Getting More from Pushing Less: Negative Specific Heat and Conductivity in Non-equilibrium Steady States

R. K. P. Zia\textsuperscript{1,2}, E. L. Praestgaard\textsuperscript{3} and O. G. Mouritsen\textsuperscript{4}
\textsuperscript{1}Center for Stochastic Processes in Science and Engineering
Department of Physics
Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0435, USA
\textsuperscript{2}Fachbereich Physik, Universität - Gesamthochschule Essen,
D-45117 Essen, Federal Republic of Germany.
\textsuperscript{3}Department of Life Sciences and Chemistry, Roskilde University
4000 Roskilde, Denmark
\textsuperscript{4}Physics Department, University of Southern Denmark-Odense
Campusvej 55, DK-5230 Odense M, Denmark
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ABSTRACT

For students familiar with equilibrium statistical mechanics, the notion of a positive specific heat, being intimately related to the idea of stability, is both intuitively reasonable and mathematically provable. However, for system in non-equilibrium stationary states, coupled to more than one energy reservoir (e.g., thermal bath), negative specific heat is entirely possible. In this paper, we present a "minimal" system displaying this phenomenon. Being in contact with two thermal baths at different temperatures, the (internal) energy of this system may increase when a thermostat is turned down. In another context, a similar phenomenon is negative conductivity, where a current may increase by decreasing the drive (e.g., an external electric field). The counter-intuitive behavior in both processes may be described as "getting more from pushing less." The crucial ingredients for this phenomenon and the elements needed for a "minimal" system are also presented.

I. INTRODUCTION

To most physicists, it is intuitively reasonable that the average internal energy, $U$, of a system in contact with a thermal bath should increase with $T$, the bath temperature. For those well versed with equilibrium statistical mechanics, it is trivial to prove this statement, usually in the form of the specific heat, $\partial U/\partial T$, being positive. Indeed, this notion is so deeply rooted in the idea of stability that its contrary may be rejected immediately, even for non-equilibrium steady states. In this paper, we show the presence of a negative specific heat in a minimal system, coupled to two thermal baths at different temperatures. We also point out a crucial ingredient which makes this phenomenon possible, namely, the presence of "barriers" which trap the system in a higher energy state. In a similar vein, we discuss negative conductivity, using again a simple model to demonstrate the phenomenon of increasing current by decreasing the drive (e.g., an external electric field). Here too, a crucial ingredient is the presence of "obstructions" which trap the system in a low current state. Noting that both processes involve a similar idea, we coin a "folksy" phrase – getting more from pushing less – to describe this class of counter-intuitive behavior.

We begin with a brief summary of standard equilibrium statistical mechanics, for which no dynamics is needed. In contrast, for non-equilibrium steady states, the underlying dynamics (which leads a system into such states) is crucial. The most convenient framework for describing both scenarios is the master equation, which we review in the next section, for the convenience of those readers unfamiliar with this approach. In this context, a clear distinction between equilibrium and non-equilibrium steady states will be presented. In section 3, we display the presence of negative specific heat in some minimal systems and a more typical, many-body system, which are coupled to two thermal baths. Similarly, negative conductivity is shown to arise in a simple hopping model in Section 4. Concluding in the last section, we recapitulate the key ingredients needed for such phenomena and draw an intuitive picture of the mechanism. For ease of reading, the details of the algebra are taken out of the main text and placed in an appendix.

II. CONTRASTS BETWEEN EQUILIBRIUM AND NON-EQUILIBRIUM STEADY STATES

To describe a physical system statistically, a complete and relevant set of microstates (or configurations: $C$) for the system must first be specified. For simplicity, let us consider finite systems with finite degrees of freedom (e.g., finite
Ising models), so that the $C$’s form a discrete, countable set. With appropriate mathematical tools, our considerations can be extended to the thermodynamic limit of systems with continuous degrees of freedom. Next, we need $P[C]$, the probability for finding the system in each $C$. From here, the average of an observable quantity (e.g., internal energy), which takes the value $O[C]$ in configuration $C$, is then given by

$$\langle O \rangle = \sum_C O[C] P[C]. \quad (1)$$

Beyond averages, fluctuations and correlations are similarly computed.

When a system is evolving, then the probability distribution is a function of time: $P[C;t]$, leading to time dependent averages, fluctuations, etc. Clearly, an “equation of motion” is needed to describe the evolution of $P[C;t]$. In principle, we should derive such an equation from, e.g., Newton’s equations. In practice, however, this is typically not feasible. Instead, let us follow the standard framework of a master equation $[1]$:

$$\frac{\partial}{\partial t} P[C;t] = \sum_C \{ R(C' \rightarrow C) P[C';t] - R(C \rightarrow C') P[C;t] \} \quad (2)$$

which is basically a continuity equation for the probability density. Here, $R(C \rightarrow C')$ stands for the rate a configuration $C$ changes to $C'$. Most frequently, these rates are not time dependent, i.e., the dynamics is invariant under time-translation. As in the case of Eq. $[1]$ itself, they can be found in principle, once we specify how our system is coupled to its environment (e.g., a thermal reservoir). Again, in practice, the task of finding these rates is prohibitively complex, so that progress in this approach relies, typically, on postulating reasonable forms, based on sound physical principles. Returning to Eq. $[2]$, we see that, being linear, the right hand side may be written as a matrix,

$$\frac{\partial}{\partial t} |P_t\rangle = L |P_t\rangle, \quad (3)$$

Explicitly, the matrix elements are

$$L_{C,C'} = R(C' \rightarrow C) - \delta(C,C') \sum_C R(C \rightarrow C'') \quad (4)$$

where $\delta(C,C')$ is the Kronecker delta.

For simplicity, let us focus on systems which eventually settle down into a unique time-independent state, i.e.,

$$\lim_{t \rightarrow \infty} P[C,t] = P^*(C). \quad (5)$$

In other words, $P^*$ satisfies $\partial P^*/\partial t = 0$ and is the eigenvector of $L$ with zero eigenvalue. Further, the real parts of all other eigenvalues are strictly negative, so that $P^*$ is a stable state.

Clearly, this approach should embrace systems which evolve towards thermal equilibrium. If we wish to reproduce the results from the theory of equilibrium statistical mechanics (e.g., the Boltzmann factor in the canonical ensemble), there must be some constraints on these rates. These constraints are known as detailed balance. Specifically, denoting the energy of a configuration of our system be given by the Hamiltonian $H[C]$, we must impose, for an isolated system with total energy $E$,

$$R(C' \rightarrow C) = R(C \rightarrow C') \quad (6)$$

if $H[C'] = H[C] = E$ and $R(C' \rightarrow C) = 0$ otherwise. Then $P^*(C) \propto 1$, which is the fundamental hypothesis (micro-canonical ensemble), clearly satisfies $L |P^*\rangle = 0$. Generalizing to the canonical case (with $\beta = 1/k_B T$), we demand

$$\frac{R(C' \rightarrow C)}{R(C \rightarrow C')} = \exp \{ \beta (H[C'] - H[C]) \} \quad (7)$$

and verify that a distribution given by the Boltzmann factor

$$P_{eq}^*(C) \propto e^{-\beta H[C]} \quad (8)$$

indeed satisfies $L |P_{eq}^*\rangle = 0$. Apart from these constraints, there is much leeway in postulating the $R$’s, corresponding to the fact that equilibrium states are independent of the details of the dynamics. In particular, it is not crucial that
\( R (C \rightarrow C') \neq 0 \) for all pairs of \((C, C')\), though there must be enough non-zero rates so that every configuration (within the desired ensemble) may be reached from any other one. As an explicit example, we give the Metropolis rate \[ R (C' \rightarrow C) = \min[1, e^{\beta(H[C'] - H[C])}] \],

which is the basis of numerous successful Monte Carlo simulations of systems in equilibrium.

From the condition of detailed balance, a stronger statement about an equilibrium state emerges. Not only is the distribution time-independent, the net (probability) current between any pair \((C, C')\) vanishes! To be more explicit, we regard the right hand side of the master equation (3) as a sum of the net currents (from \(C'\) into \(C\)):

\[
R (C' \rightarrow C) P[C'; t] - R (C \rightarrow C') P[C, t],
\]

Then detailed balance, embodied in Eqs. (4) or (5), implies the vanishing of all net currents. An analog of this situation in electrodynamics is electrostatics, where the charge distribution is stationary and no currents exist.

Next, let us turn to non-equilibrium steady states. The simplest example is a system in contact with two energy reservoirs, e.g., two thermal baths at different temperatures: \(T_1\) and \(T_2\). For physically realizable cases, we can think of a time frame during which energy flows through our system (from the hotter to the cooler bath) steadily, so that the average energy within the system is time-independent. Typically, to model the coupling of our system to such reservoirs, there is no need to respect detailed balance when specifying a set of rates. Of course, the rates are not completely free of contraints. Without going into details, let us simply restrict our considerations to those rates which eventually take the system to a unique time-independent distribution: \(P^\ast(C)\). However, without detailed balance, we should expect, generically, \(P^\ast(C) \neq P^\ast_{eq}(C)\). Now, a time-independent distribution does not imply that all currents are zero. Instead, we can expect (time independent) current loops to be present. Using the analog above, this situation corresponds to magnetostatics, in which the charge density is stationary but steady current loops prevail. In this sense, we prefer to use the term “steady states” for describing such (magnetostatic-like) systems, while reserving “stationary states” for those in equilibrium (or electrostatics). The presence of current loops also highlights another crucial difference between equilibrium and non-equilibrium steady states, namely, time reversal invariance. Since currents change sign under time reversal, only states with zero currents are invariant. In this light, the concepts of equilibrium, detailed balance, and time reversal are intimately connected.

Once \(P^\ast(C)\) is known, we can compute the “internal energy” of the system

\[
U \equiv \langle H[C] \rangle \equiv \sum_C H[C] P^\ast[C],
\]

since we have a well defined microscopic Hamiltonian. For equilibrium states with \(P^\ast_{eq}(C) = e^{-\beta H[C]} / \sum_C e^{-\beta H[C]}\), it is a simple step to check that, without knowing the details of \(H[C]\), the specific heat: \(\partial U / \partial T \propto -\partial U / \partial \beta \propto \langle (H[C] - U)^2 \rangle\) is never negative. Notice that \(\partial U / \partial T \geq 0\) is true for systems of any size, regardless of whether a proper thermodynamic limit exists or not. For non-equilibrium steady states in, e.g., systems coupled to two baths, we naturally have \(U(T_1, T_2)\) and may extend the usual definition of specific heat. Of course, in this case, there are two such response functions:

\[
C_1 \equiv \frac{\partial U}{\partial T_1} \quad \text{and} \quad C_2 \equiv \frac{\partial U}{\partial T_2}
\]

as we can separately “dial up” the temperature of either bath while keeping the other fixed. While we cannot expect both to be negative, we will show that one of them can be negative in very simple systems.

### III. SIMPLE SYSTEMS WITH NEGATIVE SPECIFIC HEAT

#### A. A minimal system with three states

We begin by considering an abstract system with only three, non-degenerate, energy levels. For reasons shown at the end of the next subsection, it is impossible to construct a system with only two microstates which displays negative specific heat. In this sense, we believe that the three state system is “minimal.”

Each configuration (or microstate) is associated with a unique energy. Using the subscript \(\alpha = 0, 1, 2\), let us denote the energies by
\[ E_{\alpha} = 0, \varepsilon_1, \varepsilon_2 \]  

(13)

with \( \varepsilon_2 > \varepsilon_1 > 0 \). Our goal is, given a set of rates \( R(\alpha \to \alpha') \), to find \( U \), the average energy in the steady state. First, we must compute \( P^*_{\alpha} \), the probability for finding the system in level \( \alpha \) when steady state has been reached. Then

\[
U \equiv \sum_{\alpha} E_{\alpha} P^*_{\alpha} = \varepsilon_1 P^*_1 + \varepsilon_2 P^*_2.
\]

(14)

Had we been interested in the equilibrium distribution, corresponding to our system being in contact with a single thermal bath, then we could use, e.g., the usual Metropolis rates (Eq. 9). Here, they are explicitly

\[
\begin{align*}
R(0 \to 1) &= e^{-\beta \varepsilon_1} ; \\
R(1 \to 0) &= 1 \\
R(0 \to 2) &= e^{-\beta \varepsilon_2} ; \\
R(2 \to 0) &= 1 \\
R(1 \to 2) &= e^{-\beta \delta} ; \\
R(2 \to 1) &= 1
\end{align*}
\]

(15)

where \( \delta \equiv \varepsilon_2 - \varepsilon_1 \). The reader may verify that, with these rates in Eq. (4), the Boltzmann form, \( P^*_1, P^*_2 = P^*_0 \exp (-\beta \varepsilon_\alpha) \), is indeed a solution to \( L |P^*\rangle = 0 \). Note further that, even if we forbid the 0 \( \leftrightarrow \) 1 transition (by setting \( R(0 \to 1) = R(1 \to 0) = 0 \)), the system will still equilibrate to the same set of \( P^*_\alpha \)’s.

Next, let us modify the dynamics by coupling the 0 \( \leftrightarrow \) 2 and 1 \( \leftrightarrow \) 2 transitions to different baths, while forbidding the 0 \( \leftrightarrow \) 1 transition entirely. To avoid confusion with subscripts, we will label the two bath temperatures by \( T_x \) and \( T_y \).

Defining

\[
x \equiv \exp \left[ -\varepsilon_2 / k_B T_x \right] \quad \text{and} \quad y \equiv \exp \left[ -\delta / k_B T_y \right]
\]

(16)

the master equation takes the simple form

\[
\begin{align*}
\partial_t P_0 &= -xP_0 + P_2 \\
\partial_t P_1 &= -yP_1 + P_2 \\
\partial_t P_2 &= xP_0 + yP_1 - 2P_2
\end{align*}
\]

(17)

The steady state distribution is trivial to find:

\[
P^*_0 = y/Z ; \quad P^*_1 = x/Z ; \quad P^*_2 = xy/Z ,
\]

(18)

where \( Z \equiv x + y + xy \). Thus, the average energy is

\[
U = \frac{x \varepsilon_1 + xy \varepsilon_2}{x + y + xy}
\]

(19)

so that the specific heats (associated with the \( x \)- and \( y \)-baths) are:

\[
C_x \equiv \frac{\partial U}{\partial T_x} = \{ \varepsilon_1 + y \varepsilon_2 \} \frac{xy \varepsilon_2}{k_B T_x^2 [x + y + xy]^2}
\]

(20)

and

\[
C_y \equiv \frac{\partial U}{\partial T_y} = \{ x \varepsilon_2 - \varepsilon_1 (1 + x) \} \frac{xy \delta}{k_B T_y^2 [x + y + xy]^2}.
\]

(21)

While the first of these never goes negative, the second clearly becomes negative for a range of \( x \). Working out the details, we find \( C_y < 0 \) (for all \( T_y \)’s), provided \( T_2 \) drops below the critical value

\[
T_{xc} \equiv \frac{\varepsilon_2}{k_B} \left[ \ln \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1} \right]^{-1}.
\]

(22)

Note that, unless baths with negative temperatures are invoked, \( \varepsilon_2 > 2 \varepsilon_1 \) is needed.

While it is easy to analyze Eq. (21) mathematically, it may be helpful to provide an explicit example. We choose \( \varepsilon_2 = 4 \varepsilon_1 \) and plot, in Fig. 1, \( C_y/k_B \) against \( T_y \) (in units \( \varepsilon_1/k_B \)) for various \( T_x \)’s. Note that, in this “minimal” system, \( C_y \) does not change sign as long as \( T_x \) is fixed.
B. An intuitive picture

To help the reader appreciate how such an unusual response arises, we provide an intuitive picture for this phenomenon. Since the effects of a thermal bath on the transition between two levels are written in terms of rates, we may think of the role of a bath as that of (a pair of) “pumps” on the “population” in these levels. If we had only two levels, there could be only one pair of rates (pumps), regardless of how many “baths” are coupled to them. In the steady state, only one ratio of populations (say, the occupancy of the higher level to that of the lower) is relevant. In this situation, the only sensible way to define “thermodynamics” of the system is to have a single bath with an effective temperature. Then, the usual intuitive picture easily emerges: if this (effective) temperature is increased, the relative occupancy of the higher level will be higher, leading to a positive specific heat. The steady state system might as well be described as “in equilibrium.” Therefore, a minimal system which can display negative specific heat must involve more than two (distinct) levels.

With three levels, there are three (sets of) rates, so that our system may be coupled to three different “thermal baths.” By forbidding the transition between the lower pair of levels (as in the simple case above), it is already possible to generate “unconventional” population changes. This restriction also reduces our consideration to only two baths. Now, let us assume that our system has settled in a steady state where the populations are given by \( (P_0, P_1, P_2) \), using the notation above. If we increase the temperature of the bath coupled to \( 1 \leftrightarrow 2 \), we will certainly deplete \( P_1 \) in favor of \( P_2 \). However, the \( 0 \leftrightarrow 2 \) transition is coupled to a different bath, with a fixed temperature, so that any increase in \( P_2 \) will be driven to increases in \( P_0 \). If this bath is very cold, then the downward pump is very strong (relative to the “up-pump”), ensuring increases in \( P_2 \) be accompanied by much larger increases in \( P_0 \). Thus, there is an effective “downward” shift of population (from \( P_1 \) to \( P_0 \)), even though the thermostat coupled to \( 1 \leftrightarrow 2 \) has been turned up! By contrast, if both transitions are coupled to the same bath, then there would be also an “upward” shift (from \( P_0 \) to \( P_2 \)), leading to the expected increase in \( U \). From these considerations, we see that forbidding the \( 1 \leftrightarrow 0 \) transition introduces an “barrier” (or “obstruction”), leading to a “local minimum”. The presence of such “obstructions” forms the key ingredient to the display of negative specific heats. In the next section, we provide another illustration of such a link, in the context of currents and drives. Of course, “the proof is in the pudding.” The heuristic argument, hopefully, helps the reader to digest the mathematical “pudding” above.

Before turning to the explicit example, we note that this simple three state system can be generalized to include a third bath, coupling to the \( 0 \leftrightarrow 1 \) transition. To be specific, let the temperature be \( T_w \) and, in addition, let the “efficiency” of this coupling be \( \eta \), so that the extra rates are

\[
R(0 \rightarrow 1) = \eta w; \quad R(1 \rightarrow 0) = \eta
\]

with

\[
w = \exp \left[ -\varepsilon_1 / k_B T_w \right].
\]

Of course, setting \( \eta \) to zero will reduce this system to the simple one above. Computing the steady state distribution and the average internal energy is a straightforward exercise. Here, we only quote the relevant result. For sufficiently small \( \eta \), there is a critical line in the \( (T_x - T_w) \) plane, given by
\[ x_c + \eta w_c = \frac{\epsilon_1 - \eta \epsilon_2}{\epsilon_2 - \epsilon_1}, \]  
(25)
on which the specific heat \( C_y \) vanishes. For temperatures (or \( x,w \)) below this line, \( C_y \) is negative.

C. An explicit example: the Driven Lattice Gas

A “realization” of the above three-level system is the “two-temperature Ising model,” \(^3\) which consists of a lattice gas coupled to two baths. The only extra complication comes from degeneracies. Otherwise, all analysis is identical to the minimal case.

Our system consists of a \( 2 \times 3 \) lattice, half filled with particles. Imposing the boundary conditions:

- brick wall in \( x \); periodic in \( y \)

the 20 possible configurations fall into three distinct classes, labeled as follows:

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\[ \text{0} \quad \text{1} \quad \text{2} \]

For energetics, we use the usual ferromagnetic Ising Hamiltonian: \(-J\) is associated with each nearest neighbor particle pair. For convenience, shift all energies by \(-3J\). As a result, the labels of the configurations are also the energy levels (in units of \( J \)). The degeneracies are, respectively, \( (2, 12, 6) \) due to translation and parity (in \( x \) and \( y \)).

To be pedantic, let us use a second label to distinguish them, so that all 20 configurations are, explicitly:

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\[ \text{0,1} \quad \text{0,2} \]

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\[ \text{1,1} \quad \text{1,2} \quad \text{1,3} \quad \text{1,4} \quad \text{1,5} \quad \text{1,6} \quad \text{1,7} \quad \text{1,8} \quad \text{1,9} \quad \text{1,10} \quad \text{1,11} \quad \text{1,12} \]

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\[ \text{2,1} \quad \text{2,2} \quad \text{2,3} \quad \text{2,4} \quad \text{2,5} \quad \text{2,6} \]

Next, let us specify the dynamics: particles may hop to nearest neighbor empty sites (Kawasaki exchange \(^4\)) according to the usual Metropolis rates (Eq. 9). The two temperature model is defined so that exchanges along \( (x, y) \) axes are coupled to baths with temperatures \( (T_x, T_y) \). As examples, the rate for \( 0,1 \rightarrow 2,1 \) is \( \exp(-2J/kT_x) \) but the rate for \( 1,1 \rightarrow 2,1 \) is \( \exp(-J/kT_y) \). Obviously, our system is reduced to the trivial equilibrium case when \( T_x = T_y \). With these rates, the master equations can be easily written. Using subscripts to denote configurations, we give only three of the 20 master equations:

\[ \begin{align*}
\partial_t P_{0,1} &= P_{2,1} + P_{2,2} + P_{2,3} - 3xP_{0,1} \\
\partial_t P_{1,1} &= P_{2,1} + P_{2,3} + P_{1,2} + P_{1,7} + P_{1,4} - (2y + 3) P_{1,1} \\
\partial_t P_{2,1} &= xP_{0,1} + y(P_{1,1} + P_{1,2} + P_{1,3} + P_{1,6}) + P_{2,5} + P_{2,6} - 7P_{2,1}
\end{align*} \]  
(26)

where
\[ x \equiv \exp(-2J/kT_x), \quad y \equiv \exp(-J/kT_y). \]  

(27)

To find the steady state \( P^* \)'s, we note that all degenerate configurations will have same probability (since they are related to each other by symmetries). So, we just write equations without the second subscript:

\[
\begin{align*}
0 &= 3P_2^* - 3xP_0^* \\
0 &= 2P_2^* - 2yP_1^* \\
0 &= xP_0^* + 4yP_1^* - 5P_2^*
\end{align*}
\]

(28)

Apart from degeneracies, the solutions are same as in the minimal example above:

\[
P_0^* = y/Z; \quad P_1^* = xZ; \quad P_2^* = xyZ,
\]

(29)

with

\[ Z = 2y + 12x + 6xy. \]

(30)

The average energy is given by

\[
\frac{U}{J} = \frac{12x + 2 \times 6xy}{Z} = 6x \frac{1 + y}{y + 6x + 3xy},
\]

so that

\[ C_y \equiv \frac{\partial U}{\partial T_y} \propto [3x - 1]. \]

(32)

(with a positive definite proportionality factor). Similar to the minimal case, we have

\[ C_y < 0 \]

(33)

for all \( T_y \), provided \( T_x \) is low enough. Note that the degeneracies of these three levels affect the critical \( T_{xc} \). A simple exercise including \( g_\alpha \) (the degeneracy of level \( \alpha \)) in the computations above leads to the general result

\[
T_{xc} \equiv \frac{\varepsilon_2}{k_B} \left[ \ln \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1} + \ln \frac{g_2}{g_0} \right]^{-1}.
\]

(34)

Interestingly, this critical value is independent of the degeneracy of the middle level. From the intuitive picture given above, this behavior is, arguably, reasonable. After all, the transition from positive to negative specific heat depends how the depopulation of the middle level is redistributed between the upper and lower levels. At the critical point, this redistribution leads to an average energy (associated with the outer levels alone) which is identical to \( \varepsilon_1 \), leading to no change in the total energy. Now, each state in the middle level would “suffer the same fate,” so that it is irrelevant how many such states there are. Thus, we have \( g_1 \) independence.

D. Energy flux

In general, a system coupled to two thermal baths will lead to a transfer of energy from the hotter bath to the colder one. On the other hand, by definition of steady state, the energy stored in our system is a constant. Thus, we may expect a constant energy flux through our system. Most remarkably, in our minimal \((\eta = 0)\) case, there is no energy flux through the system! In this sense, our system and both baths are “in equilibrium,” and detailed balance is satisfied! Indeed, the general condition for detailed balance \([3]\) is less restrictive than Eq. \((7)\), so that it is possible to have a system coupled to two baths and retain detailed balance. The ramifications of such “effectively equilibrium” systems remain to be explored.

Meanwhile, as \( T_y \) is increased (with fixed \( T_x < T_{xc} \)), the energy of the system decreases. To be more precise, suppose we take a system in steady state and suddenly replace the \( y \)-bath by another with a higher temperature. Then there must be a net flow of energy out of our system somehow, since the new steady state must have lower \( U \). This paradox cannot be solved by studying the properties of steady states alone. The resolution lies in an analysis of the full dynamics. Deferring all details to another article, we provide only the result here: less energy is transferred from the \( y \)-bath to our system than from the system to the \( x \)-bath. In the general case \((\eta > 0)\), there is a net energy flux through our system, so that similar surprising behavior appears less paradoxical.
IV. A MODEL WITH NEGATIVE CONDUCTIVITY

The counter-intuitive phenomenon of negative response is not restricted to the energy-temperature variables. In this section, we show a similar behavior in the current-drive variables, i.e., the possibility of “negative conductivity”.

A. Set up and the unobstructed case

Consider a single particle hopping in two “lanes” of \( L \) sites, periodic on the long side and “brick walls” bounding the lanes. For convenience, assume \( L \) is even, so that the sites along the lanes can be labeled by the integer \( i = -L/2, \ldots, L/2 - 1 \). Periodicity allows us to use \( i = 0, 1, \ldots, L - 1 \) interchangeably.

Let us denote the probabilities of finding the particle on the two lanes by \( P_i \) and \( Q_i \).

Symbolically, we represent this system by:

\[
\begin{array}{ccccccc}
\ldots & Q_{-2} & Q_{-1} & Q_0 & Q_1 & Q_2 & \ldots \\
\ldots & P_{-2} & P_{-1} & P_0 & P_1 & P_2 & \ldots 
\end{array}
\]

(36)

Let there be no obstructions and suppose the particle is “driven” by a uniform external “electric” field \( E \), so that the jump rates are proportional to

\[
\begin{align*}
1 & \quad \text{for crossing lanes only;} \\
x & \quad \text{for jumping “upstream” (} i \rightarrow i - 1 \text{) to either lane;} \\
1/x & \quad \text{for jumps “downstream” (} i \rightarrow i + 1 \text{) to either lane.}
\end{align*}
\]

(37)

The normalization factor is just

\[
N = \frac{1}{1 + 2x + 2/x}. 
\]

(38)

We may regard \( x \) as a Boltzmann-like rate:

\[
x = e^{-\beta E},
\]

(39)

in which case \( N = 1/(1 + 4 \cosh \beta E) \). Note that the behavior of this “charged” particle is not the same as one in free space. Instead, it represents an overdamped situation, where inertia can be neglected compared to (thermal) damping. As a result, the particle settles down to the drift velocity instantaneously. Furthermore, with the rates and normalization chosen, the limit of \( E \to \infty \) does not mean the particle will move with infinity velocity. From the rates, it should be clear that, in this limit, all that happens is that the particle moves to the next site (either lane) with unit probability. Thus, the velocity saturates at unity for “infinite drive”.

Without obstructions, the system is translationally invariant and the steady state is trivially given by

\[
P_i = Q_i = 1/2L
\]

(40)

since the particle can be located at any of the \( 2L \) locations. The uniform current density, \( J_{\text{free}} \), can be found by considering the probability of all jumps between \( i \) and \( i + 1 \). Taking into account the contributions from both lanes, we have \( 2N (P_i + Q_i) - 2xN (P_{i+1} + Q_{i+1}) \). Therefore we obtain

\[
J_{\text{free}} = \frac{2 \sinh \beta E}{(1 + 4 \cosh \beta E)L}.
\]

(41)

Needless to say, the conductivity is positive

\[
\frac{\partial J}{\partial E} > 0
\]

(42)

for all finite \( \beta E \).

Another perspective is to consider the average velocity of the particle. Since we have only a single particle, we have \( J = \rho v \). Given uniform density \((1/2L)\), we obtain \( v = 4 \sinh \beta E / (1 + 4 \cosh \beta E) \), which is a monotonically increasing function of the drive \( E \). Note that this expression is expected for both small and large \( E \). In the former case, four out of the five possible jumps contribute to the velocity, so that the conductivity is simply \((4/5)\beta\).
B. Single obstruction case

Next, let us introduce barriers at \( i = 0 \), but only for one lane. Specifically, “impenetrable walls” are placed between the site associated with \( P_0 \) and three of its neighbors (those associated with \( Q_0, P_1, \) and \( Q_1 \)). Symbolically, we draw thick lines around \( P_0 \) (Fig. 2), and, using the analogy of water flowing under gravity, we will refer to the obstruction as a “cup.” Clearly, the cup causes a blockage, which, for large \( E \), will reduce the current seriously. However, as \( E \) is lowered, the particle’s chances of backward jumps are higher and leads to a higher current, giving us a negative conductivity.

\[
\begin{array}{ccccccc}
\cdots & Q_{-2} & Q_{-1} & Q_0 & Q_1 & Q_2 & \cdots \\
\hline
P_{-2} & P_{-1} & P_0 & P_1 & P_2 & \cdots \\
\end{array}
\]

FIG. 2. Schematic display of the probability for finding the particle in each box. Thick lines borders are associated with impenetrable walls.

To see that this picture is indeed correct, we start with a careful consideration of all the master equations. Without the cup, these equations read, for all \( i \),

\[
\begin{align*}
\partial_t P_i &= \frac{1}{x} (P_{i-1} + Q_{i-1}) + x (P_{i+1} + Q_{i+1}) + Q_i - \left(1 + \frac{2}{x} + 2x\right) P_i \\
\partial_t Q_i &= \frac{1}{x} (P_{i-1} + Q_{i-1}) + x (P_{i+1} + Q_{i+1}) + P_i - \left(1 + \frac{2}{x} + 2x\right) Q_i
\end{align*}
\]

With the cup in place, the only jumps affected are those involving \( 0 \leftrightarrow 1 \). As a result, the only equations affected are:

\[
\begin{align*}
\partial_t P_0 &= \frac{1}{x} (P_{-1} + Q_{-1}) - 2x P_0 \\
\partial_t Q_0 &= \frac{1}{x} (P_{-1} + Q_{-1}) + x (P_1 + Q_1) - 2 \left(\frac{1}{x} + x\right) Q_0 \\
\partial_t P_1 &= \frac{1}{x} Q_0 + x (P_2 + Q_2) + Q_1 - \left(1 + \frac{2}{x} + x\right) P_1 \\
\partial_t Q_1 &= \frac{1}{x} Q_0 + x (P_2 + Q_2) + P_1 - \left(1 + \frac{2}{x} + x\right) Q_1
\end{align*}
\]

A factor of \( N \) has been absorbed into the time scale, an irrelevant concern for the time-independent state. Setting the left hand side of these equations to zero, we seek the unique solution corresponding to the steady state. Note that, if we set the drive to zero (\( x \to 1 \)), then the obstruction becomes irrelevant in steady state and we retrieve the expected result: the trivial flat distribution. For the \( E \neq 0 \) case, we defer all details of the calculation to the appendix, providing a few brief steps and the result here.

For convenience, define the sums and differences:

\[
\begin{align*}
S &\equiv P + Q \\
D &\equiv P - Q
\end{align*}
\]

With no obstructions, it is intuitively clear (and mathematically easy to show) that the two lanes have equal probabilities in the steady state. However, the cup enhances \( P_0 \), so that

\[
\begin{align*}
D_i &= 0 \quad \text{for} \quad i \neq 0 \\
D_0 &= \frac{1 - x^2}{1 + 2x^2} S_0 > 0
\end{align*}
\]

Invoking (probability) current conservation, we set

\[
K = \frac{2}{x} S_{i-1} - 2x S_i \quad i \neq 0, 1
\]
which is proportional to the current between \(i-1\) and \(i\). But this \(K\) must also hold for all links. In particular,

\[
K = \frac{2}{x} - 2xS_0
\]  

(49)

\[
K = \frac{2}{x}Q_0 - xS_1 = \frac{S_0 - D_0}{x} - xS_1
\]

Using Eq. (47), we find a set of equations for the \(S's\), leading to

\[
S_0 = \frac{(1 + 2x^2) (2 - x^2 - x^{2L})}{3Lx^2 + 2 + 2x^2 - Lx^{2L} - 2Lx^{2+2L} - 2x^{2L} - 2x^{2+2L}}
\]  

(50)

and

\[
K = \frac{2x (1 - x^2) (3 - x^{2(L-1)} - 2x^{2L})}{3Lx^2 - Lx^{2L} - 2Lx^{2+2L} - 2x^{2L} + 2 - 2x^{2+2L} + 2x^2}
\]  

(51)

It is instructive to check that these expressions indeed reduce to \(1/L\) and 0, respectively, in the limit \(E \to 0\) (\(x \to 1\)). Another interesting limit is \(\beta E\) diverges faster than \(\ln L\) (\(Lx \to 0\)). In this case, the probability of the particle jumping out of the cup is so low that even the entropy factor (the 2\(L\) possible locations for the particle) is not enough to overcome the barrier (\(x \to 0\)), so that “complete trapping” occurs. This expectation is borne out by

\[
[S_0]_{\text{trapped}} \to 1
\]  

(52)

and, from Eq. (47), \([D_0]_{\text{trapped}} \to 1\) also. Thus, we have

\[
[P_0]_{\text{trapped}} \to 1 \quad \text{and} \quad [Q_0]_{\text{trapped}} \to 0.
\]  

(53)

Verifying that all other probabilities also vanishes, we see that the particle is completely trapped in the cup. To complete the study of this limit, we find

\[
K_{\text{trapped}} = 3x + O(Lx^2, x^2) \to 0
\]  

(54)

Since \(J = NK\), the current \textit{vanishes} (as \(x^2\)) for large fields, rather than saturating, as in the free case. Thus, \(\partial J/\partial E\) must be negative in some range of \(E\).

Returning to Eqs. (51) and (54), we find less cumbersome forms if we consider the thermodynamic limit and drop terms of \(O(x^{2L}, Lx^{2L})\) first. The results are:

\[
S_0 = \frac{(1 + 2x^2) (2 - x^2)}{3Lx^2 + 2 + 2x^2}
\]  

(55)

\[
J_{\text{obstruction}} = NK = \frac{6x^2 (1 - x^2)}{(2 + 2x^2 + 3Lx^2) (2 + x + 2x^2)}
\]  

(56)

![FIG. 3. Current vs. \(x \equiv e^{-\beta E}\). Note increasing \(E\) corresponds to decreasing \(x\) and the linear rise of the current for small \(E\) (near \(x = 1\)). For large enough drive (small \(x\), the current drops with increasing \(E\).](image-url)
Of course, we can differentiate the current and find the critical field above which the conductivity $\partial J / \partial E$ is negative. However, it may be more instructive to provide an illustration of this expression. In Fig. 3, we plotted this current as a function of the driving field, for the case of $L = 10$. We should remind the reader that $x = \exp(-\beta E)$, so that larger $x$ corresponds to smaller $E$. Note that the curve is basically linear near the $x = 1$ end, confirming the typical constant, positive conductivity for small $E$. On the other hand, negative conductivity sets in for sufficiently large $E$ (approximately $k_B T$ in this case).

V. CONCLUDING REMARKS

In this paper, we have shown that “negative responses,” in a system coupled to thermal baths, can be easily generated, provided we consider non-equilibrium steady states. Specifically, we gave examples of exceedingly simple systems which display negative specific heat. One is an abstract system with only three energy levels, but coupled to two thermal baths. The other is a standard Ising lattice gas (3 particles in $2 \times 3$ sites), also coupled to two baths. These models are “minimal” in the sense that systems with just two energy levels can support only a single (set of) transition rates, so that an single (effective) temperature can be defined. Then, we have essentially an equilibrium system, with non-negative specific heats. There is no doubt that such systems can be extended to more complex and macroscopic cases. In particular, using Monte Carlo simulation techniques with the two-temperature Ising model, we have observed negative specific heats in, e.g., a 60 lattice for $T_g \gtrsim 1.5T_D$ with $T_x = 0.7T_D$. Another example is a two-temperature Ising model with a population of mobile impurities that couple to a heat bath with a temperature different from that of the Ising spins. This model has been proposed to mimic the non-equilibrium behavior of a biological membrane in which diffusing protein particles receive energy from a heat bath with a temperature that is different from the membrane matrix in which diffuse. Under certain conditions this has shown to lead to a negative specific heat (Fig. 4 in [6]). We also showed a second form of negative response: negative conductivity. The explicit example consists of particles hopping along two lanes of discrete sites, driven by an external field so that a non-vanishing DC current is established in the steady state. When an obstruction is introduced, the current is shown to decrease when the drive is increased (beyond some critical value). In both cases, the key ingredient (besides being in non-equilibrium steady states) is the presence of local minima or “obstructions.” When the drive, be it another thermal bath or an external field, is too large, the system is caught for longer in the obstruction. By lowering the drive, the system can respond “more positively”. Though the phenomenon has been observed for some time, e.g., in driven diffusive systems [7], it has been discovered in another context and popularized through the catchy phrase: “freezing by heating” [8]. Since this kind of counter-intuitive response is not only reserved for negative specific heat, but also negative conductivity and beyond, we may label all of them by the catch-all phrase: “getting more by pushing less.”

Though we are certain that this kind of phenomena are present in physical systems, we have not conducted a systematic search for them, nor have we proposed designs for such devices. The goal of this paper is simply to encourage those who teach statistical mechanics to keep their students’ minds open about the issue of negative specific heats. In particular, in non-equilibrium steady states, positive responses are not intimately related to stability.

To close, we should mention that “negative specific heat” is not a novel phrase. Indeed, it occurs frequently in discussions of self-gravitating systems. Evidently, Eddington wrote about how a star or star-cluster would cool down if energy is added [9]. Reading the literature, there is no doubt that this is a subtle situation of a complex system, with particles subjected to long range interactions (gravity). Furthermore, it is clear that such systems are inherently unstable, leading to “gravothermal catastrophe” and collapse. Clearly, the theoretical existence of such a kind of negative specific heat was not well received by physicists. In the opening sentence of a recent article [10], Lynden-Bell wrote, “When I first used the concept of Negative Specific Heat ...the Statistical Mechanics community thought I was talking nonsense.” By contrast, our examples are far less exotic and the phenomenon should be abundant in our neighborhood as well as amongst the distant stars. After all, every living organism can be considered as a non-equilibrium steady state, coupled to more than one reservoir of energy so that there is a constant through-flux. If we succeed in convincing other teachers to add a footnote in their course, that $\partial U / \partial T \geq 0$ is ironclad only for system in equilibrium, then this paper would have served its purpose.

VI. APPENDIX

Here we provide a few more details for finding the steady state distribution in the two-lane hopping model. Referring to the schematic diagram (36), we seek solutions to the set of equations (43,44) with zero on the right hand sides.
Recall that we have periodic boundary conditions, so that hopping rates from sites $i = L - 1$ to $i = -L$ are the same as all others (except for the obstruction).

As mentioned in the text, it is convenient to define sums and differences:

$$S \equiv P + Q$$
$$D \equiv P - Q$$

so that we have

$$0 = 2x S_{i-1} + 2x S_{i+1} - 2 \left( \frac{1}{x} + x \right) S_i$$

$$0 = -2 \left( 1 + \frac{1}{x} + x \right) D_i$$

and

$$0 = \frac{2}{x} S_{-1} + x S_1 - 2x S_0 - \frac{1}{x} (S_0 - D_0)$$

$$0 = -x S_1 - 2x D_0 + \frac{1}{x} (S_0 - D_0)$$

$$0 = \frac{1}{x} (S_0 - D_0) + 2x S_2 - \left( \frac{2}{x} + x \right) S_1$$

$$0 = - \left( 2 + \frac{2}{x} + x \right) D_1$$

from Eqs. (43,44), respectively. The advantage of this decomposition is obvious now. It proves the intuitive notion that, apart from the obstructed sites, the two lanes should have equal probabilities in the steady state. So,

$$D_i = 0 \quad \text{for } i \neq 0$$

$$D_0 = \frac{1 - x^2}{1 + 2x^2} S_0$$

Now, we have a set of equations involving only $S$:

$$0 = \frac{2}{x} S_{-1} + x S_1 - 5 + 4x^2 x S_0$$

$$0 = \frac{3x}{1 + 2x^2} S_0 + 2x S_2 - \left( \frac{2}{x} + x \right) S_1$$

$$0 = \frac{2}{x} S_{i-1} + 2x S_{i+1} - 2 \left( \frac{1}{x} + x \right) S_i \quad \text{for } i \neq 0, 1$$

To solve these, we exploit current conservation, since the physical content of these equations lies in the difference between the particle currents into and out-of site $i$ must be zero. Thus, we first consider the “unaffected” sites, just to be careful. Set $2S_{i-1}/x - 2x S_i$ to a constant:

$$K = \frac{2}{x} S_{i-1} - 2x S_i \quad i \neq 0, 1$$

which will be proportional to the steady state current. (As a reminder, given the periodic condition, $S_{L/2} = S_{-L/2}$. $K = 2S_{L/2-1} - 2x S_{-L/2}$ is part of this set of equations.) Note that this “trick” solves Eq. (58) automatically: $0 = K - K$. Next, this $K$ serves as the steady state current, so that it must hold for all jumps $i \leftrightarrow i + 1$. In particular, the jumps across $-1 \leftrightarrow 0$ leads to

$$K = \frac{2}{x} S_{-1} - 2x S_0$$

which is the same as the unaffected case. Meanwhile, the jumps across $0 \leftrightarrow 1$ provides a new equation:

$$K = \frac{2}{x} Q_0 - x S_1$$
By definition, \(2Q_0 = S_0 - D_0\), so that, using Eq. (47), we obtain

\[
2Q_0 = \frac{3x^2}{1 + 2x^2} S_0
\]  

and

\[
K = \frac{3x}{1 + 2x^2} S_0 - x S_1
\]  

All these equations with \(K\) on the left can be recast as recursion relations for the \(S_i\)'s. Specifically, we will try to express everything in terms of \(S_0\), so that we write

\[
S_1 = \frac{3}{1 + 2x^2} S_0 - \frac{1}{x} K
\]  

\[
S_{i-1} = \frac{x}{2} K + x^2 S_i \quad \text{for} \quad i \neq 1
\]  

Starting with the \(i = 0\) recursion relation Eq. (74), we work all the way around back to \(S_1\):

\[
S_{i-1} = \frac{x}{2} K + x^2 S_0 \\
S_{i-2} = \frac{x}{2} K + x^2 S_{i-1} = \frac{x}{2} (1 + x^2) K + x^4 S_0 \\
\vdots \\
S_{i-n} = \frac{x}{2} (1 + \cdots + x^{2(n-1)}) K + x^{2n} S_0 \\
= \frac{x (1 - x^{2n})}{2 (1 - x^2)} K + x^{2n} S_0 \\
\vdots \\
S_1 = S_{-L+1} = \frac{x (1 - x^{2(L-1)})}{2 (1 - x^2)} K + x^{2(L-1)} S_0
\]  

Together with Eq. (74), the last of these allows us to express \(K\) in terms of \(S_0\).

\[
K = \frac{3}{1 + 2x^2} - \frac{x^{2(L-1)}}{2 (1 - x^2)} + 1 \quad \text{on the left}
\]

\[
K = x \left[ \frac{3}{1 + 2x^2} - \frac{x^{2(L-1)}}{2 (1 - x^2)} \right] S_0
\]  

Finally, normalization \((\sum_i S_i = 1)\) will fix everything.

It may be instructive to compare the above equations with those in the free case. The only difference is that we would have one more “unaffected” step. Instead of Eq. (74), we have \([S_0]_{\text{free}} = \frac{x}{2} K_{\text{free}} + x^2 [S_1]_{\text{free}},\) so that

\[
x^{-2} [S_0]_{\text{free}} - \frac{1}{2x} K_{\text{free}} = \frac{x (1 - x^{2(L-1)})}{2 (1 - x^2)} K_{\text{free}} + x^{2(L-1)} [S_0]_{\text{free}}
\]  

i.e.,

\[
[S_0]_{\text{free}} = \frac{x}{2 (1 - x^2)} K_{\text{free}}
\]  

Note first that this expression is independent of \(L\)! This result should be expected, since we know that the average velocity must be \(L\)-independent for the free case. But the velocity is just the current divided by the particle density (i.e., probability for finding the particle at, say, site 0). To continue the check, insert this expression into the recursion relations and find that all the \(S_i\)'s are the same. So, normalization gives \([S_1]_{\text{free}} = 1/L\) and \(K_{\text{free}} = (4 \sinh \beta E) / L\).

Armed with these considerations, we return to the case with barrier and define

\[
M \equiv S_0 - \frac{x}{2 (1 - x^2)} K
\]  

13
which is a measure of the effect of the cup. Eliminating $K$ in its favor, Eq. (77) is replaced by a neater formula:

$$\left[ \frac{(1 - x^2)^L}{(1 - x^2)} + 1 \right] M = \frac{2(1 + x^2)}{(1 + 2x^2)} S_0$$  \hspace{1cm} (81)

Finally, the sum over the $S$'s is

$$S_0 + \sum_{n=1}^{L-1} S_{-n} = S_0 + \sum_{n=1}^{L-1} \left[ \frac{x(1 - x^{2n})}{2(1 - x^2)} K + x^{2n} S_0 \right]$$

$$= S_0 + \frac{x(L-1)}{2(1 - x^2)} K + \sum_{n=1}^{L-1} x^{2n} M$$  \hspace{1cm} (82)

Eliminating $K$ and setting this to unity, we have

$$1 = L S_0 + \left[ \frac{1 - x^{2L}}{1 - x^2} - L \right] M$$  \hspace{1cm} (83)

Eqs. (81,83) can now be used to obtain Eq. (50).

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[1] For more details, see, e.g., L. E. Reichl, A Modern Course in Statistical Physics 2nd edition (Wiley, N.Y., 1998).
[2] N. Metropolis, A.W. Rosenbluth, M.M. Rosenbluth, A.H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).
[3] P. L. Garrido, J. L. Lebowitz, C. Maes, and H. Spohn, Phys. Rev. A42, 1954 (1990); B. Schmittmann and R.K.P. Zia, Phys. Rev. Lett. 66, 357 (1991); E. Praestgaard, H. Larsen, and R.K.P. Zia, Europhys. Lett. 25, 447 (1994); and E. Praestgaard, B. Schmittmann, and R.K.P. Zia, Euro. Phys. J. B18, 675 (2001).
[4] K. Kawasaki, in Phase Transitions and Critical Phenomena, eds. C. Domb and M.S. Green, Vol. 2 (Academic, N.Y., 1972).
[5] D. Mukamel, in Soft and Fragile Matter: Nonequilibrium Dynamics, Metastability and Flow, eds: M R Evans and M. E. Cates (Scottish Universities Summer School in Physics, Edinburgh, 2000).
[6] J.R. Henriksen, M.C. Sabra, and O.G. Mouritsen, Phys. Rev. E62, 7070 (2000).
[7] S. Katz, J.L. Lebowitz, and H. Spohn, Phys. Rev. B 28, 1655 (1983); J. Stat. Phys 34, 497 (1984). For a review, including two temperatures models, see, e.g., B. Schmittmann and R.K.P. Zia, Phase Transitions and Critical Phenomena, Vol. 17, edited by C. Domb and J. L. Lebowitz (Academic, London, 1995).
[8] H. E. Stanley, Nature 404, 718 (2000).
[9] A.S. Eddington, Mon. Not. R. Astro. Soc. 76, 525 (1916) and The Internal Constitution of the Starts (Cambridge, 1926).
[10] D. Lynden-Bell, Physica A263, 293 (1999).