knowing the initial density matrix ρ_0 , Eq. (12), and the transition amplitudes $P(\mathbf{n}, \mathbf{l}, \mathbf{r})$, Eq. (37). That is, it can be obtained from the only knowledge of the (time independent) diagonal elements

$$\langle \mathbf{n} | \rho_t | \mathbf{n} \rangle = \sum_{\mathbf{l}, \mathbf{r}} P(\mathbf{n}, \mathbf{l}, \mathbf{r}) \frac{e^{-\beta_L E_l} e^{-\beta_R E_r}}{Z(\beta_L) Z(\beta_R)}, \quad (46)$$

with no need to calculate the off-diagonal elements $\langle \mathbf{n} | \rho_t | \mathbf{m} \rangle$, $\mathbf{n} \neq \mathbf{m}$. In fact:

$$D_{HS}^2[\rho_t, \rho_\beta] = \text{Tr} \rho_\beta^2 - 2 \text{Tr} \rho_t \rho_\beta + \text{Tr} \rho_t^2, \quad (47)$$

and

$$\text{Tr} \rho_\beta^2 = \sum_{\mathbf{n}} \frac{e^{-2\beta E_{\mathbf{n}}}}{Z_1^2(\beta)}, \quad (48)$$

$$\text{Tr} \rho_t \rho_\beta = \sum_{\mathbf{n}} \frac{e^{-\beta E_{\mathbf{n}}}}{Z_1(\beta)} \langle \mathbf{n} | \rho_t | \mathbf{n} \rangle, \quad (49)$$

$$\text{Tr} \rho_t^2 = \text{Tr} \rho_0^2 = \sum_{\mathbf{l}, \mathbf{r}} \frac{e^{-2\beta_L E_l}}{Z^2(\beta_L)} \frac{e^{-2\beta_R E_r}}{Z^2(\beta_R)}. \quad (50)$$

Using Eqs. (44-50) we calculated the minimal distance

$$D_{HS}^{\min} = \min_{\beta} D_{HS}[\rho_t, \rho_\beta], \quad (51)$$

between the final state ρ_t and the set of thermal Gibbs states. This gives both an estimate of how far the system is from equilibrium, and what the temperature $k_B \bar{T} = \beta^{-1}$ is of the closest equilibrium, where β is the value of β for which the minimum distance D_{HS}^{\min} is attained.

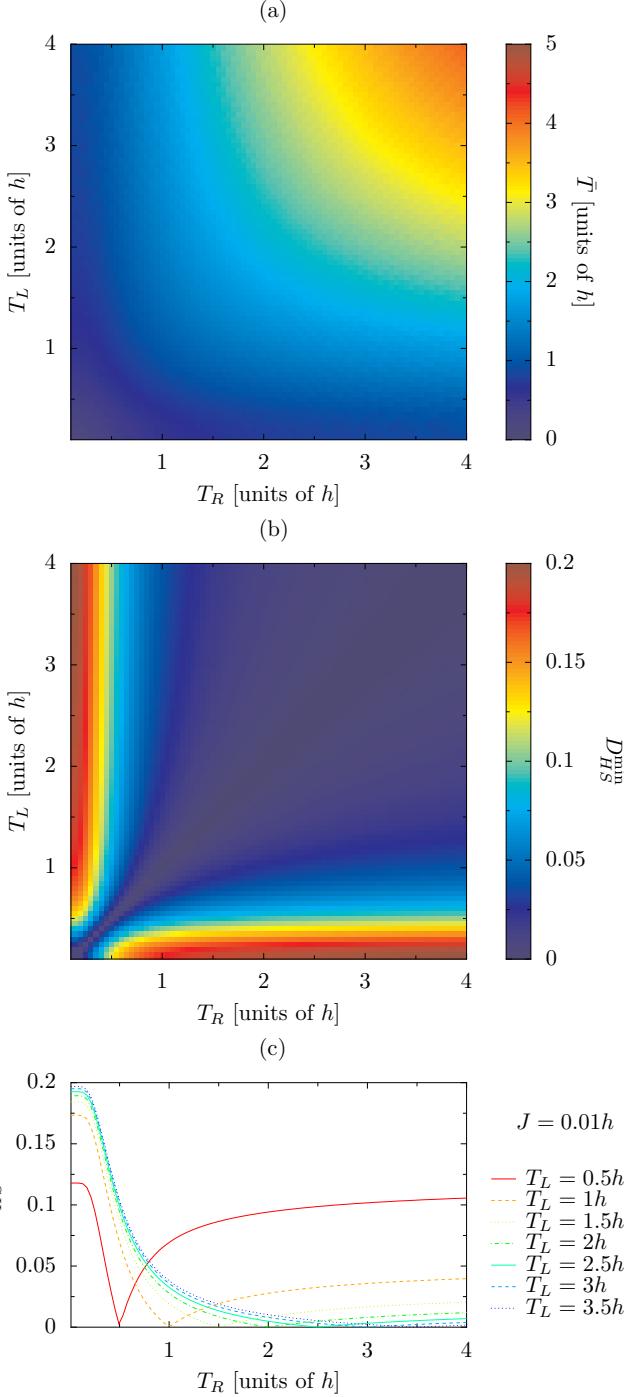


Fig. 4. (a): Temperature \bar{T} of closest equilibrium, as a function of T_L, T_R . (b): Minimal distance D_{HS}^{\min} , Eq. (51), as a function of T_R, T_R . (c): Minimal distance D_{HS}^{\min} , Eq. (51), as a function of T_R for various fixed T_L 's. Here $h = 1$, $J = 0.01h$ and $N = 8$.

Fig. 4 shows plots of \bar{T} and D_{HS}^{\min} (panels (a) and (b), respectively), as a function of T_L, T_R , at a low value of interaction strength $J = 0.01h$ and chain length $N = 8$. Panel (c) presents D_{HS}^{\min} as function of T_R for various fixed T_L 's. Panel (b) indicates that better thermalization is achieved when T_L and T_R are closer. As can be seen from

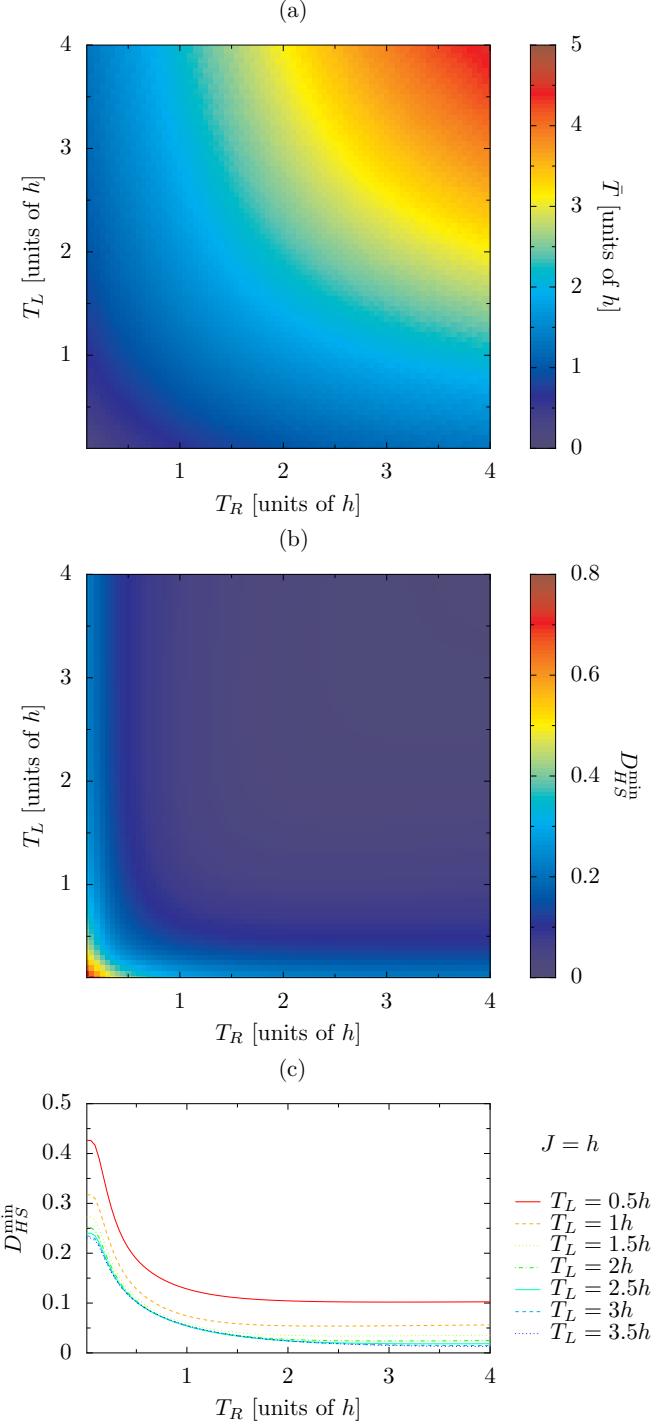


Fig. 5. (a): Temperature \bar{T} of closest equilibrium, as a function of T_L, T_R . (b): Minimal distance D_{HS}^{\min} , Eq. (51), as a function of T_R, T_R . (c): Minimal distance D_{HS}^{\min} , Eq. (51), as a function of T_R for various fixed T_L 's. Here $h = 1$, $J = h$ and $N = 8$.

panel (a), when $T_L = T_R$ it is $\bar{T} \simeq T_L = T_R$. For fixed T_L (panel (c)) we observe that as T_R grows from zero, the minimal distance D_{HS}^{\min} first decreases, then reaches a minimum, and finally grows. The minimum is in corre-

spondence to $T_R \sim T_L$ as expected, and it is sharper for low T_L 's.

Fig. 5 is like Fig. 4 with the only difference that it is for a larger interaction strength $J = h$. As compared with Fig. 4 we observe here a different structure of the plot of D_{HS}^{\min} as a function of T_L and T_R , see panel (b). Within the range of T_L, T_R considered in the plot, it appears that a smaller distance is achieved when either T_L, T_R or both grow. This different structure is reflected in the curves presented in panel (c), presenting D_{HS}^{\min} as a function of T_R , for fixed T_L 's. The structure of the plot of \bar{T} as a function of T_L, T_R , panel (a), is qualitatively similar to the corresponding plot in Fig. 4. Note that for $T_L = T_R$, the temperature of the closest equilibrium is larger than T_L , of some amount of the order of h . This is because the quench injects an energy amount of the order $J = h$ in the system. Similarly, in Fig. 4, \bar{T} was close to $T_L = T_R$ because the quench injects in that case an energy of the order $J = 0.01h$.

8 Conclusions

We have investigated numerically the change in the quantum Hertz entropy of Eq. (5), caused by a quench of two spin-chains of different temperatures into a larger single chain. Although we cannot conclude that such changes are always positive, our numerics clearly suggests that this is the typical behavior, thus providing further support to the statement that the quantum Hertz entropy of Eq. (5) is a proper quantum entropy for thermally isolated systems.

We further quantified how far the system is from equilibrium after the quench, and estimated the corresponding temperature of the closest equilibrium. For those quenches ending very close to an equilibrium state, it becomes meaningful to assign the system the equilibrium temperature \bar{T} , and the thermodynamic entropy S_1 .

The Hertz entropy S can be employed to study phase transitions and critical points in spin chains in a way analogous to Ref. [22] where the dissipated work W_{diss} signaled the crossing of a critical point as the magnetic field was incrementally and globally changed, and the chain was initially at some temperature T . Because of the strict connection between Hertz entropy and dissipated work, the Hertz entropy in that same scenario should give similar results. The present thermalization scenario, with an initial nonequilibrium state and a local quench, is not convenient though, for the study of critical points.

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Appendix

As detailed in Sec. 5, the transition probabilities $P(\mathbf{n}|\mathbf{l}, \mathbf{r})$, involve the calculation of the expectation of the operators $|\mathbf{s}\rangle\langle\mathbf{s}'|$ over the Fock states $|\mathbf{n}\rangle$. Accordingly, we have detailed how these operators may be expressed in terms of the fermionic operators b_k , whose action on the Fock states is defined in Eqs. (20,21,22). In order to calculate those expectations we expressed the fermionic operators b_k in matrix form. First we represented the Fock states $|\mathbf{n}\rangle$ as tensorial product of single-spin states:

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (52)$$

For example, the Fock state $|01\rangle$ of a chain of $N = 2$ spins read

$$|01\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad (53)$$

and similarly for larger chains. In this representation, the searched fermionic operators are represented by the following matrix tensorial products:

$$b_k = (-1)^{k-1} \underbrace{\sigma^z \otimes \dots \otimes \sigma^z}_{k-1 \text{ terms}} \otimes \sigma^- \otimes \underbrace{\mathbb{1} \otimes \dots \otimes \mathbb{1}}_{N-k \text{ terms}} \quad (54)$$

$$b_k = (-1)^{k-1} \underbrace{\sigma^z \otimes \dots \otimes \sigma^z}_{k-1 \text{ terms}} \otimes \sigma^+ \otimes \underbrace{\mathbb{1} \otimes \dots \otimes \mathbb{1}}_{N-k \text{ terms}} \quad (55)$$

$$(56)$$

where $\sigma^\pm = (\sigma^x \pm \sigma^y)/2$ are rising and lowering operators, expressed in terms of the Pauli matrices $\sigma^{x,y,z}$, and $\mathbb{1}$ is the 2×2 identity matrix.

The calculation of $P(\mathbf{n}|\mathbf{l}, \mathbf{r})$ further requires the calculation of the expectations $\langle \mathbf{l}|\mathbf{s}_L\rangle\langle\mathbf{s}'_L|\mathbf{l}\rangle$, $\langle \mathbf{r}|\mathbf{s}_R\rangle\langle\mathbf{s}'_R|\mathbf{r}\rangle$. The calculation of these proceeds exactly in the same way detailed above, with the only difference that the chain length is now $N/2$ instead of N . With all these expectations one can calculate the probabilities $P(\mathbf{n}|\mathbf{l}, \mathbf{r})$, and, in turn, via Eq. (35), the final quantum entropy.

The performance of the calculation can be greatly improved if one notices the following selection rules

$$2 \sum_{k=1}^N n_k \neq \sum_{j=1}^N s_j + N \implies \langle \mathbf{n}|\mathbf{s} \rangle = 0, \quad (57)$$

$$2 \sum_{k=1}^{N/2} l_k \neq \sum_{j=1}^{N/2} s_j + N/2 \implies \langle \mathbf{l}|\mathbf{s}_L \rangle = 0, \quad (58)$$

$$2 \sum_{k=1}^{N/2} r_k \neq \sum_{j=N/2+1}^N s_j + N/2 \implies \langle \mathbf{r}|\mathbf{s}_R \rangle = 0. \quad (59)$$

Together with Eq. (37) these rules imply that the quench at time $t = 0$ conserves the number of excitations.

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