Energy flux near the junction of two Ising chains at different temperatures

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Abstract – We consider a system in a non-equilibrium steady state by joining two semi-infinite Ising chains coupled to thermal reservoirs with different temperatures, \( T \) and \( T' \). To compute the energy flux from the hot bath through our system into the cold bath, we exploit Glauber heat-bath dynamics to derive an exact equation for the two-spin correlations, which we solve for \( T' = \infty \) and arbitrary \( T \). We find that, in the \( T' = \infty \) sector, the in-flux occurs only at the first spin. In the \( T < \infty \) sector (sites \( x = 1, 2, \ldots \)), the out-flux shows a non-trivial profile: \( F(x) \). Far from the junction of the two chains, \( F(x) \) decays as \( e^{-x/\xi} \), where \( \xi \) is twice the correlation length of the equilibrium Ising chain. As \( T \to 0 \), this decay crosses over to a power law \( (x^{-3}) \) and resembles a “critical” system. Simulations affirm our analytic results.

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Introduction. – Equilibrium statistical mechanics, formulated by Boltzmann, Gibbs, and others about a century ago, is so well established that today, it is part of the core material in typical physics programs. By contrast, statistical mechanics of systems far from equilibrium is so poorly understood that the Committee on CMMF 2010 of the National Research Council recently recognized it as one of the six most fundamental and important challenges in condensed matter and materials physics [1]. To be clear, we should distinguish two types of such systems. On the one hand, we may encounter a statistical system evolving with a dynamics which obeys detailed balance. Though it will eventually settle into an equilibrium state and can be described within the Boltzmann-Gibbs framework, its time-dependent behavior can be highly non-trivial. Good examples are slow relaxation or practically stationary states, such as aging [2] or glassy phenomena [3]. On a more difficult level, we may face a system with a dynamics which violates detailed balance. Examples abound in, e.g., the life sciences, sociology, or economics, for which macroscopic variables are more appropriate. Typically, the rules for their evolution do not obey time reversal. Even when such a system settles into a time-independent steady state, its stationary distribution is unknown in general. Much of the intuition built on equilibrium statistical mechanics fails under these circumstances. In an effort to develop insight into this class of non-equilibrium steady states (NESS), we take model systems with especially simple equilibrium properties and drive them out of equilibrium by mechanisms which are physically well motivated.

A good example of a simple model driven far from equilibrium is the kinetic Ising model, coupled to two thermal reservoirs set at different temperatures [4–8]. In previous studies, translational invariance is kept as much as possible, e.g., every other spin being updated according to the same reservoir [5,6]. As a result, the effects of being driven out of equilibrium are extensive. In this article, we study another, perhaps more common, way of coupling a system to two baths, namely, one side being kept hot and the other, cold. Specifically, we consider an Ising chain (i.e., a one-dimensional lattice with sites \( x = \ldots, -1, 0, 1, \ldots \) in which all spins with \( x \leq 0 \) are coupled to one bath while the rest are coupled to another bath. Alternatively, we can view this system as joining together two Ising chains, each being in contact with its own thermal bath. The coupling of the two spins at the ends \( (x = 0, 1) \) allows the flow of energy from the hotter bath to the cooler one, as illustrated in fig. 1.

Recently, a simpler version of this model has been investigated [9]. On a ring of \( 2N + 1 \) spins (i.e., periodic
Fig. 1: (Colour on-line) We consider two semi-infinite chains of Ising spins (red and blue) that only assume the two values $\sigma_x = \pm 1$, which we denote by “+” and “−” signs. The two boxes labeled $T'$ and $T$, with $T' > T$ represent the two thermal reservoirs to which we couple the two Ising spin chains. The red (blue) arrows denote the energy flux flowing into (out of) the chain. Narrower arrows denote a smaller flux.

The model. – In a kinetic Ising chain, spins are located on sites (labeled by an integer $x$) of a discrete lattice and assume only two values: $\sigma_x = \pm 1$. Thus, a configuration of this system is described by the set of spins $\{\sigma_x\}$. Each spin interacts with its two neighbors via the Hamiltonian: $H(\{\sigma_x\}) = -J \sum_x \sigma_x \sigma_{x+1}$, where $J$ is a coupling constant. For a finite system, boundary conditions are needed, the simplest being periodic.

While in contact with a thermal bath at temperature $T$, the kinetic Ising chain has a simple equilibrium distribution: $P_{eq}(\{\sigma_x\}) = e^{-\mathcal{H}(\{\sigma_x\})}/Z$. Its static properties (e.g., the partition function $Z$) were obtained first by Ising [12]. Its dynamical properties, on the other hand, are much more complex since they depend sensitively on how the system is endowed with time dependence. The simplest is Glauber spin-flip “heat-bath” dynamics [10]. In a Monte Carlo simulation with parallel updates, each spin $\langle \tilde{\sigma}_x \rangle$ is chosen and reset to be $\sigma_x$, with a probability that depends only on the average of its two neighboring spins: $p_x \equiv \frac{1}{2} + \gamma \sigma_x (\tilde{\sigma}_{x-1} + \tilde{\sigma}_{x+1})/4$, with $\gamma = \tanh(2J/k_BT)$. Thus, with $J$, $\gamma > 0$, the new spin will tend to be more aligned $(1+\gamma)/2$ with its neighbors than anti-aligned $(1-\gamma)/2$. The standard framework to deal with dynamics is based on the master equation for a time-dependent $P(\{\sigma_x\},t)$. In this approach, we have $P(\{\sigma_x\},t+1) = \sum_{\{\tilde{\sigma}\}} \prod_x p_x P(\{\tilde{\sigma}_x\},t)$, and at large times, the system settles into the stationary $P_{eq}(\{\sigma_x\})$. A favorite alternative update is random sequential, where only one randomly chosen spin is updated at each time step. We will use this method for the “two-temperature” Ising chain below.

One way to drive this kinetic Ising chain out of equilibrium is to couple it to more than one thermal bath. The simplest generalization is to have two baths, at $T$ and $T' > T$. Even with this simplification, there is an infinite variety of ways to couple the spins to them. One is to update each spin the same way, randomly choosing $T$ and $T'$ with fixed probabilities [4]. On average, $\gamma$ remains homogeneous and the intuitive picture of the system—same as in equilibrium but with an effective $\gamma$—proves to be correct. One may alternatively couple the two baths to every other spin [6-8,13], so that we should write $\gamma_x$ in the $p_x$ above. The master equation then takes the form

$$P(\{\sigma_x\},t+1) = \sum_{\{\tilde{\sigma}\}} W(\{\sigma_x\};\{\tilde{\sigma}_x\}) P(\{\tilde{\sigma}_x\},t),$$

(1)

where $W$ is given by

$$N^{-1}_{tot} \sum_x \left[ \frac{1}{2} + \gamma_x \sigma_x \left( \frac{\tilde{\sigma}_{x-1} + \tilde{\sigma}_{x+1}}{4} \right) \right] \prod_{y \neq x} \left[ 1 + \frac{\sigma_y \tilde{\sigma}_y}{2} \right].$$

(2)

Here, $N_{tot}$ is the total number of spins in the system, so that $N^{-1}_{tot} \sum_x$ accounts for the possibility of any spin being chosen, with equal probability, once per time step. The $\prod_{y \neq x}$ factor insures that all other spins remain unchanged. For the model in [6], we have, say, $\gamma_x = \tanh(2J/k_BT)$ and $\gamma_{2n+1} = \tanh(2J/k_BT')$ with integer $n$. A prominent aspect of this model is the non-trivial energy flux through the system, flowing from the hotter bath to the colder one. In particular, many of the properties of the energy transferred to the baths due to the updating of the
spins can be computed exactly [6,8]. Entropy production (associated with the two baths) can be defined and also computed. Due to the translationally invariant nature of the alternating couplings, both the total flux and entropy production are extensive.

In this study, we consider another way to couple the Ising chain to two baths, namely,

\[
\gamma_x \leq 0 = \tanh(2J/k_BT) \equiv \gamma', \quad (3)
\]

\[
\gamma_x > 1 = \tanh(2J/k_BT) \equiv \gamma. \quad (4)
\]

In other words, each of the two sectors of the chain is updated with a single temperature, with the left sector being hotter \((T' > T)\). This is a much more common form of coupling a system to two baths, occurring, for example, in stovetop cooking. Of course, this model is still far from being realistic, since heat is typically transported, via diffusion, from the hotter side to the colder one. Here, due to the local nature of the spin-bath coupling, non-trivial energy transfer is expected to take place close to the junction and the anomalies associated with non-equilibrium statistical mechanics should vanish for \(|x| \gg 1\). Now, translational invariance is broken and the analysis is more complex. In the next section, we provide a solution to the problem, in terms of the two-spin correlation function \((\sigma_x \sigma_y)\). Simulation data will also be presented for the case \(T' = \infty\) (\(\gamma' = 0\)), showing a consistent picture of the inhomogeneous energy flux.

Before ending, let us remark that we will, for simplicity, ignore the boundary conditions. A more rigorous way is to start with open boundaries, write modified expressions for the end spins, and ensure that they make no difference in the limit of large \(N_{\text{tot}}\). Alternatively, we can impose periodic boundary conditions, deal with two junctions, and check that the effects of the two disentangle appropriately.

**Theoretical analysis and simulation results.**

For \(W\)’s which violate detailed balance, it is generally impossible to find an explicit expression for the stationary distribution \(P^*(\{\sigma_x\})\), i.e. the solution to \(P^* = \sum W P^*\). A formal solution exists [14], but it is so cumbersome that typically, useful information cannot be extracted. An alternative approach is to seek the correlations functions in the steady state

\[
\langle \sigma_{x_1} \ldots \sigma_{x_k} \rangle \equiv \sum_{\{\sigma_x\}} \sigma_{x_1} \ldots \sigma_{x_k} P^* (\{\sigma_x\}). \quad (5)
\]

Inserting this definition into the equation for \(P^*\), we face the sum \(\sum_{\{\sigma_x\}} \sigma_{x_1} \ldots \sigma_{x_k} W (\{\sigma_x\}; \{\sigma_x\})\) which, in general, involves \(k' > k\) spins (\(\delta_s\)’s). Writing an equation for the \(k'\)-spin correlation, we encounter more spins. The result is the BBGKY hierarchy [15] involving correlations of arbitrarily many spins. However, \(W\) is linear in its arguments in our case (a salient feature of “heat-bath” dynamics), so that coupled equations do not proliferate. In particular, we find

\[
\sum_{\{\sigma_x\}} \sigma_a W = \frac{\gamma_a}{2} (\delta_{a-1} + \delta_{a+1}) + (N_{\text{tot}} - 1) \delta_a. \quad (6)
\]

We now replace the dummy \(\delta_a\) by \(\sigma_x\) and average both sides of eq. (6). The \(N_{\text{tot}}\) variable cancels and we obtain

\[
0 = \gamma_x \langle \sigma_{x-1} + \sigma_{x+1} \rangle - 2 \langle \sigma_x \rangle \quad (7)
\]

(with slight modification for the spins at the ends of the chain). Unless \(\gamma_x = 1\), the only solution to this equation is \(\langle \sigma_x \rangle = 0\). This result is hardly surprising, especially since an ordinary Ising chain displays no spontaneous magnetization for all positive temperatures.

Turning to the two-point function, we first note

\[
\langle \sigma_x \sigma_x \rangle = 1 \quad (8)
\]

and

\[
\langle \sigma_x \sigma_y \rangle = \langle \sigma_y \sigma_x \rangle \quad (9)
\]

so that we can focus on, say, \(x < y\) only. There, we obtain

\[
0 = \gamma_x (\langle \sigma_{x+1} \sigma_y \rangle + \langle \sigma_{x-1} \sigma_y \rangle) + \gamma_y (\langle \sigma_x \sigma_{y+1} \rangle + \langle \sigma_x \sigma_{y-1} \rangle) - 4 \langle \sigma_x \sigma_y \rangle. \quad (10)
\]

It is easy to verify that, for \(\gamma_x = \gamma_y = \gamma\), a familiar result emerges, i.e., \(\langle \sigma_x \sigma_y \rangle = \omega^{x-y}\), with \(\omega \equiv \tanh(J/k_BT)\).

Before we solve equation eq. (10), let us remark that all correlations with an odd number of spins vanish. Further, with our dynamics, correlations of any even number of spins can be expressed in terms of products of \(\langle \sigma_x \sigma_y \rangle\) [6,7,13,16,17]. In this sense, we have a complete picture of this non-equilibrium system.

Returning to our problem, we see it is a generalized, discrete Helmholtz equation and so, boundary conditions (BCs) are crucial. One BC is eq. (8) and the other is \(\langle \sigma_x \sigma_y \rangle \rightarrow 0\) for \(|x - y| \rightarrow \infty\). In other words, we have Dirichlet BCs for the half-space \(x \geq y\). In our case, we have only two \(\gamma\)’s. Thus, this domain can be partitioned into three regions, \(R_{++}, R_{-+}\), and \(R_{+-}\) (corresponding to \(x, y\) being positive or negative, as shown in fig. 2), in each of which the operator is homogenous. Thus, the solution can be attacked by standard, though tedious, methods. We will only indicate some key points for the general problem and provide a few more details below for the special case of \(T' = \infty\), i.e., \(\gamma' = 0\).

![Energy flux near the junction of two Ising chains at different temperatures](image-url)
Note that the operator in eq. (10) is isotropic in \( R_{++} \) and \( R_{--} \), but anisotropic in \( R_{+-} \). Since the operators are homogeneous (discrete) Laplacians within each region, we can make use of the eigenfunctions \( e^{ikx + ipy} \) with eigenvalues \( 2(\gamma_x \cos k - 1) + 2(\gamma_y \cos p - 1) \). In the regions \( R_{--} \) and \( R_{++} \), appropriate combinations must be chosen to satisfy eqs. (8), (9). The last BC is less straightforward and we will rely on the following approximation. We choose functions which vanish on the \( x = N \) line in \( R_{++} \) and the \( y = -N \) line in \( R_{--} \), and then let \( N \to \infty \) at the end. Such an approach can also be exploited in \( R_{+-} \). Finally, we must match the functions on the common boundaries \( (x = 0 \text{ and } y = 0 \text{ lines, i.e. the green lines in fig. 2}). \)

Let us consider an easier case, \( \gamma' = 0 \), so we have only one parameter left: \( \gamma \). Equation (10) immediately provides

\[
\langle \sigma_x \sigma_y \rangle = 0 \quad \text{for } y < x \leq 0,
\]

which is quite reasonable for \( R_{--} \) where spins are flipped completely randomly. Next, in \( R_{++} \), this equation simplifies to a single one, \( \langle \sigma_x \sigma_y \rangle + \langle \sigma_y \sigma_x \rangle = 4 \langle \sigma_x \sigma_y \rangle / \gamma \), for all \( y \leq 0 \) (and \( x > y \)). It is satisfied by \( \langle \sigma_x \sigma_y \rangle = e^{\mu x} \), with (real) \( \mu = \pm \cosh^{-1}(2/\gamma) \). To be careful, let us first focus on \( y < 0 \). From eq. (11) above, we have \( \langle \sigma_x \sigma_y \rangle = 0 \), which restricts us to \( \langle \sigma_x \sigma_y \rangle = A \sinh \mu x \). Imposing the BC for \( x \to \infty \), we arrive at

\[
\langle \sigma_x \sigma_y \rangle = 0, \quad \forall \ x > y.
\]

On the line \( y = 0 \), we have a different BC, since \( \langle \sigma_0 \sigma_0 \rangle = 1 \). The other BC then picks out

\[
\langle \sigma_x \sigma_0 \rangle = \bar{\omega}^x, \quad \forall \ x \geq 0,
\]

where

\[
\bar{\omega} \equiv \frac{2}{\gamma} - \sqrt{\left( \frac{2}{\gamma} \right)^2 - 1}.
\]

In other words, this particular correlation is of the same form as that for the Ising chain in equilibrium, with an effective temperature given by \( \gamma/2 \) instead of \( \gamma \). Intuitively, this result is appealing, since one spin \( \langle \sigma_0 \rangle \) is coupled to \( \gamma' = 0 \) and the other \( \langle \sigma_\gamma \rangle \) is coupled to \( \gamma \).

Finally, we turn our attention to \( R_{++} \). Here, eq. (10) is exactly the same as for the equilibrium Ising chain. Indeed, the only difference between the two problems is the BC on the \( y = 0 \) line, where we have eq. (13) instead of \( \langle \sigma_x \sigma_0 \rangle_{eq} = \omega^x \). Thus, we can simplify our problem by considering the difference

\[
S(x, y) \equiv \langle \sigma_x \sigma_y \rangle - \langle \sigma_x \sigma_y \rangle_{eq}
\]

which vanishes on two of the three boundaries of \( R_{++} \). A further advantage is that \( S \) is directly related to the quantity of interest — the flux, \( F(x) \), i.e., the average rate of energy loss when \( \sigma_x > 0 \) is updated. Specifically, from [6], one can show that

\[
F(x) = \frac{1}{4} \left[ \gamma S(x + 1, x - 1) - S(x + 1, x) - S(x, x - 1) \right].
\]
some results here. We find that eq. (23) for integers $x \geq 2$ reduces exactly to

$$F(x) = \frac{1}{\pi \gamma^{2x+1}} \int_0^1 \frac{1 - \gamma^2 \eta^4}{\eta^{2x} (1 - \gamma^2 \eta^2 + \gamma^2 \eta^4)} \left(1 - \gamma^2 \eta^2 - \gamma^2 \eta^4\right)^{2x} d\eta,$$

(25)

with a known correction for $x = 1$ [11]. To get the crossover behavior as $\gamma \rightarrow 1$ ($T \rightarrow 0$), we can arrange an asymptotic expansion of eq. (25) (for large $x$) as a sum over modified Bessel functions

$$F(x) = x^{-1} \sum_{n=0}^\infty B_n \zeta^{-n} e^\zeta K_{n+1} (\zeta),$$

(26)

where $\zeta = 2\sqrt{1 - \gamma^2}x$ and $B_n$ are explicitly known coefficients.

Intuitively, we expect $F$ to decay exponentially for $T > 0$, where the equilibrium correlation length, $\xi \equiv -1/\ln \omega$, is finite. Careful analysis [11] confirms this picture. In particular, eq. (26) leads to

$$F(x) \rightarrow \frac{1}{4} \sqrt{\frac{(1 - \omega^2)5}{\pi \omega^2 (1 + \omega^2)^3}} \omega^{2x} e^{\sqrt{x}} \{1 + O(x^{-1})\}.$$

(27)

Interestingly, we observe that the decay length is $\xi/2$, though we have no good heuristic explanation. In the extreme case of $T = 0$, these complex expressions simplify and a power law appears. The result is

$$\lim_{\gamma \rightarrow 1} F(x) = \frac{1}{2\pi x^3} + \ldots.$$

(28)

Though reminiscent of the crossover to critical exponents, we also have no simple argument in favor of the specific value $-3$. Of course, the total steady flux is finite, so that $\Sigma_{x>0} F(x)$ must converge. But this constraint only limits the power to be less than $-2$.

As further confirmation of these analytic results, we performed Monte Carlo simulations of our system. For $T' = \infty$, it is unnecessary to include any spin at $x < 0$. Instead, we study a chain with $N + 1$ spins, the first (or zero) being coupled to the infinite temperature bath. At each step, a random spin is chosen and assigned a new value according to the probabilities given above, except zero, which is assigned $\pm 1$ randomly. Using $N \approx 30$, we evolved the system for approximately $10^6$ time steps (i.e., updates per spin). When a spin flips during an update, we record the change in the energy $\Delta E$, which can take only the values $0$ and $\pm 1$ (in units of $4J$). In this manner, we have a time series $\Delta E(x, t)$ for each site. It is clear that, over a run, this quantity essentially performs a random walk. For systems in equilibrium, such walks will be unbiased. For our case, we expect biased walks. To verify this scenario, we carried out $10^5$ independent runs and computed both the average, $\Delta E(x, t)$, and the variance $[\Delta E(x, t)]^2 - (\Delta E(x, t))^2$. As illustrated in fig. 3, both the average and the variance increase with $t$ linearly (i.e., $a \approx 1$). The intercept, $b$, of the former provides us with data to compare with $F(x)$. Similarly, the intercept of the latter allows us to estimate the error bars in fig. 4. Figure 4 shows the excellent agreement with theoretical predictions and simulations.

Finally, we remark that we did not present results for the in-flux of energy, which occurs only at $x = 0$, since there are no correlations involving $\sigma_x < 0$. It is clear that its value must be just $\Sigma_{x>0} F(x)$.

Summary and outlook. – In this article, we consider joining together two Ising chains end-to-end, each coupled to a uniform (but different) temperature reservoir. As a result, when the system settles into a steady state, there is a constant flow of energy through the system, from the hotter to the colder bath. Far from the junction,
each sector of the chain is expected to behave as one in equilibrium, so that the effects of this energy flow are localized. Such a through-flux is strictly a non-equilibrium phenomenon and the stationary distribution is not simply given by some spatially dependent, effective Boltzmann factor. By choosing heat-bath spin-flip dynamics, we are able to compute all the correlation functions. In particular, we provide key points for the calculation and the results for the two-spin correlation, $\langle \sigma_x \sigma_y \rangle$. This is not simply a function of $|x - y|$, since our system is not translationally invariant. From these functions, we can compute $F(x)$, the steady flux of energy out of the system, as a result of updating the spin at $x$. When one reservoir is set at $T' = \infty$, we find explicitly that $F(x)$ decays into the sector with $T < \infty$ exponentially, with a length half of the correlation length of its equilibrium counterpart. As $T \to 0$, there is no such counterpart, as the decay crosses over to a power law: $1/x^3$. Simulations of this model verify these results.

Before closing, let us consider possible future studies, as well as related Ising-like systems far from equilibrium. The most immediate case of interest is finite $T'$, analytic results for which should be within reach. There, we expect exponentials for $F(x)$ in both sectors. It is not clear if the decay lengths continue to be as simple as what we found. In particular, $F$ must vanish as $T' \to T$. Whether this limit appears as an overall amplitude which vanishes, analytically with $(T' - T)^2$ or more singularly, would be interesting. Beyond the Ising chain, the most obvious generalization is the same model in higher dimensions, joining two systems side by side, say. Since the ordinary Ising model at equilibrium displays phase transitions in higher dimensions, more interesting questions arise. Examples include: Does $F$ decay with singular powers when $T$ is set at $T_c$, the critical temperature (with $T' > T_c$)? If so, are there new exponents (such as the dynamic exponent $z$ in model A [18]) or new combinations of existing exponents (such as $z = 4 - \eta$ in model B [18])? Setting $T < T_c$, we could expect a non-trivial magnetization profile $\langle \sigma_x \rangle$. How does it decay with $x$? Continuing along these lines, are there new singularities associated with this profile when $T'$ is lowered to $T_c$?

Another generalization of joining two Ising systems is also immediate: using Kawasaki spin-exchange dynamics [19] instead. While no new static properties are present in an equilibrium Ising model with this type of dynamics, much more surprising behavior for the two-temperature case have been observed, for both 1- and 2-d systems [20]. Beyond these, there are limitless varieties, most of which will undoubtedly provide further insight into how we may proceed in attempting to formulate an overarching principle for non-equilibrium statistical mechanics.

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