1 ABSTRACT

Glauber dynamics, applied to the one-dimensional Ising model, provides a tractable model for the study of non-equilibrium, many-body processes driven by a heat bath. We explain Glauber's dynamical Ising model in the context of a system comprising three “spins” in a 1-dimensional Ising model. We first present the model without a magnetic field and then, following Glauber, add an oscillating magnetic field. We then show that Glauber’s demonstration of the fluctuation-dissipation theorem carries over to the 3-spin case. A web-link to a simulation code and an interactive video display of the “spins” flipping from a non-equilibrium to an equilibrium configuration (zero magnetic field) is included.

2 INTRODUCTION

The study of thermodynamics traditionally deals with equilibrium properties of matter. However, as remarked by Le Bellac, et al. ([1], p. 335) “this is rather restrictive since non-equilibrium phenomena, such as heat conduction or diffusion, are of great interest and cannot be ignored.” On the other hand, our understanding of the properties of out-of-equilibrium matter is still something of a work in progress, as one might conclude from Kubo’s brief summary of modern developments in the theory of irreversible processes. ([2], p. 374).

The Ising model [3] considers arrays of coupled two-component spins, and is often discussed in connection with ferromagnetism in modern textbooks. The model lived most of its life as an equilibrium model, until, as discussed by Ràcz [4], Glauber[5] initiated an industry of kinetic spin models (currently, ”Glauber Ising” gets about 1.4 million hits on Google) by providing for single spin-flips induced by a heat bath followed by a relaxation to equilibrium. A solution for an arbitrary number of spins was subsequently given by Felderhof [6]. Kawasaki quickly followed Glauber’s paper with a spin-exchange model that conserved total spins. Garrido, et al. [8], using Glauber dynamics with competing heat baths, demonstrated the existence of non-equilibrium phase transitions in 1-dimension with short-range forces. Lage [9] extended the use of Glauber dynamics
to the Potts model, taking care to point out that the extension is not unique, that is, that there are multiple possible dynamics that could be added to the original Potts model.

Many authors have recognized that the Ising model can also serve as a lattice-gas model, the two “spin” orientations being considered as lattice occupation numbers, 0 and 1. Chomaz et al.[10] invoke such an interpretation to discuss the formation and evolution of compact stars. The Ising model has also found application to the discussion of the thermodynamic properties of Schwarzschild black holes[11] A recent paper by Mazilu and Williams[12] “introduces nonequilibrium statistical mechanics” by solving exactly a two-temperature (1-d) Ising model with four spins.

The Ising Hamiltonian for a lattice with \( N \) spins is[13]

\[
\mathcal{H} = -J \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i
\]  

with index \( N + 1 \equiv 1 \). \( H \) is the strength of an applied external magnetic field, which may be time dependent. The coupling strength \( J \) is positive for an attractive interaction that would simulate ferromagnetism if all the spins had the same value, thereby indicating alignment.

Statistical mechanics typically deals with very large systems, see e.g.[13]. Glauber’s[5] paper accordingly considers the infinite 1-d Ising chain (as well as the single spin case). Chemists and biologists, however, are often interested in very small systems, such as molecules with just a few binding sites. Ter Bush and Thompson[14] worked out the Glauber dynamics of 2-spin and 4-spin Ising chains in connection with a model for the functioning of hemoglobin.

## 3 GLAUBER-ISING WITH 3 SPINS

The 3-spin 1-d dynamic Ising model displays many of the features of larger finite Ising systems and is easily handled by elementary methods in the case of zero magnetic field. It is assumed that each individual spin, \( s_i \), flips randomly between the values \( +1, -1 \) with a probability per unit time (measured in arbitrary time units) that depends upon the orientations of the adjacent spins according to

\[
w_i(s_i) = \left[ 1 - \frac{1}{2} \gamma s_i (s_{i-1} + s_{i+1}) \right]
\]

The constant \( \gamma \) is related to the spin-coupling \( J \) and the temperature of a presumed heat bath, that drives the random orientation transitions of the individual spins, by[5]

\[
\gamma = \coth \left( \frac{2J}{kT} \right)
\]

where \( T \) is the temperature of the heat bath. Appendix A includes a table of the values of the \( w_i \)'s.

Designating the probability of a given spin configuration by \( p(s_1, s_2, s_3; t) \), where each \( s_i \) can take either of the values \( +, - \), the time dependence of the probabilities is given by the master equation

\[
\frac{dp(s_1, s_2, s_3; t)}{dt} = -\sum_i w_i(s_i)p(s_1, s_2, s_3; t) + \sum_j w_j(-s_j)p(s_{j-1}, -s_j, s_{j+1}; t)
\]
with the convention that subscripts 0 and 4 are respectively the same as 3 and 1. As pointed out in connection with Eq. 17 of [5], the coupling strength \( \gamma \) is limited to the range \([+1, -1]\), the extreme values corresponding to zero temperature of a presumed heat bath, and the negative value corresponding to a repulsive interaction between adjacent spins. The coupling vanishes in the limit of infinite temperature of the heat bath.

Now let \( V_+(V_-) \) represent the probability for the spins all having the value \(+1(-1)\), and \( X_+(X_-) \) the sum of the probabilities that exactly two spins have the values \(+1(-1)\). The individual probabilities for the latter configuration are denoted by \( x_{\pm i} \) with the "\( i \)" denoting the position of the odd spin. Also, define \( V = V_+ + V_- \), \( X = X_+ + X_- \), \( U = V_+ - V_- \), \( Y = X_+ - X_- \), \( x_i = x_{+i} + x_{-i} \), and \( y_i = x_{+i} - x_{-i} \). Clearly, in the case of three spins

\[
V + X = 1 \tag{5}
\]

4 ZERO MAGNETIC FIELD

Define a vector

\[
\Psi = \begin{bmatrix} V \\ X \\ U \\ Y \end{bmatrix} \tag{6}
\]

Then, in Glauber’s “alternative” approach, the master equation may be written as (the dot denotes time differentiation)

\[
\frac{d}{dt} \Psi \equiv \dot{\Psi} = M \Psi \tag{7}
\]

where the matrix \( M \) is

\[
\begin{bmatrix}
-3(1 - \gamma) & (1 + \gamma) & 0 & 0 \\
3(1 - \gamma) & -(1 + \gamma) & 0 & 0 \\
0 & 0 & -3(1 - \gamma) & (1 + \gamma) \\
0 & 0 & 3(1 - \gamma) & -(5 + \gamma)
\end{bmatrix}
\]

The eigenvalues of the matrix \( M \) are \( 0, -2(1-\gamma), -2(2-\gamma), -6 \). The zero eigenvalue corresponds to equilibrium. There is a “parity” symmetry in the equations of motion, corresponding to the simultaneous flipping of all three spins, so that both \( U \) and \( Y \) must be equal to zero at equilibrium, and the equilibrium solution is \( V = \frac{(1+\gamma)}{2(2-\gamma)} \), as would be expected from the static Ising model. It is evident that the six configurations with one odd spin must be equally populated.

The solutions are

\[
X(t) = X(0)e^{-2(2-\gamma)t} + \frac{3(1 - \gamma)}{2(2 - \gamma)}[1 - e^{-2(2-\gamma)t}]
\]

\[
U(t) = \frac{1}{2(2 + \gamma)}\{U(0)[(1-\gamma)e^{-6t} + 3(1+\gamma)e^{-2(1-\gamma)t} - [(1 + \gamma)Y(0)[e^{-6t} - e^{-2(1-\gamma)t}]]}
\]

\[
Y(t) = \frac{1}{2(2 + \gamma)}\{Y(0)[3(1+\gamma)e^{-6t} + (1-\gamma)e^{-2(1-\gamma)t}] - 3(1-\gamma)U(0)[e^{-6t} - e^{-2(1-\gamma)t}]\} \tag{8}
\]
The first of these equations provides for relaxation to the classical Ising equilibrium solution, as shown in the accompanying Figure, where, in the initial configuration the three spins are aligned in the positive direction \((X(0) = 0, U(0) = +1, \text{ so that } Y(0) = 0)\). The scale of the \(t\)-variable is arbitrary.

### 4.1 Average Values

Glauber also suggests that in many situations the relevant observable quantities might be average values and correlations of the individual spins, rather than the detailed configurations. Accordingly, he defines the single spin average value to be, for the \(k^{th}\) spin

\[
q_k(t) \equiv \langle s_k \rangle = \sum_s s_k p(s_1, s_2, s_3; t) \quad (9)
\]

where the sum is over the eight possible values of the three spins. The time dependence of the \(q_k\) is given by

\[
\dot{q}_k(t) = -\left[ q_k(t) - \frac{\gamma}{2}[q_{k-1}(t) + q_{k+1}(t)] \right] \quad (10)
\]

The solution to Eq. (10) is (see Appendix B)

\[
q_k(t) = \frac{1}{3}[q_k(0)(e^{-(1-\gamma)t} + 2e^{-(1+\frac{3}{2})t}) + [q_{(k-1)}(0) + q_{k+1}(0)][e^{-(1-\gamma)t} - e^{-(1-\frac{3}{2})t}]] \quad (11)
\]

Evidently, at equilibrium, reached from any starting configuration, the average value of each spin is zero, as might be expected.
4.2 2-spin correlations

The 2-spin correlation function is defined [5], in the 3-spin case, by

\[ r_{j,k}(t) \equiv \langle s_j s_k \rangle = \sum_s s_j s_k p(s_1, s_2, s_3; t) \] (12)

which guarantees that \( r_{j,j} \equiv 1 \). The \( r' \)s are, of course, symmetric in the two indices. The time dependences are given by

\[
\begin{align*}
\dot{r}_{i,i+1} &= -2r_{i,i+1} + \frac{\gamma}{2} [r_{i,i-1} + r_{i-1,i+1}] + \gamma \\
\dot{r}_{i,i-1} &= -2r_{i,i-1} + \frac{\gamma}{2} [r_{i,i+1} + r_{i-1,i+1}] + \gamma \\
\dot{r}_{i-1,i+1} &= -2r_{i-1,i+1} + \frac{\gamma}{2} [r_{i,i-1} + r_{i,i+1}] + \gamma
\end{align*}
\] (13)

The solutions are (see Appendix C)

\[
\begin{align*}
\dot{r}_{i,j}(t) &= r_{i,j}(0)e^{-\frac{\gamma}{2}(4+\gamma)t} + \frac{1}{3} R(0)[e^{-(2-\gamma)t} - e^{-(\frac{3}{2}(4+\gamma)t)}] + \frac{\gamma}{2(2-\gamma)}[1 - e^{-(2-\gamma)t}] 
\end{align*}
\] (14)

where \( R \) is the sum of the three independent correlation functions. The final term of Eq 14 indicates that the 3 spins are partially correlated at all times.

5 MAGNETIC FIELD

Glauber observes that a dynamic Ising model with a magnetic field \( H \) will have the same equilibrium solution as the static Ising model if \( w_i \) in Eq 2 is replaced by

\[
w'_i(s_i) = w_i(s_i)[1 - \beta s_i]
\] (15)

where

\[
\beta \equiv \tanh\left(\frac{\mu H}{kT}\right)
\] (16)

and \( \mu \) is the magnetic moment associated with one of the spins. The Matrix \( M \) of the previous section is then replaced by

\[
\begin{bmatrix}
-3(1-\gamma) & (1+\gamma) & 3(1-\gamma)\beta & (1+\gamma)\beta \\
3(1-\gamma) & -(1+\gamma) & -3(1-\gamma)\beta & -(1+\gamma)\beta \\
3(1-\gamma)\beta & (1+\gamma)\beta & -3(1-\gamma) & (1+\gamma) \\
-3(1-\gamma)\beta & (3-\gamma)\beta & 3(1-\gamma) & -(5+\gamma)
\end{bmatrix}
\] (17)
5.1 Zero Temperature: A Phase Transformation?

The zero temperature ($\gamma = \beta = 1$) eigenvalues are readily found to be 0 and 4, each occurring twice. The solutions may be written as

$$
X(t) = \{X(0) + 2t[X0 − Y(0)]\}e^{-4t}
$$

$$
Y(t) = \{Y(0) + 2t[X0 − Y(0)]\}e^{-4t}
$$

$$
U(t) = \{U(0) + X(0)(1 − e^{-4t}) − 2t[X0 − Y(0)]\}e^{-4t}
$$

$$
V(t) = 1 − X(t)
$$

(18)

The equilibrium solution, which depends upon the initial conditions, has no counterpart in the original Ising model, where the concept of “initial” plays no role. The system ultimately relaxes to the configuration

$$
V(t) \sim 1
$$

$$
U(t) \sim U(0) + X(0) \equiv 1 − 2V.0
$$

(19)

where the last identity results from the fact that there are only three spins.

A number of authors have treated the zero temperature limit of an Ising system as a phase boundary (see, generally, Privman in [4]). That this is a tempting analogy may be seen from the fact that in the zero temperature limit, the parameter $|\beta|$ is 1 when a magnetic field, no matter how small, is present, and 0 if the field is absent. This parameter breaks the “parity” symmetry of the equilibrium solutions, resulting in the non-zero asymptotic values of $Y(t)$ and $U(t)$.

5.2 Magnetic Field at Low, but Non-Zero Temperature

The eigenvalues of the Master Equation matrix, Eq. 17 must, in general, be determined from a cubic equation. I have investigated the solutions for the low, but non-zero, temperature case
where $\gamma = \beta = 0.90$. I find the 3 non-zero eigenvalues to be approximately $-4.81, -3.05$, and $-0.538$. These may be compared with the values $-6, -2.2, -0.2$, in the absence of a magnetic field ($\beta = 0$), and $-4, -3.8, -6[-1, 2(1 + \gamma), -6(1 - \gamma)]$ in the presence of a very large magnetic field ($\beta = 1$). The magnetic field obviously breaks the parity symmetry, favoring $+\text{-}\text{spins over } -\text{-}\text{spins (for positive } \mu H)\text{.}

The secular equation for the eigenvalues of the Master Equation matrix involve the parameter $\beta$ to at least the second power, so that to linear order in the magnetic field the eigenvalues are unchanged from their zero-field values. To linear order in $\beta$ the relaxation rates are just the zero-field rates. The solutions to the same order in $\beta$, for a time dependent external field $\beta = \beta_0 e^{-i\omega t}$ are:

$$
\Delta U = -\frac{\beta_0}{2+\gamma} \langle [X(0) - 3(1 - \gamma)] \frac{4\gamma(1 + \gamma)}{2 + i\omega} (e^{-[2(2-\gamma)+i\omega]t} - e^{-2(1-\gamma)t}) + \frac{2(2-\gamma)}{2(1+\gamma-i\omega)} (e^{-[2(2-\gamma)+i\omega]t} - e^{-6t}) - \frac{3(1 - \gamma)^2}{2(1 - \gamma - i\omega)} \frac{2 + \gamma}{2 - \gamma} (e^{-i\omega t} - e^{-2(1-\gamma)t})
$$

$$
\Delta Y = -\frac{\beta_0}{2+\gamma} \langle [X(0) - 3(1 - \gamma)] \frac{4\gamma(1 + \gamma)}{2 + i\omega} (e^{-[2(2-\gamma)+i\omega]t} - e^{-6t}) - \frac{3(1 - \gamma)^2}{2(1 - \gamma - i\omega)} \frac{2 + \gamma}{2 - \gamma} (e^{-i\omega t} - e^{-2(1-\gamma)t})
$$

(20)

The equilibrium values are given by

$$
U(t) \sim \frac{12\beta_0(1-\gamma)}{(1-\gamma^2)[2(2-\gamma)-i\omega]} e^{-i\omega t}
$$

$$
Y(t) \sim \frac{12\beta_0(1-\gamma)^2}{(1-\gamma^2)[2(2-\gamma)+i\omega]} e^{-i\omega t}
$$

(21)

Setting $\omega = 0$ makes it obvious that the magnetic field breaks the up-down symmetry of the no-field solutions.

### 5.3 Average Values with a Weak Magnetic Field

In place of Eq [10] the average value of spin k must satisfy, in the presence of a (weak) magnetic field $H = H_0 \exp^{i\omega t}$

$$
\dot{q}_k = -q_k + \frac{\gamma}{2} (q_{k-1} + q_{k+1}) + \beta[1 - \frac{\gamma}{2} \{r_{k-1,k} + r_{k,k+1}\}]
$$

(22)

We suppose that the system is close to equilibrium, and approximate by using the equilibrium value $\frac{\gamma}{2}$ of the correlation functions $r_{i,k}$. The solution, after the transients have died off, is

$$
q_k(t) \sim 3\beta_0 \frac{2 + \gamma}{2 - \gamma} \frac{1 - \gamma}{1 - \gamma - i\omega} e^{-i\omega t}
$$

(23)

The average value of Glauber’s stochastic magnetization”, $< M(t) > \equiv \mu \sum_k q_k(t)$, is then

$$
< M(t) > = 3\mu^2 H \frac{2 + \gamma}{kT} \frac{1 - \gamma}{1 - \gamma - i\omega} e^{-i\omega t}
$$

(24)
The time-delayed correlation function \( < M(0)M(t) > \) (see Appendix D) is
\[
< M(0)M(t) > = 3\mu^2 \left( \frac{1 + \frac{\gamma}{2}}{1 - \frac{\gamma}{2}} \right) e^{-(1-\gamma)|t|} \tag{25}
\]

The frequency-dependent susceptibility \( \chi(\omega) \), defined by \( < M(t) > = \chi(\omega)H \) is then
\[
\chi(\omega) = 3\mu^2 \frac{2 + \gamma}{kT} \left( \frac{1 - \gamma}{1 - \gamma - i\omega} \right) \tag{26}
\]

5.4 The Fluctuation-Dissipation Theorem

The fluctuation-dissipation theorem, see e.g., [18], was probably motivated by Johnson’s discovery of electrical “noise” voltage across otherwise isolated resistors [16].

Nyquist [17] subsequently related Johnson’s voltage to “thermal agitation” of charges in the resistor, and predicted the magnitude of the voltage \( V \) in a frequency interval \( d\nu \) to depend upon the values of the ambient temperature \( T \) and the resistance \( R \), according to
\[
V^2 d\nu = 4RkT d\nu \tag{27}
\]
In the present context, following Glauber, we can let the magnetic field frequency \( \omega \) simulate the frequency of the “thermal agitation”. Then the Fourier transform of the magnetization correlation function, Eq 25 is
\[
\int_{-\infty}^{\infty} dt < M(0)M(t) > e^{i\omega t} = 3\mu^2 \left( \frac{1 + \frac{\gamma}{2}}{1 - \frac{\gamma}{2}} \right) \frac{2(1-\gamma)}{(1-\gamma)^2 + \omega^2} = \frac{2kT}{\omega} Im\chi(\omega) \tag{28}
\]
Thus \( \frac{2kT}{\omega} \) times the imaginary, or absorptive, part of the susceptibility, in this magnetic example, plays the role of the resistance in the case of Johnson noise. As Glauber points out, relations such as this may be useful in finding the effect of a weak field upon general functions of the spin variables in Ising-type models.

6 Discussion and Conclusions

The dynamic Ising model in one dimension would seem, at first blush, to be somewhat insipid—it can do nothing except relax to equilibrium. The paths to equilibrium, however, can involve all eight of the possible configurations, in the case of three spins. This raises the possibility of interesting patterns occurring in similar systems with larger numbers of spins. Even the three-spin model becomes more interesting, when used interactively, that is, by repeatedly shifting the equilibrium temperature. This is done by repeatedly changing the value of the \( \gamma \) parameter, randomly or otherwise.

The three-spin model with a weak magnetic field shows an amusing relationship to the infinite-spin model considered by Glauber. The susceptibility in Glauber’s Eq. 94 (see also his Eq. 56) contains a term \( \frac{1}{1+\eta} \), which can be re-expressed as \( \sqrt{\frac{1+\eta}{2}} \). The equivalent three-spin term in Eq 26 is just the small \( \gamma \) (weak-coupling) approximation to Glauber’s expression.
**Acknowledgements**

I am deeply indebted to Dr. Jason Green for introducing me to the notion of thermodynamics of small systems, to Cosmas Zachos for bringing Glauber’s paper to my attention, and to both of them for many pleasant and fruitful discusions, and Dr. Robert Blair for assistance with the manuscript. This work was supported in part by the U.S. Department of Energy, Division of High Energy Physics, under Contract DE-AC02-06CH11357.

**APPENDICES**

**A TRANSITION PROBABILITIES**

\[
\begin{array}{cccccc}
  s_1 & s_2 & s_3 & w_{1}s_1 & w_{2}(s_2) & w_{3}s_3 \\
  +1 & +1 & +1 & 1 - \gamma & 1 - \gamma & 1 - \gamma \\
  +1 & +1 & -1 & 1 & 1 & 1 + \gamma \\
  +1 & -1 & +1 & 1 & 1 + \gamma & 1 \\
  +1 & -1 & -1 & 1 + \gamma & 1 & 1 \\
  -1 & +1 & +1 & 1 + \gamma & 1 & 1 \\
  -1 & +1 & -1 & 1 & 1 + \gamma & 1 \\
  -1 & -1 & +1 & 1 & 1 + \gamma & 1 \\
  -1 & -1 & -1 & 1 - \gamma & 1 - \gamma & 1 - \gamma
\end{array}
\]

**B AVERAGE VALUE SOLUTIONS**

Summing Eq. (10) over k (for arbitrary number of spins N), and defining \( Q(t) \equiv \sum_k q_k(t) \) gives the equation

\[
\dot{Q}(t) = -(1 - \gamma)Q(t)
\]

with the solution

\[
Q(t) = Q(0)e^{-(1-\gamma)t}
\]

Then, in the present instance of 3 spins we can rewrite Eq (10 ( [14] Eq 32 et seq))

\[
\dot{q}_k(t) = -(1 + \frac{\gamma}{2})q_k(t) + \frac{\gamma}{2}Q(t)
\]

which has the solution

\[
q_k(t) = e^{-(1+\frac{\gamma}{2})t}[q_k(0) + \frac{\gamma}{2}Q(0)\int_0^t e^{\frac{-\gamma}{2}r}d\tau]
\]

which, in turn, gives Eq (11).

**C AVERAGE CORRELATION FUNCTION SOLUTION**

In keeping with the approach in Appendix B, we can define a quantity

\[
R = \sum_{i<k=1}^3 r_{i,k}
\]
The sum of the three equations (13) then gives

$$\dot{R} = -(2 - \gamma)R + 3\gamma$$  \hspace{1cm} (34)

from which we deduce that

$$R(t) = R(0)e^{-(2-\gamma)t} + \frac{3\gamma}{2-\gamma}[1 - e^{-(2-\gamma)t}]$$  \hspace{1cm} (35)

but each of the equations (13) may be written as

$$\dot{r}_{i,k} = \frac{\gamma}{2}(R - r_{i,k}) + \gamma$$  \hspace{1cm} (36)

from which the solution given by Eq (14) may readily be obtained by standard methods.

D  TIME DELAYED CORRELATION AND MAGNETIZATION

The average two-spin time-delay correlation function

$$< s_j(0)s_k(t) > = r_{i,j}(0)e^{-(1-\gamma)t}$$  \hspace{1cm} (37)

is

$$< s_j(0)s_k(t) > =$$

$$\frac{1}{3} < s_j(0)[s_k(0)[2\exp^{-(1+\gamma)t} + \exp^{-(1-\gamma)t}]$$

$$[s_{k-1}(0) + s_{k+1}(0)] > [\exp^{-(1-\gamma)t} - \exp^{-(1+\gamma)t}] =$$

$$\frac{1}{3} [r_{j,k}(0)(2\exp^{-(1+\gamma)t} + \exp^{-(1-\gamma)t} - [r_{j,k-1}(0) + r_{j,k+1}(0)]$$

$$\exp^{-(1+\gamma)t} - \exp^{-(1-\gamma)t}) = r_{i,j}(0)\exp^{-(1-\gamma)t}$$  \hspace{1cm} (38)

where the last equality reflects the fact that the $r_{j,k}$'s are all equal at equilibrium. Summing over both indices (remembering that $r_{j,j} = 1$) and multiplying by $\mu^2$ then leads directly to Eq. 25.

E  SIMULATION AND VIDEO DISPLAY

There are eight possible configurations of the three two-valued spins. We number these as states $N = 1, ..., 8$ according to the scheme:

$N = 1(8)$ for configurations $V_+ (V_-)$

$N = 1 + i$ for configurations $x+i$

$N = 3 + i$ for configurations $x-i$.

The eight states are shown in eight .jpg files.
Transitions among the states, starting from some arbitrarily chosen initial state, with $\gamma$ set in the range [-1,1], are encoded in an interactive python program which may be downloaded from [http://www.hep.anl.gov/may/jlu/ThermoWith3spins/index.html](http://www.hep.anl.gov/may/jlu/ThermoWith3spins/index.html). Just download and open the .tar file at that location and see the resulting README file for more information.

The program simulates the relaxation to equilibrium of a 3-element Ising chain, and is reproduced at the end of this Appendix, augmented with a graphics display. Programs, files and other supporting information can be found at the Web URL address cited above. The Web site also presents results of simulation runs as a graphical comparison of the simulation results with the a corresponding solution of the Master Equation.

The graphical display of a run shows three arrows making transitions among the eight possible states. Each transition is one that is accomplished with a single-spin flip, as illustrated in the "cube" file. also available at the URL cited above. The transition rates, given in Appendix A, are assumed to be the rates of Poisson Processes [22], where the values in Appendix A are multiples of a basic rate “r” specified in The body of the program.

The program starts with the python loop command "while k != numberOfIter". As presently set up, this loop is first entered with the spins in the "ferromagnetic“ state 1”, displayed according the the variable “back1”. Prior to the loop we define functions including eight functions denoted by “$A_n$” (n=1..8), and a function “exponen(x)”. Each $A_n$ function is called when the system is in the state corresponding to the value of “n” and returns three parameters on exit, namely, which of the three possible transitions will be made to a successor state, the rate at which the transition will be made, and the time spent in the current state prior to the transition.

The Poisson flip rate for the successor state is given by the parameter “x”, specified in calling the exponen(x) function. That function randomly determines a waiting time $z$ in the successor state in accordance with the exponential distribution of waiting times for the first event of a Poisson process. The probability, $p(z)$, that the first event has occurred after elapsed time $z$

$$p(z) = \exp(-zx)$$

where $p(z)$ is a random number in the range [0, 1] and $z$ is the elapsed time variable (in the range [0, $\infty$]. Accordingly.

$$z = -\frac{\ln\text{randomnumberfrom}[0,1]}{x}$$

as has been emphasized by Gillespie [21]. The variable $z$ obviously represents the time spent in the successor state.

During a single run of the simulation the fluctuations among the 8 possible states are large, making it difficult to “eyeball” an average time behavior to compare with the X(t), Y(t), ... functions given by the solution to the master equation. The conventional method is to use ensemble averaging [23], by running the simulation using the same initial state but with different random number seeds. The states as a function of time are combined and sorted into small time bins for which the average values of X(t), Y(t),... are easily calculated. Typically results from 50 to 100 runs are sufficient to obtain values in which the fluctuations are sufficiently small (i.e. standard deviation values for X(t) of 0.0806 and 0.0672 respectively) for reasonable comparisons to the master equation solutions. Both the master equation relaxation times and asymptotic values are well reproduced by the simulation. Plots of these are available at the web site.
For a single interactive display run of the simulation which shows the 3-spin state as a function of time, we also show a plot of the X(t) and Y(t) function using a different averaging technique to give the user an indication of how the system relaxes to equilibrium. The algorithm accumulates, at each instant, the time spent in each of the states from time zero, thereby estimating the probabilities of each state as a function of time. This method reproduces the general behavior of the X(t), Y(t), and asymptotic values.

A Python program to simulate the behavior of a 3 spin system using a Stochastic Monte Carlo Approach:

```python
#!/usr/bin/python # this is a code to do a stochastic simulation of the dynamic time evolution of a state consisting of # 3 spin 1/2 objects based on a state transition diagram which specifies the available transitions # among the 8 possible states and the forward and backward transition rates. # Jack Uretsky and Ed May 2011 # this is glauber3spinSimulation3.py # this is revised to use exponential distribution in the A_ functions # to calculate the time of the next transition based on the rate local to the # A_ function # A graphical display (based on Tk functions) of the state and the X and Y functions as a function # of the iteration step. The display updates in the time determined by the simulation

import sys import time import random import math
debugevel = 0

def expon(x) : z = random.random() expValue = -math.log(z)/x return expValue

if len(sys.argv) >= 1: print "Usage: view3spinSimulation3.py stateid gamma numberOfIterations seed" print "For example: view3spinSimulation3.py 1 0.25 325 1379" time.sleep(2) # sleep for 2 seconds then continue with the simulation using default configuration #sys.exit() graphicsmode = "Tkinter" # view3spinSimulation3.py [ Tkinter ] stateid gamma numberOfIterations runN seed # view3spinSimulation3.py stateid gamma numberOfIterations seed # 1 2 3 4 5 # decode the command argument list to get initial parameters k=0 for arg in sys.argv: #print "Command line",arg,k k=k+1 graphicsmode =
```
Tkinter

initialstateid = 1  # all spins Up if len(sys.argv) 
>= 2 : initialstateid = int(sys.argv[1]) initialgamma = 0.25
if len(sys.argv) >= 3 : initialgamma = float(sys.argv[2])
numberOfIter = 325  # fills the iteration length of the
display
if len(sys.argv) >= 4 : numberOfIter = int(sys.argv[3])
initialrunN = 1
initialseed = 137
if len(sys.argv) >= 5 : initialseed = int(sys.argv[4])

if initialgamma <=-1.0 :
    print "Unphysical value for gamma...Exit"
    exit()

if initialgamma >=+1.0 :
    print "Unphysical value for gamma...Exit"
    exit()

print
print "User requested graphicsmode=",graphicsmode,"initialstateid=",initialstateid
print "gamma=",initialgamma,"numberOfIter=",numberOfIter, "initialseed=",initialseed
print
from sys import exit
import time
import random
from math import *
global gamma
gamma = initialgamma
runN=initialrunN
# setup structures to communicate with A_ functions
global RET
RET = [0,0,0]  # will contain the triple state, rate, time given by the A_ functions
global state
global r
global N

# setup a dictionary to store state spin patterns for 3 spins 0=spin down 1=spin up
def bits(state) :
    s=''
# The A_ functions change the state at time t based on state diagram

def A_1():
    state = 1  # current state
    r = 1 - gamma
    f = random.randint(0, 2)
    g = f + 2  # destination
    t = expon(3*r)
    RET = [g, r, t]  # g is new state after time t
    return RET

def A_2():
    state = 2
    global r2
    r2 = 1 + gamma
    f = random.random()
    if f > 2. / (3 + gamma):
        g = 1
    elif f > 1. / (3 + gamma):
        g, r2 = 7, 1
    else:
        g, r2 = 6, 1
    t = expon(r2 + 2.0)
    RET = [g, r2, t]
    return RET

def A_3():
    state = 3
    global r3
    r3 = 1 + gamma
    f = random.random()
    if f > 2. / (3 + gamma):
        g = 1
    elif f > 1. / (3 + gamma):
        g, r3 = 7, 1
    else:
        g, r3 = 5, 1
    t = expon(r3 + 2.0)
```python
RET = [g,r3,t]
return RET

def A_4():
    state = 4
    global r4
    r4 = 1. + gamma
    f = random.random()
    if f > 2./(3. + gamma):
        g = 1
    elif f > 1./(3. + gamma):
        g, r4 = 5, 1
    else:
        g, r4 = 6, 1
    t = expon(r4+2.0)
    RET = [g, r4, t]
    return RET

def A_5():
    state = 5
    global r5
    r5 = 1. + gamma
    f = random.random()
    if f > 2./(3. + gamma):
        g = 8
    elif f > 1./(3. + gamma):
        g, r5 = 4, 1
    else:
        g, r5 = 3, 1
    t = expon(r5+2.0)
    RET = [g, r5, t]
    return RET

def A_6():
    state = 6
    global r6
    r6 = 1. + gamma
    f = random.random()
    if f > 2./(3. + gamma):
        g = 8
    elif f > 1./(3. + gamma):
```
g, r6 = 4, 1
else:
g, r6 = 2, 1
t = expon(r6 + 2.0)
RET = [g, r6, t]
return RET

def A_7():
    state = 7
    global r7
    r7 = 1. + gamma
    f = random.random()
    if f > 2. / (3. + gamma):
g = 8
    elif f > 1. / (3. + gamma):
g, r7 = 3, 1
    else:
g, r7 = 2, 1
    t = expon(r7 + 2.0)
    RET = [g, r7, t]
    return RET

def A_8():
    state = 8
    global r8
    r8 = 1. - gamma
    f = random.randrange(3)
    g = f + 5
    t = expon(3 * r8)
    RET = [g, r8, t]
    return RET

# dictionaries
Adestin = {1: A_1, 2: A_2, 3: A_3, 4: A_4, 5: A_5, 6: A_6, 7: A_7, 8: A_8}
apics = {1: 'IMAGES/a_1.jpg', 2: 'IMAGES/a_2.jpg', 3: 'IMAGES/a_3.jpg', 4: 'IMAGES/a_4.jpg',
         5: 'IMAGES/a_5.jpg', 6: 'IMAGES/a_6.jpg', 7: 'IMAGES/a_7.jpg', 8: 'IMAGES/a_8.jpg'}
state = initialstateid
print "Beginning state=", state
iseed = initialiseed
random.seed(iseed)
# open a data output file to store simulation data for this run
openfile=open('glauber3spinSimulation.data','w')
# open a data output file to store configuration parameters for this run, used for plotting
openfileconf=open('glauber3spinSimulation.conf','w')

back1 = apics[state]  # setup the initial state

if graphicsmode == "Tkinter" :
    # Setup Tkinter graphics
    # create the canvas, size in pixels
    canvas = Canvas(width = 700, height = 750, bg = 'yellow')
    # pack the canvas into a frame/form
    canvas.pack(expand = YES, fill = BOTH)
    # create the X axis (ie iteration count)
    for i in range(50,700) :
        canvas.create_text(i,625,fill='black',text='-',
        asymX = (3*(1-gamma))/(2*(2-gamma))
        j=625-100*asymX
        for i in range(650,700) :
            canvas.create_text(i,j,fill='black',text='.')
    canvas.create_text(600,625,fill='black',text='iteration')
    canvas.create_text(600,525,fill='red',text='X() simulation')
    canvas.create_text(600,545,fill='blue',text='Y() simulation')
    # create the Y axis at x=50
    for i in range(525,725) :
        canvas.create_text(50,i,fill='black',text='.')
    # create the Y axis tick marks
    for i in range(45,55) :
        canvas.create_text(i,525,fill='black',text='.')
        canvas.create_text(i,625,fill='black',text='-')
        canvas.create_text(i,725,fill='black',text='.')
        canvas.create_text(30,525,fill='black',text='1.0')
        canvas.create_text(30,625,fill='black',text='0.0')
        canvas.create_text(30,725,fill='black',text='-1.0')
    canvas.update()

k=0
vPlusCnt=0.
vMinusCnt=0.
xPlusCnt=0.
xMinusCnt=0.
pXsum=0.0
pX=0.0
pY=0.0
arbTime = 0.
xAtTime = 0.
xAtZero=0.0
statePop=[]
for i in range(8):
    statePop.append(0)

# write configuration data information
openfile.write('# iseed = '+str(iseed)+' init state = '+str(state)+' gamma = '+str(initialgamma)+'
openfile.write('# numberOfIterations = '+str(numberOfIter) + '
')

# write out header
openfile.write('# rowIndex'+' '+'state'+' '+'arbTime'+' '+'runN'+' '+'pX'+' '+'pY'+'
')

# write out starting state information
openfile.write(str(k)+' '+str(state)+' '+str(arbTime)+' '+str(runN)+'
')

while k <= numberOfIter :
    startTime = time.time()
    oldState=state
    k = k+1
    back1 = apics[state]
    RET = Adestin[state]() # this executes the appropriate A_ function to get a
destin = RET[0]
r = RET[1]
state = destin
if graphicsmode == "Tkinter" :
    # display the state using Tkinter graphics
    filename = 'IMAGES/a_'+str(state)+'.gif'
    filename = 'IMAGES/a_'+str(oldState)+'.gif'
    gifimage = PhotoImage(file = filename)
    canvas.create_image(20, 10, image = gifimage, anchor = NW)
    j= 625-100*pX
    k2 = 2*k+50
    canvas.create_text(k2,j,fill='red',text='x')
    j= 625-100*pY
    canvas.create_text(k2,j,fill='blue',text='+')
canvas.update()

# get time generated in the A_ functions
rest = RET[2]
arbTime=arbTime+rest
statePop[oldState-1] += rest # update a time weighted state
state1Prob = float(statePop[0])/arbTime
#
#={1:'111', 2:'011', 3:'101', 4:'110', 5:'100', 6:'010', 7:'001', 8:'000'} # jacks 21oct10
#if (state==1) : vPlusCnt=vPlusCnt+1
#if (state==8) : vMinusCnt=vMinusCnt+1
#if (state==2 or state==3 or state==4) : xPlusCnt=xPlusCnt+1
#if (state==5 or state==6 or state==7) : xMinusCnt=xMinusCnt+1
# calculate various time weighted average for various X,Y,U,V functions at current time
vPlusCnt = statePop[0]
vMinusCnt= statePop[7]
xPlusCnt = statePop[1]+statePop[2]+statePop[3]
xMinusCnt= statePop[4]+statePop[5]+statePop[6]
vPlus = float(vPlusCnt)/arbTime
vMinus = float(vMinusCnt)/arbTime
v = vPlus + vMinus
pVplus = float(vPlusCnt)/arbTime
pVminus = float(vMinusCnt)/arbTime
pV = pVplus + pVminus
pXplus = float(xPlusCnt)/arbTime
pXminus = float(xMinusCnt)/arbTime
pX = pXplus + pXminus
pY = pXplus - pXminus

#pXave = pXsum/arbTime
#
xAtTime=xAtZero*exp(-2*(2-gamma)*arbTime) +(3*(1-gamma)*(1.0 - exp(-2*(2-gamma)*arbTime)))/arbTime)
#
print "\r\rAt iteration=%d state=%s pX=%6.4f time=%6.3f % (k,bits(oldState),pX,arbTime),
sys.stdout.flush()
openfile.write(str(k)+' '+str(state)+' '+str(arbTime)+' '+str(runN)+' '+str(pX)+' '+str(pY)+'

time.sleep(rest)

print "\n"
\[ pU = pV_{\text{plus}} - pV_{\text{minus}} \]
\[ pY = pX_{\text{plus}} - pX_{\text{minus}} \]

print "At end of iterations X=%5.3f Y=%5.3f V=%5.3f U=%5.3f" % (pX,pY,pV,pU)
if ( debuglevel > 0 ) :
    for i in range(8):
        print "%5.3f " % statePop[i-1],
    print
    for i in range(8):
        print "%5.3f " % (float(statePop[i-1])/arbTime),
    print

print
print "lastTime = %8.3f" % arbTime
print "gamma =",gamma
print "Running at single spin flip rate (flips/sec) = %5.3f" % (numberOfIter/arbTime)
print "initialseed =",initialseed
print "Master Equation prediction at gamma = ", gamma," and t--> infinity",
print "X=%5.3f" % ( (3*(1-gamma))/(2*(2-gamma)) )

openfileconf.write("lastTime = "+str(arbTime)+'\n')
onopenfileconf.write("gamma = "+str(gamma)+'\n')
onopenfileconf.write("initialseed = "+str(initialseed)+'\n')
print "end of program"

openfile.close()
onopenfile.close()
print '\a', '\a', '\a' # ring terminal bell
time.sleep(10)

print "That's All, Folks!"

References

[1] M. Le Bellac, F. Mortessagne and G. Batrouni *Equilibrium and Non-Equilibrium Statistical Thermodynamics* Cambridge University Press, Cambridge, U. K., 2004)

[2] R. Kubo, *Statistical Mechanics* (Elsevier, Amsterdam, The Netherlands, 1985)

[3] W. Lenz, *Physik.Z.*, 21 (1920)613; History in S. Brush RevModPhys. 39(1967)883

[4] Racz, Zoltan, in Privman (Ed.), *Nonequilibrium Statistical Mechanics in One Dimension* (Cambridge University Press, Cambridge 1997)

[5] R.J.Glauber, *J. Math. Phys.*, 4, 204 (1963)
[6] B.U. Felderhof, *Rep. on Math. Phys.* 1 (1971)215; Erratum *Id.* 2((1971)151

[7] K. Kawasaki, *Phys. Rev.* 145 (1966) 310

[8] P.L. Garrido, A. Labaria, and J. Marro, *J. Stat. Phys.* 49, (1987) 314

[9] J. S. Lage, *J. Phys. A:* Math. Gen. 18 (1985) 2289-2299

[10] P. Chomaz, *et al.* Nucl. Phys. A797 (2007) 603;nucl-th/070610007; see also, Buendia, *et al.* J. Chem. Phys. 121 (2004) 4193 cond-mat/0402537

[11] H. Kastrup, *Phys. Lett.* B413 (1997) 267; gr-qc/970032v1

[12] I. Mazilu and H.T. Williams, *Am J. of Phys.* 77 (2009) 458

[13] K Huang, *Statistical Mechanics* (John Wiley & Sons, New York 1963)

[14] R. Ter Bush and C. J. Thompson, *Bipolymers* 10 (1971) 961

[15] Terrell L. Hill, *J. Chem. Phys.* 36 (1962) 3182 and subsequent papers.

[16] J. B. Johnson, *Nature* 119 (1927)50

[17] H. Nyquist, *Phys. Rev.*12 (1928) 110

[18] J. M. Rubi, in *Lecture Notes in Physics,* Vol. 100, 233 (Springer, 1984)

[19] Brian D. Ripley, *Stochastic Simulation* (Wiley, New York 1987) Algorithm 3.3, p.55

[20] William Feller. *An Introduction to Probability Theory and its Applications* (Wiley, New York, 2d Ed. 1971) Vol.II, p.11ff

[21] Daniel T. Gillespie, *A General Method for Numerically Simulating the Stochastic Time Evolution of Coupled Chemical Reactions.* Journal of Computational Physics 22 (4): 403?434, (1976).

[22] William Feller, *An Introduction to Probability Theory and Its Applications,* Vol. I, 3d Edition, John Wiley & Sons, New York (1968).

[23] M. E. J. Newman and G. T. Barkema, *Monte Carlo Methods in Statistical Physics* Monte Carlo Methods in Statistical Physics, Oxford, U.K.: Oxford University Press, (1999).