Nonequilibrium statistical mechanics: A solvable model

I. Mazilu and H. T. Williams

Department of Physics and Engineering, Washington and Lee University, Lexington, Virginia 24450

(Received 10 December 2008; accepted 26 January 2009)

A two-temperature linear spin model is presented as an introduction to nonequilibrium statistical physics. The model involves the concepts that are typical of more realistic nonequilibrium models, but has straightforward steady state solutions and, for small systems, development of the full time dependence for configuration probabilities. The model is accessible to upper-level undergraduates and provides a good check of computer models for larger systems. © 2009 American Association of Physics Teachers.

[DOI: 10.1119/1.3081423]

I. INTRODUCTION

The statistical mechanics of systems in thermal equilibrium is a well-established part of the core physics curriculum. Yet, thermal equilibrium is the exception rather than the rule. If we look around us, we see a world far from equilibrium: from the intricate dynamics of living cells to more complex biological organisms; from ripples on a pond to global weather patterns.

The study of systems far from thermal equilibrium is challenging and rewarding. The reward comes from the chance to better understand the vast collection of nonequilibrium real-life systems. The challenge is obvious: we step outside the comfort of the familiar Gibbs framework for equilibrium systems, and thus we have to develop new tools to achieve understanding and classification of non-equilibrium behavior. Over the last three decades an increasing number of physicists have been studying the complex collective behavior of far-from-equilibrium systems using methods ranging from easily accessible computer simulations to sophisticated field theoretic techniques.

Nonequilibrium statistical physics is a relatively new field and is not yet part of the physics curriculum at the undergraduate level. Nonetheless, the methods and results of nonequilibrium statistical physics are being employed in fields as diverse as molecular biology, computer science, economics, and politics. Thus it is advantageous to introduce undergraduate students to the field.

This paper introduces nonequilibrium statistical physics via a simple model that retains the essence of the difficulties of far-from-equilibrium systems. The two-temperature kinetic Ising model has two appealing features. First, multi-temperature systems are fairly common. Examples include a water tank with an immersion heater, nuclear magnetic resonance in an external magnetic field, and a lattice of nuclei in a solid prepared at a specified spin temperature. Second, the model can be solved analytically for small system sizes using only basic linear algebra, and can also be modeled via Monte Carlo simulations without much difficulty. For these reasons this model has great pedagogical value. Undergraduate students in a traditional course in statistical physics can extend principles learned there to gain their first exposure to far-from-equilibrium systems.

This paper is structured as follows. In Sec. II we give an overview of nonequilibrium statistical physics and compare it with its equilibrium counterpart. In Sec. III we introduce the two-temperature kinetic Ising model as a simple example of a nonequilibrium system. We solve the master equation exactly Sec. IV for some small system sizes to obtain the probability distribution. In Sec. V we comment on the probability currents, a fundamental feature of far-from-equilibrium systems in the steady state. By direct calculations in Sec. VI we also find the time dependence of the probability distribution for a small system.

II. IN AND OUT OF EQUILIBRIUM: COMPARISON AND CONTRAST

Statistical mechanics enables us to predict macroscopic behavior of a system, knowing the quantitative properties of molecular interactions. The foundation of equilibrium statistical mechanics rests upon a fundamental hypothesis, as stated by Boltzmann:3

If an isolated macroscopic system is ergodic, it will reach thermal equilibrium after a sufficiently long time. Then every configuration (or microstate) available to the system can be found with equal probability.

Completely isolated systems are unrealistic, so typically we consider systems in contact with a heat reservoir. Equilibrium is reached after a sufficiently long time, meaning that the average net energy flux between the system and the heat reservoir vanishes and the system reaches the fixed temperature $T$ of the reservoir. For these conditions the probability of finding the system in a configuration $\sigma$ is given by the canonical distribution:

$$P_{eq}(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z},$$  \hspace{1cm} (1)

where $\beta=1/(k_B T)$, $k_B$ is Boltzmann’s constant, and the partition function $Z$ ensures the normalization of the probability. Thus, once we have specified a labeling of the microscopic configurations, $\{\sigma\}$, and have determined the microscopic Hamiltonian, $H(\sigma)$, that is, the energy of each configuration, we can calculate in principle the partition function of the equilibrium system and average values of time-independent observables. Some of the configurational sums may not be obtainable exactly, but the fundamental framework for a solution is well established.

The jump from the idealization of thermal equilibrium to the full, possibly turbulent, dynamics of the real world is too great for our limited present understanding of nonequilibrium systems, and we will focus on the simplest extension of
equilibrium systems, namely, non-equilibrium steady states. This category of systems is characterized by time-independent macroscopic behavior, which results from applying a driving force. We will model the external driver as a second temperature bath, at a different temperature than the first, thus feeding energy into the system or removing it. The long-time behavior of such a two-bath system exhibits constant energy flow through the system. A simple example of such a system is a current-carrying electrical resistor that gains energy from a current source and loses it as heat to the environment. The resistor is not in equilibrium because there is a nonzero energy flux flowing through it; yet, after a sufficient long time, it reaches a steady state with time-independent macroscopics. Understanding such a system in the steady state involves finding the associated stationary probability distribution of configurations, which is the long-time limit of the time-dependent configuration probability distribution.

A starting point for the study of these systems is the master equation, which expresses the conservation of configurational probabilities. We consider a continuous time dynamics, with a finite and discrete configuration space $\sigma$. The time-dependent probability $P(\sigma,t)$ for finding the system in configuration $\sigma$ at time $t$ changes due to the transfer of probability into $\sigma$ from other configurations, or from $\sigma$ into others, such that $\sum_\sigma P(\sigma,t)=1$ at all times. The evolution of $P(\sigma,t)$ is dictated by a set of transition rates $c[\sigma \to \sigma']$ that describe the evolution of the system from configuration $\sigma$ to a different configuration $\sigma'$ per unit time. For example, for a spin system, one configuration leads into another via a spin flip. The evolution of $P(\sigma,t)$ is given by a balance (continuity) equation with the right-hand side consisting of two sums: the first is a gain term which sums over all configurations from which configuration $\sigma$ can result, and the second is a loss sum which accounts for all configurations into which $\sigma$ can evolve:

$$\frac{dP(\sigma,t)}{dt} = \sum_{\sigma'} \{c[\sigma' \to \sigma]P(\sigma',t) - c[\sigma \to \sigma']P(\sigma,t)\}. \tag{2}$$

The transition rate $c[\sigma \to \sigma']$ from configuration $\sigma$ to another configuration $\sigma'$ defines the model. To solve the steady-state problem we need to find the stationary solution of this equation, $P^*(\sigma)=\lim_{t \to \infty} P(\sigma,t)$, for which the left-hand side of Eq. (2) vanishes:

$$0 = \frac{dP^*(\sigma)}{dt} = \sum_{\sigma'} \{c[\sigma' \to \sigma]P^*(\sigma') - c[\sigma \to \sigma']P^*(\sigma)\}. \tag{3}$$

The steady state distribution $P^*(\sigma)$ depends on the transition rates. For rather general conditions on the $c$’s, this solution will be unique, and thus independent of initial conditions.

For a system in thermal equilibrium with a single heat bath, we know its steady state distribution must be given by $P_{\text{eq}}(\sigma)$ in Eq. (1). Hence we must choose the rate terms $c[\sigma \to \sigma']$ to be consistent with the canonical distribution result. Rates which satisfy the detailed balance condition provide the required consistency: $\frac{c[\sigma' \to \sigma]}{c[\sigma \to \sigma']} = \frac{P_{\text{eq}}(\sigma)}{P_{\text{eq}}(\sigma')}$. Because $P_{\text{eq}}(\sigma) \propto \exp(-\beta H)$, we choose the rates such that

$$\frac{c[\sigma' \to \sigma]}{c[\sigma \to \sigma']} = \exp(\beta \Delta H), \tag{4}$$

where

$$\Delta H = H(\sigma') - H(\sigma). \tag{6}$$

For systems in equilibrium the detailed balance condition is an intrinsic property and is related to their microscopic reversibility. This condition assures the invariance of the long time limit of the probability distribution. This constraint on the transition rates is necessary when modeling (via Monte Carlo simulations, for instance) systems in thermal equilibrium.

A key feature of a system far from thermal equilibrium is the violation of detailed balance: its steady state distribution $P^*(\sigma)$ does not satisfy Eq. (4). For a nonequilibrium system in its steady state, the question becomes how we can generalize the detailed balance condition such that, when the “drive” is turned off, the equilibrium solution is recovered.

A more intuitive way to discuss the detailed balance condition is to describe it in terms of probability currents. We consider a series of configurations $\sigma_1, \sigma_2, \ldots, \sigma_n$ which form a cycle, each successive state reachable in a single step from its predecessor (likewise for states $\sigma_n$ and $\sigma_1$): We define the products of the rates around the cycle as

$$\Pi_1 = c[\sigma_1 \to \sigma_2]c[\sigma_2 \to \sigma_3] \cdots c[\sigma_n \to \sigma_1], \tag{7a}$$

$$\Pi_2 = c[\sigma_2 \to \sigma_1]c[\sigma_3 \to \sigma_2] \cdots c[\sigma_n \to \sigma_2]r. \tag{7b}$$

Detailed balance holds if and only if

$$\Pi_1 = \Pi_2 \tag{8}$$

for all cycles, which is equivalent to saying that the net probability current between any two configurations vanishes in the steady state:

$$c[\sigma' \to \sigma]P^*(\sigma') - c[\sigma \to \sigma']P^*(\sigma) = 0. \tag{9}$$

If the rates violate the detailed balance condition, there will be nontrivial current loops:

$$c[\sigma' \to \sigma]P^*(\sigma') - c[\sigma \to \sigma']P^*(\sigma) \neq 0. \tag{10}$$

The presence of these current loops is a key characteristic of nonequilibrium steady states and a signal of the microscopic irreversibility of these systems. For a complete and unique characterization of a nonequilibrium steady state we need to specify the configurational probability distribution and the distribution of the probability currents. The choice of the transition rates is not unique. The transition rates we will use (see Sec. III) for our two-temperature kinetic model have been studied and lead to equilibrium solutions. We will examine the specific probability currents for our model to illustrate the profound differences between equilibrium and nonequilibrium systems.

From a pedagogical point of view these calculations provide students an opportunity to learn important statistical physics concepts such as choice of transition rates, balance equations, steady state, probability distributions, equivalence classes, and boundary conditions. These analytical calculations complement straightforward computer simulations of nonequilibrium states.

In Sec. III we introduce the model and present some sample calculations and results for an $N=4$ lattice. It is in-

I. Mazilu and H. T. Williams 459

III. THE TWO-TEMPERATURE KINETIC MODEL

The Ising model was introduced by Lenz in 1925 to understand the nature of phase transitions in ferromagnets. Students already familiar with the Ising model can quickly consider. The two heat baths at temperatures \( T_c \) and \( T_o \) experience a rate \( c_n \). The ising model was introduced by Lenz in 1925 to understand the nature of phase transitions in ferromagnets. Students already familiar with the Ising model can quickly consider. The two heat baths at temperatures \( T_c \) and \( T_o \) experience a rate \( c_n \). The Ising model was introduced by Lenz in 1925 to understand the nature of phase transitions in ferromagnets. Students already familiar with the Ising model can quickly consider. The two heat baths at temperatures \( T_c \) and \( T_o \) experience a rate \( c_n \).

The nonequilibrium version of this one-dimensional kinetic model has been studied. The magnetization (average over all spins) and the two-spin correlations (average over all pairs of spins) were calculated for both the steady state and the time-dependent case. So far, there is no compact expression for the steady state probability distribution. In the following we exhibit an exact expression for the full probability distribution, but at the price of restricting ourselves to very small systems.

IV. PROBABILITY DISTRIBUTION

The master equation, Eq. (2), tells us how a particular configuration evolves in time and can be rewritten as:

\[
\partial_t P(\{\sigma\}, t) = \sum_{n=1}^{\infty} [c_n(\{\sigma[n]\})P(\{\sigma[n]\}, t) - c_*n(\{\sigma\})P(\{\sigma\}, t)],
\]

where the state \( \{\sigma[n]\} \) differs from \( \{\sigma\} \) by a flip of the nth spin and the rates are given by Eq. (12). We seek the steady state solution:

\[
P^* (\{\sigma\}) = \lim_{t \to \infty} P(\{\sigma\}, t).
\]

To simplify the problem we note that configurations that are related by symmetries of the dynamics will occur with the same probability. For example, the configurations \( +++++ \) and \( +++++ \) have the same probability in an \( N=4 \) system, because they differ from each other by a translation modulo 2. Similarly, \( +++++ \) and \( +++++ \) are related by a global spin flip. We can define equivalence classes, each class consisting of those configurations related to one an-

<table>
<thead>
<tr>
<th>Class</th>
<th>Configuration</th>
<th>Degeneracy</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>+++++</td>
<td>2</td>
<td>( P_0 )</td>
</tr>
<tr>
<td>1</td>
<td>+++++</td>
<td>4</td>
<td>( P_1 )</td>
</tr>
<tr>
<td>2</td>
<td>+++++</td>
<td>4</td>
<td>( P_2 )</td>
</tr>
<tr>
<td>3</td>
<td>+++++</td>
<td>2</td>
<td>( P_3 )</td>
</tr>
<tr>
<td>4</td>
<td>+++++</td>
<td>2</td>
<td>( P_4 )</td>
</tr>
<tr>
<td>5</td>
<td>+++++</td>
<td>2</td>
<td>( P_5 )</td>
</tr>
<tr>
<td>6</td>
<td>+++++</td>
<td>2</td>
<td>( P_6 )</td>
</tr>
<tr>
<td>7</td>
<td>+++++</td>
<td>2</td>
<td>( P_7 )</td>
</tr>
<tr>
<td>8</td>
<td>+++++</td>
<td>2</td>
<td>( P_8 )</td>
</tr>
<tr>
<td>9</td>
<td>+++++</td>
<td>2</td>
<td>( P_9 )</td>
</tr>
<tr>
<td>10</td>
<td>+++++</td>
<td>2</td>
<td>( P_{10} )</td>
</tr>
<tr>
<td>11</td>
<td>+++++</td>
<td>2</td>
<td>( P_{11} )</td>
</tr>
</tbody>
</table>

(a) Equivalence classes for 1x4 two temperature kinetic model (non-equilibrium).

<table>
<thead>
<tr>
<th>Class</th>
<th>Configuration</th>
<th>Degeneracy</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>+++++</td>
<td>2</td>
<td>( P_0 )</td>
</tr>
<tr>
<td>1</td>
<td>+++++</td>
<td>6</td>
<td>( P_1 )</td>
</tr>
<tr>
<td>2</td>
<td>+++++</td>
<td>6</td>
<td>( P_2 )</td>
</tr>
<tr>
<td>3</td>
<td>+++++</td>
<td>6</td>
<td>( P_3 )</td>
</tr>
<tr>
<td>4</td>
<td>+++++</td>
<td>6</td>
<td>( P_4 )</td>
</tr>
<tr>
<td>5</td>
<td>+++++</td>
<td>6</td>
<td>( P_5 )</td>
</tr>
<tr>
<td>6</td>
<td>+++++</td>
<td>6</td>
<td>( P_6 )</td>
</tr>
<tr>
<td>7</td>
<td>+++++</td>
<td>6</td>
<td>( P_7 )</td>
</tr>
<tr>
<td>8</td>
<td>+++++</td>
<td>6</td>
<td>( P_8 )</td>
</tr>
<tr>
<td>9</td>
<td>+++++</td>
<td>6</td>
<td>( P_9 )</td>
</tr>
<tr>
<td>10</td>
<td>+++++</td>
<td>6</td>
<td>( P_{10} )</td>
</tr>
<tr>
<td>11</td>
<td>+++++</td>
<td>6</td>
<td>( P_{11} )</td>
</tr>
</tbody>
</table>

(b) Equivalence classes for 1x6 two temperature kinetic model (non-equilibrium).

<table>
<thead>
<tr>
<th>Class</th>
<th>Configuration</th>
<th>Degeneracy</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>+++++</td>
<td>2</td>
<td>( P_0 )</td>
</tr>
<tr>
<td>1</td>
<td>+++++</td>
<td>12</td>
<td>( P_1 )</td>
</tr>
<tr>
<td>2</td>
<td>+++++</td>
<td>12</td>
<td>( P_2 )</td>
</tr>
<tr>
<td>3</td>
<td>+++++</td>
<td>12</td>
<td>( P_3 )</td>
</tr>
<tr>
<td>4</td>
<td>+++++</td>
<td>12</td>
<td>( P_4 )</td>
</tr>
<tr>
<td>5</td>
<td>+++++</td>
<td>12</td>
<td>( P_5 )</td>
</tr>
<tr>
<td>6</td>
<td>+++++</td>
<td>12</td>
<td>( P_6 )</td>
</tr>
<tr>
<td>7</td>
<td>+++++</td>
<td>12</td>
<td>( P_7 )</td>
</tr>
<tr>
<td>8</td>
<td>+++++</td>
<td>12</td>
<td>( P_8 )</td>
</tr>
<tr>
<td>9</td>
<td>+++++</td>
<td>12</td>
<td>( P_9 )</td>
</tr>
<tr>
<td>10</td>
<td>+++++</td>
<td>12</td>
<td>( P_{10} )</td>
</tr>
<tr>
<td>11</td>
<td>+++++</td>
<td>12</td>
<td>( P_{11} )</td>
</tr>
</tbody>
</table>

(c) Equivalence classes for 1x4 kinetic model (equilibrium).

<table>
<thead>
<tr>
<th>Class</th>
<th>Configuration</th>
<th>Degeneracy</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>+++++</td>
<td>2</td>
<td>( P_0 )</td>
</tr>
<tr>
<td>1</td>
<td>+++++</td>
<td>30</td>
<td>( P_1 )</td>
</tr>
<tr>
<td>2</td>
<td>+++++</td>
<td>30</td>
<td>( P_2 )</td>
</tr>
<tr>
<td>3</td>
<td>+++++</td>
<td>30</td>
<td>( P_3 )</td>
</tr>
<tr>
<td>4</td>
<td>+++++</td>
<td>30</td>
<td>( P_4 )</td>
</tr>
<tr>
<td>5</td>
<td>+++++</td>
<td>30</td>
<td>( P_5 )</td>
</tr>
<tr>
<td>6</td>
<td>+++++</td>
<td>30</td>
<td>( P_6 )</td>
</tr>
<tr>
<td>7</td>
<td>+++++</td>
<td>30</td>
<td>( P_7 )</td>
</tr>
<tr>
<td>8</td>
<td>+++++</td>
<td>30</td>
<td>( P_8 )</td>
</tr>
</tbody>
</table>

(d) Equivalence classes for 1x6 kinetic model (equilibrium).

Fig. 1. Equivalence classes for \( N=4 \) and \( N=6 \).
other by a symmetry transformation. We need solve only for the probability associated with one member of each equivalence class, thus greatly reducing the number of unknown probabilities below the total number of configurations, $2^N$.

We now pursue this program for $N=4$, presenting the calculations in detail, and also show the results for $N=6$. The exact stationary probabilities will be determined and studied as functions of the parameter $\gamma_e$ for a fixed value of $\gamma_o$. The equilibrium limit is represented by $\gamma_e = \gamma_o$.

For $N=4$ there are six equivalence classes, numbered (in arbitrary order) $i=0, 1, \ldots, 5$. The degeneracy $d_i$ of each class is the number of configurations in this class. $P_i^*$ denotes

---

Fig. 2. (a) Probability distribution for $N=4$ as a function of $\gamma = \tanh (2J/k_BT)$ in the equilibrium case, when even and odd sites are in contact with heat baths at the same temperature. (b) The probability distribution for $N=4$ as a function of $\gamma_e$ in the driven case with $\gamma_o=0.5$. 
the stationary probability associated with class $i$. In Fig. 1 we present the equivalence classes with one representative of each class. The 12 equivalence classes for $N=6$ are also listed.

To write the steady state equation for $P_0$, we need to identify the “neighbors” of class 0 in configuration space, that is, those configurations that can be reached from $P_0$ via a single spin flip and vice versa: these configurations belong to classes 1 or 2. Similarly, class 1 is a neighbor to classes 0, 3, 4, and 5. The master equation leads us to a set of six rate equations:

$$2\tau_i P_0 = 2(1 + \gamma_c)P_1 + 2(1 + \gamma_0)P_2 - 2(2 - \gamma_c - \gamma_0)P_0,$$

(16a)

$$2\tau_1 P_1 = (1 - \gamma_0)P_0 + P_3 + P_4 + (1 + \gamma_c)P_5 - 4P_1,$$

(16b)

$$2\tau_1 P_2 = (1 - \gamma_0)P_0 + P_3 + P_4 + (1 + \gamma_c)P_5 - 4P_2,$$

(16c)

$$2\tau_1 P_3 = 2P_1 + 2P_2 - 4P_3,$$

(16d)

$$2\tau_1 P_4 = 2P_1 + 2P_2 - 4P_4,$$

(16e)

$$2\tau_1 P_5 = (1 - \gamma_0)P_0 + (1 - \gamma_c)P_1 - (2 + \gamma_c + \gamma_0)P_5.$$  

(16f)

Because the probabilities are normalized, we have one additional equation, namely

$$1 = \sum_{i=0}^5 d_i P_i.\quad \text{(17)}$$

The probabilities for the equilibrium case $\gamma_0=\gamma_c=\gamma$ are given by the Boltzmann factor, $\exp(-\beta H)$. In this case the probabilities differ only if their configurational energies are distinct, producing an even greater reduction in the number of distinct cases. With a little algebra we can convert the exponentials into functions of $\gamma$ to arrive at

$$P_1 = P_2 = P_3 = P_4 = P_0 \frac{(1 - \gamma)}{(1 + \gamma)},\quad \text{(18a)}$$

$$P_5 = P_0 \frac{(1 - \gamma)^2}{(1 + \gamma)^2}.\quad \text{(18b)}$$

If we use the normalization condition Eq. (17), we find

$$P_0 = \frac{1}{8} \frac{(1 + \gamma)^2}{2 - \gamma^2}.\quad \text{(19)}$$

These equilibrium results can also be found by solving the rate equations, Eq. (14), with the left-hand sides set to zero, along with Eq. (17).

In equilibrium only three different probabilities remain, reflecting the three possible values of the configurational energy: (a) class 0: no broken (that is, $+-$) bonds; (ii) classes 1, 2, 3, 4: two broken bonds; and (iii) class 5: four broken bonds. In Fig. 2a we show their dependence on $\gamma$. All probabilities become equal for $\gamma \to 0$, which corresponds to the infinite temperature limit, and all except $P_0$ vanish for $\gamma \to 1$, that is, $T \to 0$. The situation for $N=6$ is similar [see Fig. 3(a)]. There are four distinct probabilities, all of which are zero at infinite temperature, and three of which vanish at zero temperature.

The problem becomes more difficult when $\gamma_0 \neq \gamma_c$, and it is necessary to solve simultaneously for the probabilities. Steady state solutions are achieved by considering Eq. (14), resulting from the master equation, with the partial time derivatives all set to zero. The normalization condition, Eq. (17), implies that the six equations of Eq. (14) must be redundant. A solution emerges if we solve the inhomogeneous set of linear equations resulting from taking five of the equations from Eq. (14) along with Eq. (17). This solution is easily found using algebraic software and produces the results

$$P_1 = \frac{8 + \gamma_0^2 - 6 \gamma_0 \gamma_c - 3 \gamma_c^2}{64(2 - \gamma_c \gamma_e)},$$

(20a)

$$P_2 = \frac{8 - 3 \gamma_0^2 - 6 \gamma_0 \gamma_c + \gamma_c^2}{64(2 - \gamma_c \gamma_e)},$$

(20b)

$$P_3 = \frac{8 - \gamma_0^2 - 6 \gamma_0 \gamma_c - \gamma_c^2}{64(2 - \gamma_c \gamma_e)},$$

(20c)

$$P_4 = \frac{8 - 2 \gamma_0 \gamma_c - 3 \gamma_c^2 + 8 \gamma_c + 8 \gamma_c}{64(2 - \gamma_c \gamma_e)},$$

(20d)

$$P_0 = \frac{8 + 3 \gamma_0^2 + 2 \gamma_0 \gamma_c + 3 \gamma_c^2 + 8 \gamma_c + 8 \gamma_c}{64(2 - \gamma_c \gamma_e)}.$$  

(20f)

We exhibit these probabilities in Fig. 2(b), where we plot each probability versus $\gamma_c$ for $\gamma_0=0.5$.

Note that there are more distinct probabilities than for the equilibrium case. Equation (20) shows that each equivalence class behaves differently, except for the added degeneracy that results from the dynamics we have chosen: $P_3=P_4$. The crossings at the point where $\gamma_c=\gamma$, reproduce the equilibrium results for $\gamma=0.5$. We also note that $P_0$ remains the most probable configuration. Finally, we observe a grouping of probabilities: The probabilities of configurations that share equal configurational energy track each other closely, and those associated with different configurational energy never cross. We might be tempted to conjecture that this property is a generic feature of this simple nonequilibrium system, but it does not persist for larger system sizes such as $N=8$.

This calculation also allows us to seek configurations that are unrelated by symmetry which would occur with the same probability. In equilibrium, such configurations would all have the same energy, that is, degeneracies (beyond symmetry) are controlled by the energy. Far from equilibrium it is not known which quantity controls such degeneracies. The difference between equilibrium and nonequilibrium probabilities is dramatic, and any connections between the two are not obvious.

V. PROBABILITY CURRENTS

The presence of current loops marks a fundamental difference between nonequilibrium and equilibrium systems. We illustrate this difference for $N=4$. In Sec. II we defined these probability current loops as
Due to the detailed balance condition, these current loops vanish in equilibrium for any pair of configurations in the steady state. For \( N = 4 \) we can calculate these currents in the steady state as

\[
J_0 = (1 - \gamma_e)P_0 - (1 + \gamma_e)P_1, \quad J_1 = (1 - \gamma_e)P_1 - (1 + \gamma_e)P_0, \quad J_{12} = (1 - \gamma_e)P_2 - (1 + \gamma_e)P_3, \quad J_{13} = (1 - \gamma_e)P_1 - (1 + \gamma_e)P_4, \quad J_{14} = (1 - \gamma_e)P_0 - (1 + \gamma_e)P_5.
\]

Due to the detailed balance condition, these current loops vanish in equilibrium for any pair of configurations in the steady state. For \( N = 4 \) we can calculate these currents in the steady state as

\[
J_0 = (1 - \gamma_e)P_0 - (1 + \gamma_e)P_1, \quad J_1 = (1 - \gamma_e)P_1 - (1 + \gamma_e)P_0, \quad J_{12} = (1 - \gamma_e)P_2 - (1 + \gamma_e)P_3, \quad J_{13} = (1 - \gamma_e)P_1 - (1 + \gamma_e)P_4, \quad J_{14} = (1 - \gamma_e)P_0 - (1 + \gamma_e)P_5.
\]

Fig. 3. (a) Probability distribution for \( N = 6 \) as a function of \( \gamma_e = \gamma_o = \tanh (2J/k_BT) \) in the equilibrium case, when even and odd sites are in contact with heat baths at the same temperature. (b) The probability distribution for \( N = 6 \) as a function of \( \gamma_e \) in the driven case with \( \gamma_o = 0.5 \).
where $J_{ik}$ represents the current between configurations $i$ and $j$, with $i, j = 0, \ldots, 5$.

Figure 4 shows these currents as functions of $\gamma_e$ for $\gamma_0 = 0.5$. We see that all the currents vanish at equilibrium, where $\gamma_e = \gamma_0 = 0.5$, in accordance with the detailed balance condition.

**VI. TIME DEPENDENCE**

In principle, the model can be solved analytically for the time dependence of the configuration probabilities, given any initial set of probabilities as an initial condition. The master equation, Eq. (14), leads to a set of coupled, first-order differential equations in time that can be solved using standard methods. However, the number of equations grows very quickly with the number of spins, making a straightforward approach difficult and rendering computer simulations a much more reasonable approach. Nonetheless, it is instructive to look at the nontrivial case of $N=4$ for which complete solutions can be found.

As we have seen, this case allows $2^4 = 16$ distinct spin configurations, leading to 16 distinct time-dependent probability functions. When examining the asymptotic time behavior the probabilities group into six equivalence classes, leaving a tractable $6 \times 6$ linear algebraic system to solve for the asymptotic probabilities. This simplification is not available for arbitrary times, because the initial conditions need not obey the symmetries of the asymptotic situation.

Figure 5. Time dependence of the configuration probabilities for $N=4$ with $\gamma_e = \gamma_0 = 0.5$ and the $++++$ configuration as the initial condition. The vertical axis is the absolute probability; the time units are arbitrary.
It is straightforward to set up the 16 time-dependent equations for the probabilities that follow from the master equation. They can be represented by

\[ \frac{d}{dt} \mathbf{P} = \mathbf{A} \mathbf{P}, \]

where \( \mathbf{P} \) is a 16-component vector whose components are the configurational probabilities, and \( \mathbf{A} \) is the matrix of coefficients of the probabilities from the right-hand side of the master equation. If we assume a time dependence for the vector \( \mathbf{P} \) of \( \exp(-\lambda t) \), Eq. (23) reduces to the eigenvalue equation for the matrix \( \mathbf{A} \): its eigenvalues \( \lambda_i \) are proportional to the decay coefficients \( \lambda \) with \( \lambda_i = \lambda_i/(2\tau) \). A standard algebraic software packages such as Maple can easily identify the eigenvalues of this system as a function of \( \gamma_e \) and \( \gamma_o \) as 0, 2, 4, 6, 8, 2(1 ± \( \sqrt{\gamma_e \gamma_o} \)), 4(1 ± \( \sqrt{\gamma_e \gamma_o} \)), and 6(1 ± \( \sqrt{\gamma_e \gamma_o} \)). The eigenvalues 2 and 6 are both twofold degenerate, and 4 is fourfold degenerate. Note that these eigenvalues are coincident with the set given by Glauber\(^6\) for the one-temperature model in the limit \( \gamma_e = \gamma_o \).

The general time-dependent solution is

\[ \mathbf{\tilde{P}}(t) = \sum_i c_i \tilde{V}_i \exp(-\lambda_i t), \quad (24) \]

where \( \mathbf{\tilde{P}}(t) \) is a 16-component vector, \( \tilde{V}_i \) is the eigenvector of \( \mathbf{A} \) corresponding to eigenvalue \( \lambda_i \), and the sum runs over all eigenvectors. For degenerate eigenvalues a linearly independent set of eigenvectors is chosen. The constants \( c_i \) are determined by the initial probabilities:

\[ \mathbf{\tilde{C}} = \mathbf{V}^{-1} \mathbf{\tilde{P}}_I, \]

where \( \mathbf{\tilde{C}} \) is the vector with components \( c_i \), \( \mathbf{V} \) is a matrix whose columns are the eigenvectors of \( \mathbf{A} \), and \( \mathbf{\tilde{P}}_I \) is the vector with components equal to the initial probabilities.

From the general solution, Eq. (24), it is clear that the asymptotic time behavior results from the term corresponding to the \( \lambda = 0 \) eigenvalue. The associated normalized eigenvector coincides with the collection of probabilities derived for the steady state solution.

As an example, we present graphs of the time-dependent behavior for \( N=4 \). The system at \( t=0 \) is in the configuration

![Fig. 6. Time dependence of the four largest configuration probabilities for \( N=4 \) with \( \gamma_e=0.2, \gamma_o=0.8 \), and the ++ + + configuration as the initial condition. The vertical axis is the absolute probability; the time units are arbitrary.](image-url)
In the first, simpler case the two temperature baths are at the same temperature, so that the eventual behavior of the system goes to equilibrium. The time dependence of the probabilities for this system is exhibited in Fig. 5. Because of the simplicity of the initial state and the symmetry introduced by the equal temperatures, only 5 of the 16 configuration probabilities show distinct time behavior. At large values of $t$ these five probabilities collapse into three values corresponding to the equivalence classes shown in Fig. 1(c). Even in this simple case some probabilities grow from zero to a maximum before falling to their asymptotic values. For the same initial condition, but for two distinct temperatures, $\gamma_e=0.2$ and $\gamma_o=0.8$, the system never reaches equilibrium, but eventually achieves a steady state. As shown in Figs. 6 and 7, 8 of the 16 configurations evolve distinctly, eventually reaching the steady state of the six equivalence classes listed in Fig. 1(a). As for the former example, there are configuration probabilities that grow or decay monotonically from their initial to final values, but others that initially grow past their steady state values before relaxing to them. Because we can describe all physical properties of the system as functions of the configuration probabilities, this behavior suggests the possibility of time-dependent peaks in some of these properties.

**VII. CONCLUSIONS**

We have presented a simple, intuitive way to introduce students to nonequilibrium statistical physics using a one-dimensional spin system, the two-temperature kinetic Ising model. We solved the master equation exactly for $N=4$ and found the probability distribution for both the steady state and the time-dependent case. By comparing the steady state probability spectrum with its equilibrium counterpart, we were able to see the dramatic differences between the two cases. For example, the nonequilibrium steady state probability distribution is governed not only by the configurational energy (which is the case for equilibrium), but by other factors that remain to be explored. The time-dependent probability spectrum offers new features that are worth pursuing (for example, local maxima that may be indicative of oscillatory behavior of the system before settling into its steady
state). We also emphasized the presence of the probability currents—a defining feature of nonequilibrium systems.

From a pedagogical point of view this project offers students the opportunity to learn about the novel behavior of a driven system, and to face the challenges of a lack of theoretical framework for nonequilibrium systems. We plan to study bigger system sizes with the help of Monte Carlo computer simulations. Besides being an essential tool in the study of various theoretical models, computer simulations are very appealing and accessible to undergraduate students.

ACKNOWLEDGMENTS

The authors would like to express their gratitude to B. Schmittmann and R. K. P. Zia for their very helpful and encouraging discussions and communications. This work was supported in part by Thomas F. and Kate Miller Jeffress Grant No. J-763 and by Robert E. Lee Research Fund for undergraduate research.

Electronic mail: mazilui@wlu.edu
Electronic mail: williamsh@wlu.edu

12 A fuller discussion of the role of the detailed balance condition can be found in the work of Zia and Schmittmann (Ref. 5).

Rotator Accessories. A device for rotating objects is still in the demonstration room of many physics departments. This collection of accessories for the rotator is at Hobart and William Smith Colleges in Geneva, New York, and was bought in the later 1920s from Max Kohl of Chemnitz, Germany. The apparatus at the left is a figure of the earth demonstration, and at the right is a centripetal force device. A set of toothed Savart’s wheels can be seen in the center. The Y-shaped device in the center is used to demonstrate buoyancy effects in a rotating field. In front is a siren disk. The large and small balls on the horizontal sliding rod form the demonstration showing that a two body system will rotate about its center of mass. (Photograph and Notes by Thomas B. Greenslade, Jr., Kenyon College)