The distribution of heat exchanged between two quantum spin chains

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We study the distribution of heat values exchanged between two quantum XX chains prepared at different temperatures. It is found that the system approximately obeys the Jarzynski-Wójcik exchange fluctuation theorem for large chain sizes and/or small coupling constant. We also analyze the average heat and find that finite chains do not thermalize, not even on average. In the thermodynamic limit, the other hand, thermalization does occur. However, the average heat as a function of time is not necessarily a monotonically changing function, but may oscillate toward equilibrium depending on the initial temperatures of the chains.

The basic laws of equilibrium statistical mechanics have been established over 100 years ago by Maxwell, Boltzmann, Gibbs and others. These laws allow us to relate the macroscopic properties of matter to the corresponding microscopic configurations, one of the central programs in condensed matter physics. Conversely, the laws describing systems out of equilibrium are still unknown, a fact which has motivated substantial research in the past decades. One of the most promising directions toward understanding non-equilibrium systems concerns the so called fluctuation theorems, which relate probabilities between a certain process and its time reverse. These theorems are valid for systems arbitrarily far from equilibrium and have allowed us to understand in more detail the physics which takes place in non-equilibrium situations. For this reason, in the quest to understand the laws governing systems out of equilibrium, it becomes important to study the fluctuation theorems within the context of specific many-body models.

One particularly interesting fluctuation theorem is that due to Jarzynski and Wójcik. In their setting two systems, 1 and 2, are initially prepared in equilibrium at different temperatures, 1 and 2, and suppose that \( T_2 > T_1 \). The central result in [6] is that:

\[
P_t(Q_1) = e^{\Delta \beta Q_1},
\]

where \( \Delta \beta = \frac{1}{T_1} - \frac{1}{T_2} \). Thus, although heat may flow in both directions, it is exponentially more likely that it will flow from hot to cold. From Eq. (1) it immediately follows that \( \langle e^{-\Delta \beta Q_1} \rangle_t = 1 \) and \( \langle Q_1 \rangle_t \geq 0 \).

We may interpret this as a generalization of the second law of thermodynamics in the Clausius formulation, valid for systems of arbitrary size and in the absence of work: on average, heat flows from hot to cold. It is worth noting that Eq. (1) holds for both classical and quantum systems. For the latter, in particular, a procedure to experimentally measure the heat distribution was recently proposed [18].

The fluctuation theorem in Eq. (1) is true whether or not the two systems eventually thermalize. If this will in fact occur actually depends on the system in question. In fact, all small systems studied so far [11, 19] do not thermalize, not even on average. As for many-body systems, to my knowledge this setup has never been studied, due mainly to the overwhelming complexity of the calculations.

The purpose of this paper is to fill this gap. We consider the case of two quantum XX chains prepared at different temperatures and allowed to interact by an XX coupling, exactly as in the Jarzynski and Wójcik setting. Using perturbation theory in the interaction term we compute both \( P_t(Q_1) \) and \( \langle Q_1 \rangle_t \) for arbitrary chain sizes, including the thermodynamic limit. It is shown that finite systems never thermalize, not even on average. In the thermodynamic limit, however, thermalization does occur. However, even in this case, \( \langle Q_1 \rangle_t \) may not be a monotonically increasing function of \( t \). But rather, it may oscillate toward equilibration.

Two other points motivate the present study. First, Eq. (1) was derived under the approximation that the energy contained in the interaction between the two systems is small. It is therefore interesting to see how this actually manifests itself in a many-body problem. Secondly, while classical many-body systems may always be simulated numerically, the same is not true for their quantum counterparts. It is thus important to search for methods that can be useful for different types of systems. Indeed, the present approach may be readily extended to study a broad variety of fluctuation theorems in a broad number of systems.
We begin by describing the quantum implementation of the Jarzynski and Wójcik fluctuation theorem. Let $H_1$ and $H_2$ be the Hamiltonian of the two systems, with simultaneous eigenbasis $|n\rangle = |n_1, n_2\rangle$ and energies $E_{n_1}^1$ and $E_{n_2}^2$. Each system is initially prepared in thermal equilibrium at temperatures $T_1$ and $T_2$. At $t = 0$ we unplug them from the heat baths and measure their energies. The value $E_{n_1}^1 + E_{n_2}^2$ is thus obtained with probability

$$p_n = \frac{e^{-\beta_1 E_{n_1}^1} e^{-\beta_2 E_{n_2}^2}}{Z_1 Z_2}$$

where $\beta_i = 1/T_i$ and $Z_1$ and $Z_2$ are the corresponding partition functions.

Immediately after this measurement we turn on an interaction $V$ and allow them to evolve unitarily under the total Hamiltonian $H = H_1 + H_2 + V$. After a time $t$ has elapsed we again measure both systems, this time to find the values $E_{n_1}^1$ and $E_{n_2}^2$. We then define the heat that entered each subsystem as

$$Q_1 = E_{m_1}^1 - E_{n_1}^1, \quad Q_2 = E_{m_2}^2 - E_{n_2}^2$$

The probability distribution for $Q_1$ at time $t$ is, therefore,

$$P_t(Q_1) = \sum_{n,m} \langle m|U(t)|n\rangle^2 p_n \delta(Q_1 - (E_{m_1}^1 - E_{n_1}^1))$$

where $U(t) = e^{-iHt}$. A similar formula holds for $P_t(Q_2)$. Due to the enormous number of allowed transitions, actually finding these probabilities for many-body systems is always a very complicated task.

The average heats are $\langle Q_1 \rangle_t = \langle H_1 \rangle_t - \langle H_1 \rangle_0$ and $\langle Q_2 \rangle_t = \langle H_2 \rangle_t - \langle H_2 \rangle_0$, where $\langle H_i \rangle_0 \equiv U(T_{1,2})$ is the internal energy of each system in thermal equilibrium. Since the dynamics is unitary we must have $\langle Q_1 \rangle_t + \langle Q_2 \rangle_t = \langle V \rangle_t - \langle V \rangle_0$. The right-hand side is the energy contained in the interaction. Note that $\langle V \rangle_0$ is the energy required to turn it on at $t = 0$, a process which requires the expenditure of work. In fact, the statistics of the work distribution for this procedure within the context of the XX chain was studied recently in [20] for small chain sizes.

We now apply this to the problem of two one-dimensional XX chains, each with $N$ spins described by Pauli operators $\sigma_i^x$, $\sigma_i^y$ and $\sigma_i^z$. The Hamiltonians $H_1$ and $H_2$, and the interaction term $V$, are:

$$H_1 = \frac{h}{2} \sum_{i=1}^{N} \sigma_i^z + \frac{J}{2} \sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)$$
$$H_2 = \frac{h}{2} \sum_{i=N+1}^{2N} \sigma_i^z + \frac{J}{2} \sum_{i=N+1}^{2N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)$$
$$V = \frac{g_0}{2} (\sigma_N^x \sigma_{N+1}^x + \sigma_N^y \sigma_{N+1}^y)$$

To diagonalize $H_1$ and $H_2$ we introduce Fermionic operators $c_k = \left[ \prod_{j=1}^{k-1} (-\sigma_j^z) \right] \sigma_k^z$, which satisfy $\{c_k, c_l^\dagger\} = \delta_{k,l}$. Then $H_1$ becomes

$$H_1 = h \sum_{k=1}^{N} c_k^\dagger c_k + J \sum_{k=1}^{N} (c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k) = \sum_{k,l=1}^{N} A_{k,l} c_k^\dagger c_l$$

where $A_{k,l} = h \delta_{k,l} + J(\delta_{k+1,l+1} + \delta_{k,l-1})$.

The eigenvalues of $A$ are

$$\lambda_k = h + 2J \cos \left( \frac{\pi k}{N+1} \right)$$

and the corresponding eigenvectors are $x_{k,l} = \sqrt{\frac{2}{N+1}} \sin \left( \frac{\pi k}{N+1} \right)$. If we define a new set of Fermionic operators by means of $b_k = \sum_{j=1}^{N} x_{jk} c_j$, we obtain

$$H_1 = \sum_{k=1}^{N} \lambda_k b_k^\dagger b_k$$

which puts $H_1$ in diagonal form. The procedure for $H_2$ is identical. We choose to number the operators $b_k$ with $k = 1, \ldots, 2N$ so that $H_2 = \sum_{k=1}^{N} \lambda_k b_{k+N}^\dagger b_{k+N}$, whereas $V$ in Eq. (8) becomes

$$V = \sum_{k,l=1}^{N} G_{k,l} (b_k^\dagger b_{l+N} + b_{l+N}^\dagger b_k)$$

with $G_{k,l} = \frac{2g_0}{N+1} \sin \left( \frac{\pi k}{N+1} \right) \sin \left( \frac{\pi l}{N+1} \right)$. This equation has a simple physical interpretation: each term in $V$ destroys a $b$-fermion in one chain and creates a $b$-fermion in the other. Note also that $V$ depends on $g = 2g_0/(N+1)$, which will be small if either $g$ is small or $N$ is large.

Since quadratic forms of Fermionic operators commute, the partition function becomes simply $Z_1 = \prod_{k=1}^{N} (1 + e^{-\beta_1 \lambda_k})$ and the internal energy of each chain reads

$$U(T) = \sum_{k=1}^{N} \frac{\lambda_k}{\exp(\lambda_k/T) + 1} = \sum_{k=1}^{N} \lambda_k E_k(T)$$

where $E_k(T)$ is the internal energy of the $k$th chain.
where $E_k(T) = (e^{\lambda_k/T} + 1)^{-1}$ and $T$ may be either $T_1$ or $T_2$. These formulas may be approximated by integrals in the thermodynamic limit. But we shall not do that now since we are interested in chains of any size.

The energy eigenvalues of each chain can be divided in bands containing different numbers of b-fermions. This is illustrated in Fig. 1(a) for $J = 1$ and $h = 10$. The zeroth band contains only the ground state with zero energy and no b-fermions. The first band contains a single b-fermion with a total of $N$ energy levels of the form $\lambda_k$. The second band contains 2 b-fermions with $N(N - 1)/2$ levels of the form $\lambda_k + \lambda_{\ell}$. And so on and so forth. When $h$ is small the bands will overlap, but when $h$ is large a band gap may form between the first few bands, as illustrated in the figure.

The total Hamiltonian $H = H_1 + H_2 + V$ conserves the number of b-fermions in the two chains combined. In other words, $H$ factors into subspaces containing fixed numbers of b-fermions. This strongly restricts the allowed transitions in $\langle m|U(t)|n \rangle$ [cf. Eq. (1)]. Unfortunately, however, this alone does not suffice for the computation of $P_t(Q_1)$ since the number of possible transitions is still overwhelming.

However, if we assume that the temperature is low and $h$ is large (so as to induce a band gap), the thermal probabilities $p_\ell$ [Eq. (2)] for exciting states to the second or higher bands will be overwhelmingly smaller than the probability of excitation to the first band. If this is the case, we may focus only on those transitions where the composite chain starts with a single b-fermion. This sub-

space has dimension $2N$ and may be described by the Fock basis $\{|k, 0\}, |0, k\}$. Under this approximation, the allowed values of $Q_1$ are reduced to three categories. In the first, chain 1 started with zero b-fermions and, after a time $t$, acquired a single b-fermion from chain 2. This is represented by a transition of the form $|0, k\rangle \rightarrow |\ell, 0\rangle$ leading to $Q_1 = \lambda_{\ell}$ and

$$P(Q_1 = \lambda_{\ell}) = \sum_{k=1}^{N} |\langle \ell, 0|U|0, k\rangle|^2 e^{-\beta_2 \lambda_k} Z_1 Z_2$$

The second possibility is that chain one started with one b-fermion and, after a time $t$, lost it to chain 2. In this case $Q_1 = -\lambda_{\ell}$ and

$$P(Q_1 = -\lambda_{\ell}) = \sum_{k=1}^{N} |\langle 0, \ell|U|k, 0\rangle|^2 e^{-\beta_1 \lambda_k} Z_1 Z_2$$

Finally, there is the possibility that chain 1 started with a b-fermion of energy $\lambda_k$ and, after a time $t$, continued to have a single b-fermion but now with energy $\lambda_{\ell}$. In this case we would have $Q_1 = \lambda - \lambda_k$ and

$$P(Q_1 = \lambda - \lambda_k) = \sum_{k=1}^{N} |\langle 0, k|U|k, 0\rangle|^2 e^{-\beta_1 \lambda_k} Z_1 Z_2$$

Of course, there is also the probability that $Q_1 = 0$, which may occur in several ways, including the case where both chains started with no b-fermions. But we may simply take this probability as a normalization constant.

To compute the transition probabilities appearing in Eqs. (13)-(16) we first note that in the basis $\{|k, 0\}, |0, k\}$, the total Hamiltonian $H$ reads

$$H^{(3)} := W = \begin{bmatrix} \Lambda & G \\ G^T & \Lambda \end{bmatrix}$$

where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_N)$ and $G$ is the matrix with entries $G_{k\ell}$ [cf. Eq. (1)]. The off-diagonal entries depend on $g$ and may thus be treated perturbatively by assuming that either the interaction strength $g_0$ is small, or that the system size $N$ is large (recall that $g = 2g_0/(N + 1)$).

When $g = 0$ (no interaction) the eigenstates $|k, 0\rangle$ and $|0, k\rangle$ of $W$ are degenerate with energy $\lambda_k$. The presence of $G$ lifts this degeneracy. Using degenerate perturbation theory [22] within these two-dimensional subspaces, we find that the perturbed energies are, to first order in $g$, $\omega_k = \lambda_k + sG_k$ where $G_k = G_{kk}$ and $s = \pm 1$. The new eigenvectors are $|\omega_k^\pm\rangle = \frac{1}{\sqrt{2}}(|k, 0\rangle + s|0, k\rangle)$.

With these results the transition probabilities become

$$|\langle \ell, 0|U(t)|0, k\rangle|^2 = \delta_{k, \ell} \sin^2(G_{k\ell} t) + O(g^2)$$

$$|\langle \ell, 0|U(t)|k, 0\rangle|^2 = \delta_{k, \ell} \cos^2(G_{k\ell} t) + O(g^2)$$

We indicate that the next correction will be of order $g^2$, as can be inferred by extending the perturbation theory to
higher orders. The actual formulas are too cumbersome and have thus been omitted. We only note that these terms contain off-diagonal elements.

Inserting Eqs. (17) and (18) in Eqs. (13)-(15) yields

\[ P_t(Q_1 = \lambda_k) = \frac{e^{-\beta_2 \lambda_k}}{Z_1 Z_2} \sin^2(G_k t) + \mathcal{O}(g^2) \quad (19) \]

\[ P_t(Q_1 = -\lambda_k) = \frac{e^{-\beta_2 \lambda_k}}{Z_1 Z_2} \sin^2(G_k t) + \mathcal{O}(g^2) \quad (20) \]

\[ P_t(Q_1 = \lambda_k - \lambda_k) = \mathcal{O}(g^2) \quad (21) \]

We see that to first order in \( g \) the only allowed transitions are of the form \(|k,0\rangle \rightarrow |0,k\rangle \) and vice-versa. In these transitions no energy is placed in the interaction term \( V \) so that \( \langle Q_1 \rangle_t = -\langle Q_2 \rangle_t \). Consequently, these probabilities satisfy the fluctuation theorem in Eq. (11):

\[
\frac{P_t(Q_1 = \lambda_k)}{P_t(Q_1 = -\lambda_k)} = e^{\Delta \beta \lambda_k} + \mathcal{O}(g^2)
\]

The distribution of \( P_t(Q_1) \) is illustrated in Fig. 1(b) and (c) for \( N = 300 \) at two different times. See also the videos in the supplementary material. Of course, the probability is not exactly zero in the middle region, but it is of order \( g^2 \) and thus negligible when \( g \) is small.

The average heat may be computed from Eqs. (19) and (20). It reads

\[
\langle Q_1 \rangle_t = \frac{1}{Z_1 Z_2} \sum_{k=1}^{N} \lambda_k (e^{-\beta_2 \lambda_k} - e^{-\beta_1 \lambda_k}) \sin^2(G_k t) \quad (22)
\]

The behavior of \( \langle Q_1 \rangle_t \) as a function of time is presented in Fig. 2 for different chain sizes. The result is divided by \( q_1 \), Eq. (3), which is the total heat that would have been exchanged if the two systems had thermalized. As can be seen, finite systems never thermalize. The larger the size, the larger is the amount of time that heat can be exchanged in a monotonically ordered fashion. For all sizes, however, there eventually comes a point where intense oscillations start and never seize. This instant of time increases with size. We also see that the heat evolves with a characteristic relaxation time

\[
\tau = \frac{1}{g} = \frac{N+1}{2g_0} \quad (23)
\]

This is in agreement with what is expected from classical thermodynamics \( \tau \), where the relaxation time is of the order of the dimension of the system. We illustrated this in the inset of Fig. 2 which shows the same data as the main figure, but plotted against \( gt \) instead of \( t \).

Before we analyze the thermodynamic limit, we shall first find a formula for \( \langle Q_1 \rangle_t \) that is valid for any temperature (but which is still calculated perturbatively in \( g \)). This equation will reduce to Eq. (22) in the particular case where both temperatures are low. Let \( \theta_{kl} = \langle b_k^\dagger b_l \rangle \).

Then it can be shown that

\[
\frac{d\theta}{dt} = i[W, \theta] \quad (24)
\]

where \( W \) is the matrix defined in Eq. (16). This equation is exact. It is subject to the initial condition that both chains are initially in equilibrium, which translates to

\[
\theta(0) = \begin{bmatrix} E(T_1) & 0 \\ 0 & E(T_2) \end{bmatrix}
\]

where \( E(T) \) are diagonal matrices with entries \( E_k(T) \) [cf. Eq. (24)].

Using the same perturbation method as before we now find

\[
\langle Q_1 \rangle_t = \sum_{k=1}^{N} \lambda_k [E_k(T_2) - E_k(T_1)] \sin^2(G_k t) \quad (25)
\]

which clearly reduces to Eq. (22) at low temperatures. Within the same approximation we get \( \langle Q_2 \rangle_t = -\langle Q_1 \rangle_t \).

In the thermodynamic limit \( (N \rightarrow \infty) \) we may approximate the sum in Eq. (25) by an integral; viz,

\[
\langle Q_1 \rangle_t = \frac{N}{\pi} \int_0^\pi dx \lambda(x)[E(T_2, x) - E(T_1, x)] \sin^2(g_0 t \sin^2 x) \quad (26)
\]

where \( \lambda(x) = h + 2J \cos(x) \). The only assumption in computing this result is that \( g \) is small. In the thermodynamic limit this is certainly true since \( g = 2g_0/(N+1) \).

Hence we conclude that Eq. (26) becomes exact in the thermodynamic limit. If \( gt \rightarrow \infty \) the sine term in the integral will oscillate very rapidly with \( x \) and we may replace \( \sin^2(g_0 t \sin^2 x) \simeq 1/2 \). This gives \( \langle Q_1 \rangle_\infty = q_1 \), as
shown in Eq. [5]. Hence, in the thermodynamic limit the system does thermalize.

The average heat in the thermodynamic limit is presented in Fig. 3 for different values of $\beta_1$ with $\beta_2 = \beta_1 - 0.1$. As can be seen, at low temperatures the average heat increases monotonically toward the new equilibrium value. However, for higher temperatures, it is seen to oscillate toward equilibrium, with the oscillations becoming larger as the temperature is increased further. Despite the oscillatory behavior, thermalization always takes place in the thermodynamic limit, albeit much more slowly.

The derivation of Eq. (26) did not require the assumption of large $h$ (which was previously used to induce a band gap). Hence, we may study $\langle Q_1 \rangle_t$ for different values of $h$. Results for $h = 0$ are shown in the inset of Fig. 3. As can be seen, the situation now reverses: the lower the temperature, the larger are the oscillations. This transition occurs at $h = 1$, which is precisely where the system undergoes a quantum phase transition (at $T = 0$) from a ferromagnetic to a paramagnetic phase.

FIG. 3. $\langle Q_1 \rangle_t$ in the thermodynamic limit for different values of $\beta_1$ and $\beta_2 = \beta_1 - 0.1$, with $J = 1$, $h = 10$ and $g_0 = 0.1$. The inset shows the same thing, but for $h = 0$.

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