Interacting spins in a heat bath

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The master equation for two ferromagnetically coupled Ising spins is considered. The system is assumed to be in contact with a heat bath at temperature T. Accordingly, the transition rates in master-equation are chosen so that the system relaxes to equilibrium at temperature T. The solution of the master equation is derived and the relaxation of the magnetization of the system is obtained.

SYSTEM DESCRIPTION

The system consists of two Ising spins s_1 and s_2. In approriate units, these variables can take two values: $s_i = \pm 1$. The interaction between the spins are ferromagnetic (prefering aligned spins), described by the following interaction energy

$$E(s_1, s_2) = -J s_1 s_2 \,, \tag{1}$$

where J is a positive constant setting the energy scale.

The spins are in contact with a heat bath of temperature T, and so, after a long time, the spins will be in equilibrium at T which means that the probability of a state (s_1, s_2) is given by

$$P^{(e)}(s_1, s_2) = \frac{1}{Z} e^{-\beta E(s_1 s_2)} = \frac{1}{Z} e^{\beta J s_1 s_2} \,, \tag{2}$$

where β is the inverse temperature $\beta = 1/(k_B T)$ and Z is the partition function obtained from the condition

$$\sum_{s_1=\pm 1} \sum_{s_2=\pm 1} P^{(e)}(s_1, s_2) = \frac{1}{Z} \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J s_1 s_2} = 1 \,. \tag{3}$$

Introducing $K \equiv \beta J$, one finds from the above equation

$$Z = 2(e^{2K} + e^{-2K}) \,, \tag{4}$$

and substituting this expression into eq.(2), one obtains the equilibrium distribution

$$P^{(e)}(s_1, s_2) = \frac{e^{K s_1 s_2}}{2(e^{2K} + e^{-2K})} \,. \tag{5}$$

There are two low-energy states with energy $E(\uparrow\uparrow) = E(\downarrow\downarrow) = -J$ and two high-energy states with $E(\downarrow\uparrow) = E(\uparrow\downarrow) = J$, and the corresponding equilibrium probabilities are as follows

$$P^{(e)}(\uparrow\uparrow) = P^{(e)}(\downarrow\downarrow) = \frac{e^K}{Z} \,, \tag{6}$$

$$P^{(e)}(\downarrow\uparrow) = P^{(e)}(\uparrow\downarrow) = \frac{e^{-K}}{Z} \,. \tag{7}$$

KINETIC ISING MODEL FOR 2 SPINS

We introduce dynamics by allowing the 1st or 2nd spin to flip by some rate $w_1(s_1, s_2)$ and $w_2(s_1, s_2)$. Then the master equation for the time-dependent, nonequilibrium distribution $P(s_1, s_2; t)$ is written as

$$\frac{\partial P(s_1, s_2; t)}{\partial t} = -[w_1(s_1, s_2) + w_2(s_1, s_2)] P(s_1, s_2; t) + w_1(-s_1, s_2) P(-s_1, s_2; t) + w_2(s_1, -s_2)] P(s_1, -s_2; t) \,. \tag{8}$$

The first two terms on the right-hand side describe the going out of the state (s_1, s_2) while the last two terms are related to the going into the state (s_1, s_2) by flipping the first or second spin in the $(-s_1, s_2)$ and $(s_1, -s_2)$ states, respectively.

We would like to have a system which relaxes to equilibrium. Since the detailed balance should be satisfied in equilibrium, we have the following conditions for the flip rates:

$$\begin{aligned} w_1(s_1, s_2) P^{(e)}(s_1, s_2) &= w_1(-s_1, s_2) P^{(e)}(-s_1, s_2) \\ w_2(s_1, s_2) P^{(e)}(s_1, s_2) &= w_2(s_1, -s_2) P^{(e)}(s_1, -s_2) \,. \end{aligned} \tag{9}$$

Using eq.(5), the above conditions can be rewritten as

$$\frac{w_1(s_1, s_2)}{w_1(-s_1, s_2)} = \frac{e^{-2K s_1 s_2}}{1} = \frac{1}{e^{2K s_1 s_2}} \tag{10}$$

$$\frac{w_2(s_1, s_2)}{w_2(s_1, -s_2)} = \frac{e^{-2K s_1 s_2}}{1} = \frac{1}{e^{2K s_1 s_2}} \tag{11}$$

One can easily see that the above equations are satisfied with the following choice of flip rates

$$w_1(\uparrow\uparrow) = w_2(\uparrow\uparrow) = w_1(\downarrow\downarrow) = w_2(\downarrow\downarrow) \;=\; e^{-2K} \tag{12}$$

$$w_1(\uparrow\downarrow) = w_2(\uparrow\downarrow) = w_1(\downarrow\uparrow) = w_2(\downarrow\uparrow) \;=\; 1 \,. \tag{13}$$

The above flip rates are frequently used. They correspond to the choice of rates of $w = 1$ if the flip decreases the energy while $w = e^{-\beta \delta E}$ if the flip increases the energy ($\delta E > 0$).

Note that the dimension of the flip rate w is 1/time, so one should multiply the rates in eqs.(12,13) by $1/\tau$ where τ is a characteristic time of the spin-flip process. It is treated as a parameter of the model, and setting $\tau = 1$ means that the time is measured in units of τ.

MASTER EQUATION IN MATRIX FORM

Using the spin-flip rates (12,13), the master equation (8) can be written as

$$\begin{aligned}
\partial_t P(\uparrow\uparrow,t) &= -2e^{-2K}P(\uparrow\uparrow,t) + P(\downarrow\uparrow,t) + P(\downarrow\uparrow,t) + 0 && (14)\\
\partial_t P(\downarrow\uparrow,t) &= e^{-2K}P(\uparrow\uparrow,t) - 2\,P(\downarrow\uparrow,t) + 0 + e^{-2K}P(\downarrow\downarrow,t) && (15)\\
\partial_t P(\uparrow\downarrow;t) &= e^{-2K}P(\uparrow\uparrow,t) + 0 - 2\,P(\uparrow\downarrow,t) + e^{-2K}P(\downarrow\downarrow,t) && (16)\\
\partial_t P(\downarrow\downarrow;t) &= 0 + P(\uparrow\downarrow,t) + P(\downarrow\uparrow,t) - 2e^{-2K}P(\downarrow\downarrow,t)\,. && (17)
\end{aligned}$$

Introducing the notation

$$\vec{P}(t) = \begin{pmatrix} P(\uparrow\uparrow,t) \\ P(\downarrow\uparrow,t) \\ P(\downarrow\uparrow,t) \\ P(\downarrow\downarrow,t) \end{pmatrix}, \tag{18}$$

we can write the master equation (14-17) in a matrix form

$$\partial_t \vec{P}(t) = \mathbb{A}\vec{P}(t) \tag{19}$$

where the matrix $\mathbb{A}$ is called the evolution matrix, and is obtained from the comparison of eqs.(14-17) with eqs. (18) and (19)

$$\mathbb{A} = \begin{pmatrix} -2e^{-2K} & 1 & 1 & 0 \\ e^{-2K} & -2 & 0 & e^{-2K} \\ e^{-2K} & 0 & -2 & e^{-2K} \\ 0 & 1 & 1 & -2e^{-2K} \end{pmatrix}. \tag{20}$$

The equilibrium distribution is a stationary solution of the master equation which means that the vector

$$\vec{P}^{(e)} = \frac{1}{2(e^K + e^{-K})} \begin{pmatrix} e^K \\ e^{-K} \\ e^{-K} \\ e^K \end{pmatrix}, \tag{21}$$

is an eigenvector of the matrix $\mathbb{A}$ with eigenvalue $\lambda_1 = 0$. This can be easily verified by just calculating $\mathbb{A}\vec{P}^{(e)}$.

In order to describe the time evolution starting from any initial state $\vec{P}(0)$, we must find the remaining three eigenvalues λ_i $(i = 2, 3, 4)$ and the corresponding eigenvectors $\vec{P}^{(i)}$. Indeed, once we have accomplished this task, we know that the time evolution of the i-th eigenvector is given by

$$\vec{P}^{(i)}(t) = a_i e^{\lambda_i t}\vec{P}^{(i)} \tag{22}$$

where $\vec{P}^{(i)}(0) = a_i\vec{P}^{(i)}$. Then we can write a general solution in the form

$$\vec{P}(t) = \vec{P}^{(e)} + \sum_{i=2}^{4} a_i e^{\lambda_i t}\vec{P}^{(i)}, \tag{23}$$

and the coefficients a_i are determined from the initial condition

$$\vec{P}(0) = \vec{P}^{(e)} + \sum_{i=2}^{4} a_i\vec{P}^{(i)}. \tag{24}$$

Note that, written out for the components of the vectors, we have here 4 equations for 3 coefficients a_i $(i = 2, 3, 4)$. There is, however, the normalization condition

$$\sum_{i=1}^{4}\vec{P}(t) = \sum_{i=1}^{4}\vec{P}(0) = 1 \tag{25}$$

and so we really have only three coefficients to determine.

DIAGONALIZING THE EVOLUTION MATRIX

Looking at the equilibrium distribution vector $\vec{P}^{(e)}$ [see eq.(21)], one can notice that the vector has the following symmetry: $\vec{P}^{(e)}(s_1, s_2) = \vec{P}^{(e)}(-s_1, -s_2)$, i.e. the probability of a state remains the same when both spins are flipped. This is understandable since the sytem has a symmetry: The expression of the energy is invariant under the flipping of both spins, $E(s_1, s_2) = -Js_1s_2 = E(-s_1, -s_2)$ and, consequently, the Boltzmann factors $\sim e^{-\beta E}$ have the same symmetry.

There is, however, something more general here. For systems of such up-down symmetry one has the following results from group theory: All the eigenvectors of the matrix $\mathbb{A}$ are either symmetric or antisymmetric under the simultaneous flipping of all the spins. It follows then that we can search for the eigenvectors of $\mathbb{A}$ by assuming the following forms (of course, we may also just try to find such eigenvectors without any reference to group theory)

$$\vec{P}^{(i)}_{\text{sym}} \sim \begin{pmatrix} a \\ b \\ b \\ a \end{pmatrix} \quad \text{or} \quad \vec{P}^{(i)}_{\text{antisym}} \sim \begin{pmatrix} c \\ d \\ -d \\ -c \end{pmatrix}. \tag{26}$$

Let us begin by finding the symmetric eigenvectors. The four algebraic equations obtained from the components of the eigenvalue equation

$$\mathbb{A}\vec{P}^{(i)}_{\text{sym}} = \lambda_i\vec{P}^{(i)}_{\text{sym}} \tag{27}$$

are not independent. They yield only two equations

$$-2e^{-2K}a + 2b = \lambda_i a \quad , \quad 2e^{-2K}a - 2b = \lambda_i b\,. \tag{28}$$

Adding up the above equations, we obtain

$$\lambda_1(a+b) = 0\,, \tag{29}$$

and the two solutions of the above equation are $\lambda_1 = 0$ and $b = -a$.

For the case of $\lambda_1 = 0$, we should get the equilibrium distribution and, indeed, setting $\lambda_1 = 0$ in the equations (28), we find $b = e^{-2K}a$, and normalizing the distribution leads to eq.(21), and thus

$$\lambda_1 = 0 \quad , \quad \vec{P}^{(1)} = \vec{P}^{(e)}\,. \tag{30}$$

For the second case of $b = -a$ we obtain from eqs.(28)

$$\lambda_2 = -2(1+e^{-2K}) \quad , \quad \vec{P}^{(2)} = \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}\,. \tag{31}$$

Let us turn now to the antisymmetric eigenvectors. The eigenvalue equation

$$\mathbb{A}\vec{P}^{(i)}_{\text{antisym}} = \lambda_i \vec{P}^{(i)}_{\text{antisym}} \tag{32}$$

yields again two equations for the parameters c and d

$$-2e^{-2K}c = \lambda_i c \quad , \quad -2d = \lambda_i d\,. \tag{33}$$

The two soulutions of the above equations are $\lambda_3 = -2e^{-2K}$ with $d = 0$ and $\lambda_4 = -2$ with $c = 0$. Thus the remaining eigenvalues and eigenvevtors are as follows:

$$\lambda_3 = -2e^{-2K} \quad , \quad \vec{P}^{(3)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}\,, \tag{34}$$

and

$$\lambda_4 = -2 \quad , \quad \vec{P}^{(4)} = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}\,. \tag{35}$$

All the eigenvalues and eigenvectors of the dynamical matrix (eqs.30,31,34,35) have been found, and we can see that apart from the zero eigenvalue ($\lambda_1 = 0$) related to the equilibrium state, all other eigenvalues are negative ($\lambda_i < 0$ for $i = 2,3,4$). Thus any initial perturbation described by the eigenvectors $\vec{P}^{(i)}$ with $i = 2,3,4$ die out in the $t \to \infty$ limit and the system relaxes to the equilibrium state. Note that this is not surprising. We have here a discrete, irreducible state space and so the Perron-Frobenius theorem applies.

Having the eigenvalues and eigenvectors of the dynamical matrix, we can turn now to the calculation of the relaxation of the total magnetization $m(t) = \langle s_1 + s_2\rangle_t$ of the system.

RELAXATION OF THE TOTAL MAGNETIZATION

The time evolution of the average of a physical quantity $\langle Q(s_1,s_2)\rangle$ is obtained by averaging over the time-dependent distribution $P(s_1,s_2;t)$

$$Q(t) \equiv \langle Q\rangle_t \equiv \sum_{s_1=\pm1}\sum_{s_2=\pm1} Q(s_1,s_2)P(s_1,s_2;t)\,. \tag{36}$$

Since we would like to calculate the time-evolution of the magnetization of the system, $Q = s_1 + s_2$ in our case, and we have

$$m(t) = \sum_{s_1=\pm1}\sum_{s_2=\pm1}(s_1+s_2)P(s_1,s_2;t)\,. \tag{37}$$

In order to evaluate the above expression we should find $P(s_1,s_2;t)$. To do this, we need some initial condition. For concreteness, let us assume that initially, the system is completely aligned in the + direction ($m(t=0) = 2$), i.e. $P(\uparrow\uparrow, t=0) = 1$ and all the other probabilities are zero

$$\vec{P}(t=0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}\,. \tag{38}$$

Then the coefficient a_i in the general solution of the master equation (23) can be determined using the initial condition (24) which, written out for the components take the form

$$1 = \frac{e^K}{Z}a_1 + a_2 + a_3 \tag{39}$$

$$0 = \frac{e^{-K}}{Z}a_1 - a_2 + a_4 \tag{40}$$

$$0 = \frac{e^{-K}}{Z}a_1 - a_2 - a_4 \tag{41}$$

$$0 = \frac{e^K}{Z}a_1 + a_2 - a_3\,. \tag{42}$$

Subtracting (41) from (40), we find $a_4 = 0$ while subtracting (42) from (39) resluts in $a_3 = 1/2$. Using these values, eqs.(39) and (40) yield $a_1 = 1$ and $a_2 = e^{-K}/Z$ [note that we did not assume that the coefficient in front of $\vec{P}^{(e)}$ would be unity, it emerged from the equations as it should since the equilibrium distribution (21) is already normalized].

Using the coefficints a_i as well as the eigenvalues related to the ith eigenvector, the solution of the master equation satisfying the initial condition (38) can be written as

$$\vec{P}(t) = \frac{1}{Z}\begin{pmatrix} e^K \\ e^{-K} \\ e^{-K} \\ e^K \end{pmatrix} + e^{-2(1+e^{-2K})t}\,\frac{e^{-K}}{Z}\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix} + e^{-2e^{-2K}t}\,\frac{1}{2}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} . \quad (43)$$

Collecting the components, we have

$$\vec{P}(t) = \begin{pmatrix} \frac{e^K}{Z} + e^{-2(1+e^{-2K})t}\,\frac{e^{-K}}{Z} + e^{-2e^{-2K}t}\,\frac{1}{2} \\ \frac{e^{-K}}{Z} - e^{-2(1+e^{-2K})t}\,\frac{e^{-K}}{Z} \\ \frac{e^{-K}}{Z} - e^{-2(1+e^{-2K})t}\,\frac{e^{-K}}{Z} \\ \frac{e^K}{Z} + e^{-2(1+e^{-2K})t}\,\frac{e^{-K}}{Z} - e^{-2e^{-2K}t}\,\frac{1}{2} \end{pmatrix} . \quad (44)$$

We have now all $P(s_1, s_2, t)$ and can evaluate $m(t)$ as given by (37). Looking at the sum (37), we can notice that $s_1+s+2 = 0$ for the $\downarrow\uparrow$ and $\uparrow\downarrow$ states, while $s_1+s_2 = 2$ for the $\uparrow\uparrow$ and $s_1+s_2 = -2$ for the $\downarrow\downarrow$ states. Thus the sum reduces to the following expression

$$m(t) = 2\,[\,P(\uparrow\uparrow, t) - P(\downarrow\downarrow, t)\,] \,. \quad (45)$$

Using now the $\vec{P}(t)$ components from (44), we find

$$m(t) = 2\,e^{-2e^{-2K}t} \,. \quad (46)$$

Thus the magnetization of the system relaxes exponentially with a relaxation time given as the inverse of one of the eigenvalues of the dynamical matrix

$$\tau_{relax} = \frac{1}{2}e^{2K} = \frac{1}{2}e^{2J/k_BT} \,. \quad (47)$$

As can be seen, the relaxation time diverges as the temperature goes to zero. It is understandable, the characteristic thermal energy coming from the heat bath is k_BT, and it is not enough to overturn the spins since the energy of overturning is J and $J \gg k_BT$ at low temperatures.