On the Ising spin model

František Štampach

MAFIA student conference

August 18-21, 2015

Contents

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.

The general Ising model

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.
- It can be thought of as a model of a magnet.

The general Ising model

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.
- It can be thought of as a model of a magnet.
- Consider a lattice of cells (particles, molecules,...) labelled by $n = 1, 2, \ldots, N$.

The general Ising model

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.
- It can be thought of as a model of a magnet.
- Consider a lattice of cells (particles, molecules,...) labelled by $n = 1, 2, \ldots, N$.
- Suppose that each particle n has two possible configurations (spin):

$$\sigma_n = +1, \text{ (parallel, spin up, “+”)} \qquad \sigma_n = -1, \text{ (anti-parallel, spin down, “-”)}$$

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.
- It can be thought of as a model of a magnet.
- Consider a lattice of cells (particles, molecules,...) labelled by $n = 1, 2, \dots, N$.
- Suppose that each particle n has two possible configurations (spin):

$$\sigma_n = +1, \text{ (parallel, spin up, “+”)} \qquad \sigma_n = -1, \text{ (anti-parallel, spin down, “-”)}$$

- The vector of all N spins is a configuration of the system:

$$\sigma = (\sigma_1, \dots, \sigma_N).$$

The general Ising model

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.
- It can be thought of as a model of a magnet.
- Consider a lattice of cells (particles, molecules,...) labelled by $n = 1, 2, \ldots, N$.
- Suppose that each particle n has two possible configurations (spin):

$$\sigma_n = +1, \text{ (parallel, spin up, “+”)} \qquad \sigma_n = -1, \text{ (anti-parallel, spin down, “-”)}$$

- The vector of all N spins is a configuration of the system:

$$\sigma = (\sigma_1, \ldots, \sigma_N).$$

- The energy of the system is made up by two parts:

$$E(\sigma) = E_0(\sigma) + E_1(\sigma)$$

where $E_0 \ldots$ “intermolecular forces”; $E_1 \ldots$ “spin–external field interaction”.

The general Ising model

- Classical model of equilibrium statistical mechanics proposed by Ising in 1925.
- It can be thought of as a model of a magnet.
- Consider a lattice of cells (particles, molecules,...) labelled by $n = 1, 2, \dots, N$.
- Suppose that each particle n has two possible configurations (spin):

$$\sigma_n = +1, \text{ (parallel, spin up, “+”)} \qquad \sigma_n = -1, \text{ (anti-parallel, spin down, “-”)}$$

- The vector of all N spins is a configuration of the system:

$$\sigma = (\sigma_1, \dots, \sigma_N).$$

- The energy of the system is made up by two parts:

$$E(\sigma) = E_0(\sigma) + E_1(\sigma)$$

  where $E_0 \dots$ “intermolecular forces”; $E_1 \dots$ “spin–external field interaction”.
- In the Ising model we set:

$$E_0(\sigma) = -\sum_{i,j} J_{i,j}\sigma_i\sigma_j \quad \text{and} \quad E_1(\sigma) = -\sum_i H_i\sigma_i$$

  where $J_{i,j}$ stands for spin interaction intensity and H_i the component of external magnetic field in the direction of preferred axis at the i-th site.

Simplifications

1. Dimensionality of the lattice:

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

- In most physical systems the intermolecular forces are effectively short ranged.

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

- In most physical systems the intermolecular forces are effectively short ranged.
- For instance, in inert gases they decay as $\sim r^{-7}$.

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44], on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

- In most physical systems the intermolecular forces are effectively short ranged.
- For instance, in inert gases they decay as $\sim r^{-7}$.
- Thus, most models assume particles interact with their nearest neighbours only.

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

- In most physical systems the intermolecular forces are effectively short ranged.
- For instance, in inert gases they decay as $\sim r^{-7}$.
- Thus, most models assume particles interact with their nearest neighbours only.

3. Constant interaction strength and external fields:

Simplifications

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

- In most physical systems the intermolecular forces are effectively short ranged.
- For instance, in inert gases they decay as $\sim r^{-7}$.
- Thus, most models assume particles interact with their nearest neighbours only.

3. Constant interaction strength and external fields:

- $J_{i,j} = J$, $H_i = H$.

1. Dimensionality of the lattice:

- 1-dimension: most solvable models - treated here [Ising25, Glauber65].
- 2-dimension: very few are solvable ($H = 0$), [Onsager44],
  on the other hand, they are physically very interesting since there are polymers with crystals which have strong horizontal and weak vertical interactions (K_2NiF_4, Rb_2MnF_4), phase transitions, spontaneous magnetization,....
- Higher dimensions: Monte-Carlo simulations, conformal bootstrap method,....

2. Nearest-neighbour interaction:

- In most physical systems the intermolecular forces are effectively short ranged.
- For instance, in inert gases they decay as $\sim r^{-7}$.
- Thus, most models assume particles interact with their nearest neighbours only.

3. Constant interaction strength and external fields:

- $J_{i,j} = J$, $H_i = H$.
- Thus, the Hamiltonian is often of the form

$$E(\sigma) = -J \sum_{i,j} \sigma_i \sigma_j - H \sum_i \sigma_i$$

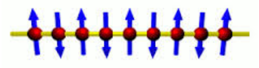
where indices of the first sum ranges “trough nearest-neighbors” only.

Contents

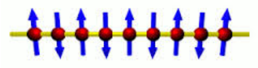
Time evolution of many-spin system

- From now we assume one-dimensional model with no external field ($H = 0$).

- From now we assume one-dimensional model with no external field ($H = 0$).
- In addition, we assume the particles are arranged in regularly spaced linear array.



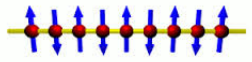
- From now we assume one-dimensional model with no external field ($H = 0$).
- In addition, we assume the particles are arranged in regularly spaced linear array.



- The system is assumed to be under influence of “external agency” (heat reservoir) causing spins of particles to flip between values ± 1 randomly (in time).

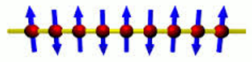
Time evolution of many-spin system

- From now we assume one-dimensional model with no external field ($H = 0$).
- In addition, we assume the particles are arranged in regularly spaced linear array.



- The system is assumed to be under influence of “external agency” (heat reservoir) causing spins of particles to flip between values ± 1 randomly (in time).
- Denote by $p(\sigma; t)$ the probability that the system is in configuration σ at time t.

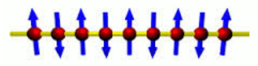
- From now we assume one-dimensional model with no external field ($H = 0$).
- In addition, we assume the particles are arranged in regularly spaced linear array.



- The system is assumed to be under influence of "external agency" (heat reservoir) causing spins of particles to flip between values ± 1 randomly (in time).
- Denote by $p(\sigma; t)$ the probability that the system is in configuration σ at time t.
- 2^N stochastic functions $p(\sigma; t)$ are unknown.

Time evolution of many-spin system

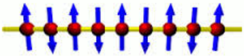
- From now we assume one-dimensional model with no external field ($H = 0$).
- In addition, we assume the particles are arranged in regularly spaced linear array.



- The system is assumed to be under influence of “external agency” (heat reservoir) causing spins of particles to flip between values ± 1 randomly (in time).
- Denote by $p(\sigma; t)$ the probability that the system is in configuration σ at time t.
- 2^N stochastic functions $p(\sigma; t)$ are unknown.
- However, for the model, it is assumed we know the rate of probability transitions (probability of change of configuration per unit time).

Time evolution of many-spin system

- From now we assume one-dimensional model with no external field ($H = 0$).
- In addition, we assume the particles are arranged in regularly spaced linear array.



- The system is assumed to be under influence of "external agency" (heat reservoir) causing spins of particles to flip between values ± 1 randomly (in time).
- Denote by $p(\sigma; t)$ the probability that the system is in configuration σ at time t.
- 2^N stochastic functions $p(\sigma; t)$ are unknown.
- However, for the model, it is assumed we know the rate of probability transitions (probability of change of configuration per unit time).
- We may, for example, introduce a tendency for a particular spin σ_n to correlate with its neighboring spins by assuming the rate depends appropriately on the momentary spin values of the other particles.

General form:

$$\frac{d}{dt}P(\mathcal{C};t) = \sum_{\mathcal{C}'} \left(w_{\mathcal{C}' \to \mathcal{C}} P(\mathcal{C}';t) - w_{\mathcal{C} \to \mathcal{C}'} P(\mathcal{C};t) \right)$$

General form:

$$\frac{d}{dt}P(\mathcal{C};t) = \sum_{\mathcal{C}'} \left(w_{\mathcal{C}'\to\mathcal{C}} P(\mathcal{C}';t) - w_{\mathcal{C}\to\mathcal{C}'} P(\mathcal{C};t) \right)$$

Specialization to our case:

- Let $w_n(\sigma)$ be the probability per unit time that the nth spin flips from the value σ_n to $-\sigma_n$, while the others remain fixed.

General form:

$$\frac{d}{dt}P(\mathcal{C};t) = \sum_{\mathcal{C}'} \left(w_{\mathcal{C}'\to\mathcal{C}}P(\mathcal{C}';t) - w_{\mathcal{C}\to\mathcal{C}'}P(\mathcal{C};t)\right)$$

Specialization to our case:

- Let $w_n(\sigma)$ be the probability per unit time that the nth spin flips from the value σ_n to $-\sigma_n$, while the others remain fixed.
- The master equation reads:

$$\frac{d}{dt}p(\sigma;t) = \sum_n w_n(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N)p(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N;t) - \left(\sum_n w_n(\sigma)\right)p(\sigma;t)$$

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.

Glauber Dynamics

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.
- In addition, it can be desirable to add a tendency for each spin to align itself parallel to its nearest neighbors.

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.
- In addition, it can be desirable to add a tendency for each spin to align itself parallel to its nearest neighbors.
- Glauber's choice for linear spin chain with $H = 0$:

$$w_n(\sigma) = \frac{\alpha}{2}\left[1 - \frac{1}{2}\gamma\sigma_n\left(\sigma_{n-1} + \sigma_{n+1}\right)\right]$$

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.
- In addition, it can be desirable to add a tendency for each spin to align itself parallel to its nearest neighbors.
- Glauber's choice for linear spin chain with $H = 0$:

$$w_n(\sigma) = \frac{\alpha}{2}\left[1 - \frac{1}{2}\gamma\sigma_n\left(\sigma_{n-1} + \sigma_{n+1}\right)\right]$$

- It takes 3 possible values:

$$w_n(\sigma) = \begin{cases} \frac{\alpha}{2}, & \text{if } \sigma_{n-1} = -\sigma_{n+1}, \\ \frac{\alpha}{2}(1-\gamma), & \text{if } \sigma_{n-1} = \sigma_n = \sigma_{n+1}, \\ \frac{\alpha}{2}(1+\gamma), & \text{if } \sigma_{n-1} = -\sigma_n = \sigma_{n+1}. \end{cases}$$

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.
- In addition, it can be desirable to add a tendency for each spin to align itself parallel to its nearest neighbors.
- Glauber's choice for linear spin chain with $H = 0$:

$$w_n(\sigma) = \frac{\alpha}{2}\left[1 - \frac{1}{2}\gamma\sigma_n\left(\sigma_{n-1} + \sigma_{n+1}\right)\right]$$

- It takes 3 possible values:

$$w_n(\sigma) = \begin{cases} \frac{\alpha}{2}, & \text{if } \sigma_{n-1} = -\sigma_{n+1}, \\ \frac{\alpha}{2}(1-\gamma), & \text{if } \sigma_{n-1} = \sigma_n = \sigma_{n+1}, \\ \frac{\alpha}{2}(1+\gamma), & \text{if } \sigma_{n-1} = -\sigma_n = \sigma_{n+1}. \end{cases}$$

- If $\gamma > 0$, then the parallel configurations are longer-lived (ferromagnetic case).

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.
- In addition, it can be desirable to add a tendency for each spin to align itself parallel to its nearest neighbors.
- Glauber's choice for linear spin chain with $H = 0$:

$$w_n(\sigma) = \frac{\alpha}{2}\left[1 - \frac{1}{2}\gamma\sigma_n\left(\sigma_{n-1} + \sigma_{n+1}\right)\right]$$

- It takes 3 possible values:

$$w_n(\sigma) = \begin{cases} \frac{\alpha}{2}, & \text{if } \sigma_{n-1} = -\sigma_{n+1}, \\ \frac{\alpha}{2}(1-\gamma), & \text{if } \sigma_{n-1} = \sigma_n = \sigma_{n+1}, \\ \frac{\alpha}{2}(1+\gamma), & \text{if } \sigma_{n-1} = -\sigma_n = \sigma_{n+1}. \end{cases}$$

- If $\gamma > 0$, then the parallel configurations are longer-lived (ferromagnetic case).
- If $\gamma < 0$, then the antiparallel configurations are longer-lived (antiferromagnetic case).

- Transition rates $w_n(\sigma)$ may be chosen to depend on neighboring spins values as well as on σ_n.
- In addition, it can be desirable to add a tendency for each spin to align itself parallel to its nearest neighbors.
- Glauber's choice for linear spin chain with $H = 0$:

$$w_n(\sigma) = \frac{\alpha}{2}\left[1 - \frac{1}{2}\gamma\sigma_n\left(\sigma_{n-1} + \sigma_{n+1}\right)\right]$$

- It takes 3 possible values:

$$w_n(\sigma) = \begin{cases} \frac{\alpha}{2}, & \text{if } \sigma_{n-1} = -\sigma_{n+1}, \\ \frac{\alpha}{2}(1-\gamma), & \text{if } \sigma_{n-1} = \sigma_n = \sigma_{n+1}, \\ \frac{\alpha}{2}(1+\gamma), & \text{if } \sigma_{n-1} = -\sigma_n = \sigma_{n+1}. \end{cases}$$

- If $\gamma > 0$, then the parallel configurations are longer-lived (ferromagnetic case).
- If $\gamma < 0$, then the antiparallel configurations are longer-lived (antiferromagnetic case).
- It has to be assure $|\gamma| \leq 1$.

Parameter γ - correspondence with the Ising model

- When the Ising model has reached equilibrium at temperature T the probability of the system being in a state σ is
$$\frac{1}{Z}\exp(-E(\sigma)/kT)$$
where Z is the (Gibbs) partition function and k stands for the Boltzmann's constant.

Parameter γ - correspondence with the Ising model

- When the Ising model has reached equilibrium at temperature T the probability of the system being in a state σ is
$$\frac{1}{Z}\exp(-E(\sigma)/kT)$$
where Z is the (Gibbs) partition function and k stands for the Boltzmann's constant.
- Recall we have
$$E(\sigma) = -J\sum_{n}\sigma_n\sigma_{n+1}.$$

Parameter γ - correspondence with the Ising model

- When the Ising model has reached equilibrium at temperature T the probability of the system being in a state σ is
$$\frac{1}{Z}\exp(-E(\sigma)/kT)$$
where Z is the (Gibbs) partition function and k stands for the Boltzmann's constant.
- Recall we have
$$E(\sigma) = -J\sum_{n}\sigma_n\sigma_{n+1}.$$
- Denote by $p_n(\sigma)$ the probability that the nth spin will take on the value σ_n as opposed to $-\sigma_n$ (other spins remain fixed). Then one has
$$\frac{p_n(\ldots,-\sigma_n,\ldots)}{p_n(\ldots,\sigma_n,\ldots)} = \frac{\exp\left(-(J/kT)\sigma_n(\sigma_{n-1}+\sigma_{n+1})\right)}{\exp\left((J/kT)\sigma_n(\sigma_{n-1}+\sigma_{n+1})\right)}.$$

Parameter γ - correspondence with the Ising model

- When the Ising model has reached equilibrium at temperature T the probability of the system being in a state σ is
$$\frac{1}{Z}\exp(-E(\sigma)/kT)$$
where Z is the (Gibbs) partition function and k stands for the Boltzmann's constant.
- Recall we have
$$E(\sigma) = -J\sum_{n}\sigma_n\sigma_{n+1}.$$
- Denote by $p_n(\sigma)$ the probability that the nth spin will take on the value σ_n as opposed to $-\sigma_n$ (other spins remain fixed). Then one has
$$\frac{p_n(\ldots,-\sigma_n,\ldots)}{p_n(\ldots,\sigma_n,\ldots)} = \frac{\exp\left(-(J/kT)\sigma_n(\sigma_{n-1}+\sigma_{n+1})\right)}{\exp\left((J/kT)\sigma_n(\sigma_{n-1}+\sigma_{n+1})\right)}.$$
- On the other hand, in the equilibrium, it has to hold that
$$w_n(\ldots,-\sigma_n,\ldots)p_n(\ldots,-\sigma_n,\ldots) = w_n(\ldots,\sigma_n,\ldots)p_n(\ldots,\sigma_n,\ldots).$$

- When the Ising model has reached equilibrium at temperature T the probability of the system being in a state σ is
$$\frac{1}{Z}\exp(-E(\sigma)/kT)$$
where Z is the (Gibbs) partition function and k stands for the Boltzmann's constant.
- Recall we have
$$E(\sigma) = -J\sum_{n}\sigma_n\sigma_{n+1}.$$
- Denote by $p_n(\sigma)$ the probability that the nth spin will take on the value σ_n as opposed to $-\sigma_n$ (other spins remain fixed). Then one has
$$\frac{p_n(\ldots,-\sigma_n,\ldots)}{p_n(\ldots,\sigma_n,\ldots)} = \frac{\exp\left(-(J/kT)\sigma_n(\sigma_{n-1}+\sigma_{n+1})\right)}{\exp\left((J/kT)\sigma_n(\sigma_{n-1}+\sigma_{n+1})\right)}.$$
- On the other hand, in the equilibrium, it has to hold that
$$w_n(\ldots,-\sigma_n,\ldots)p_n(\ldots,-\sigma_n,\ldots) = w_n(\ldots,\sigma_n,\ldots)p_n(\ldots,\sigma_n,\ldots).$$
- With the Glauber's choice for the rates one finds
$$\frac{p_n(\ldots,-\sigma_n,\ldots)}{p_n(\ldots,\sigma_n,\ldots)} = \frac{w_n(\ldots,\sigma_n,\ldots)}{w_n(\ldots,-\sigma_n,\ldots)} = \frac{1-\frac{1}{2}\gamma\sigma_n(\sigma_{n-1}+\sigma_{n+1})}{1+\frac{1}{2}\gamma\sigma_n(\sigma_{n-1}+\sigma_{n+1})}.$$

Expression for the parameter γ

- Equating the two expressions for the ratio $p_n(\dots, -\sigma_n, \dots)/p_n(\dots, \sigma_n, \dots)$ one gets the formula

$$\gamma = \tanh(2J/kT)$$

Quantities of interest 1/2

- Functions $p(\sigma; t)$ which are solutions of the master equation

$$\frac{d}{dt}p(\sigma; t) = \sum_n w_n(\sigma_1, \dots, -\sigma_n, \dots, \sigma_N)p(\sigma_1, \dots, -\sigma_n, \dots, \sigma_N; t) - \left(\sum_n w_n(\sigma)\right) p(\sigma; t)$$

contain the most complete description of the system available.

Quantities of interest 1/2

- Functions $p(\sigma; t)$ which are solutions of the master equation

$$\frac{d}{dt}p(\sigma; t) = \sum_n w_n(\sigma_1, \ldots, -\sigma_n, \ldots, \sigma_N)p(\sigma_1, \ldots, -\sigma_n, \ldots, \sigma_N; t) - \left(\sum_n w_n(\sigma)\right) p(\sigma; t)$$

  contain the most complete description of the system available.
- Nevertheless, it is usually not possible to find them explicitly.

- Functions $p(\sigma; t)$ which are solutions of the master equation

$$\frac{d}{dt}p(\sigma;t) = \sum_n w_n(\sigma_1,\ldots,-\sigma_n,\ldots,\sigma_N)p(\sigma_1,\ldots,-\sigma_n,\ldots,\sigma_N;t) - \left(\sum_n w_n(\sigma)\right)p(\sigma;t)$$

  contain the most complete description of the system available.
- Nevertheless, it is usually not possible to find them explicitly.
- However, it is not necessary, since they contain vastly more information than we usually require in practice.

Quantities of interest 1/2

- Functions $p(\sigma; t)$ which are solutions of the master equation

$$\frac{d}{dt}p(\sigma;t) = \sum_n w_n(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N)p(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N;t) - \left(\sum_n w_n(\sigma)\right)p(\sigma;t)$$

  contain the most complete description of the system available.
- Nevertheless, it is usually not possible to find them explicitly.
- However, it is not necessary, since they contain vastly more information than we usually require in practice.
- To answer the most familiar physical questions about the system it suffices to know two macroscopic variables.

- Functions $p(\sigma;t)$ which are solutions of the master equation

$$\frac{d}{dt}p(\sigma;t)=\sum_{n}w_n(\sigma_1,\ldots,-\sigma_n,\ldots,\sigma_N)p(\sigma_1,\ldots,-\sigma_n,\ldots,\sigma_N;t)-\left(\sum_{n}w_n(\sigma)\right)p(\sigma;t)$$

  contain the most complete description of the system available.
- Nevertheless, it is usually not possible to find them explicitly.
- However, it is not necessary, since they contain vastly more information than we usually require in practice.
- To answer the most familiar physical questions about the system it suffices to know two macroscopic variables.
- Expectation value of the spins (magnetization):

$$q_n(t):=\langle\sigma_n(t)\rangle=\sum_{\sigma}\sigma_n p(\ldots,\sigma_n,\ldots;t).$$

Quantities of interest 1/2

- Functions $p(\sigma; t)$ which are solutions of the master equation

$$\frac{d}{dt}p(\sigma; t) = \sum_n w_n(\sigma_1, \ldots, -\sigma_n, \ldots, \sigma_N)p(\sigma_1, \ldots, -\sigma_n, \ldots, \sigma_N; t) - \left(\sum_n w_n(\sigma)\right) p(\sigma; t)$$

  contain the most complete description of the system available.
- Nevertheless, it is usually not possible to find them explicitly.
- However, it is not necessary, since they contain vastly more information than we usually require in practice.
- To answer the most familiar physical questions about the system it suffices to know two macroscopic variables.
- Expectation value of the spins (magnetization):

$$q_n(t) := \langle \sigma_n(t) \rangle = \sum_\sigma \sigma_n p(\ldots, \sigma_n, \ldots; t).$$

- Spin correlations:

$$r_{n,k}(t) := \langle \sigma_n(t)\sigma_k(t) \rangle = \sum_\sigma \sigma_n \sigma_k p(\ldots, \sigma_n, \ldots, \sigma_k, \ldots; t).$$

  Note that $r_{n,n}(t) = 1$.

Quantities of interest 2/2

- Alternatively, quantities of interest are probabilities that individual spins or pairs of spins occupy specified states.

$$p_n(\sigma_n; t) = \sum_{\sigma;\ \sigma_n \text{ fixed}} p(\sigma_1, \dots, \sigma_N; t),$$

$$p_{n,k}(\sigma_n, \sigma_k; t) = \sum_{\sigma;\ \sigma_n, \sigma_k \text{ fixed}} p(\sigma_1, \dots, \sigma_N; t).$$

- Alternatively, quantities of interest are probabilities that individual spins or pairs of spins occupy specified states.

$$p_n(\sigma_n;t) = \sum_{\sigma;\ \sigma_n\ \mathit{fixed}} p(\sigma_1,\dots,\sigma_N;t),$$

$$p_{n,k}(\sigma_n,\sigma_k;t) = \sum_{\sigma;\ \sigma_n,\sigma_k\ \mathit{fixed}} p(\sigma_1,\dots,\sigma_N;t).$$

- It can be shown that these probabilities can be expressed in terms of magnetization and spin correlation:

$$p_n(\sigma_n;t) = \frac{1}{2}\left(1+\sigma_n q_n(t)\right),$$

$$p_{n,k}(\sigma_n,\sigma_k;t) = \frac{1}{4}\left(1+\sigma_n q_n(t)+\sigma_k q_k(t)+\sigma_n\sigma_k r_{n,k}(t)\right).$$

Contents

Evolution equation for magnetization

- Recall the master equation:

$$\frac{d}{dt}p(\sigma;t)=\sum_n w_n(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N)p(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N;t)-\sum_n w_n(\sigma)p(\sigma;t)$$

Evolution equation for magnetization

- Recall the master equation:

$$\frac{d}{dt}p(\sigma;t) = \sum_n w_n(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N)p(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N;t) - \sum_n w_n(\sigma)p(\sigma;t)$$

- Multiply both sides by σ_k and sum over all values of σ:

$$\frac{d}{dt}q_k(t) = -2\sum_\sigma \sigma_k w_k(\sigma_1,\dots,\sigma_k,\dots,\sigma_N)p(\sigma_1,\dots,\sigma_k,\dots,\sigma_N;t) = -2\langle\sigma_k w_k(\sigma)\rangle$$

Evolution equation for magnetization

- Recall the master equation:

$$\frac{d}{dt}p(\sigma;t) = \sum_n w_n(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N)p(\sigma_1,\dots,-\sigma_n,\dots,\sigma_N;t) - \sum_n w_n(\sigma)p(\sigma;t)$$

- Multiply both sides by σ_k and sum over all values of σ:

$$\frac{d}{dt}q_k(t) = -2\sum_\sigma \sigma_k w_k(\sigma_1,\dots,\sigma_k,\dots,\sigma_N)p(\sigma_1,\dots,\sigma_k,\dots,\sigma_N;t) = -2\langle\sigma_k w_k(\sigma)\rangle$$

- Substitute the Glauber's expression for the rate w_k:

$$\frac{1}{\alpha}\frac{d}{dt}q_k(t) = -q_k(t) + \frac{1}{2}\gamma\left(q_{k-1}(t) + q_k(t)\right)$$

- Matrix form of the equation for the time evolution of the magnetization ($\alpha = 1$):

$$\dot{q}(t) = -M\, q(t)$$

where

$$M = \begin{pmatrix} 1 & -\gamma/2 & 0 & \dots & 0 \\ -\gamma/2 & 1 & -\gamma/2 & \dots & 0 \\ 0 & -\gamma/2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \qquad q(t) = \begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix}$$

- Matrix form of the equation for the time evolution of the magnetization ($\alpha = 1$):

$$\dot{q}(t) = -M\,q(t)$$

where

$$M = \begin{pmatrix} 1 & -\gamma/2 & 0 & \dots & 0 \\ -\gamma/2 & 1 & -\gamma/2 & \dots & 0 \\ 0 & -\gamma/2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \qquad q(t) = \begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix}$$

- The solution reads:

$$q(t) = \exp(-tM)q(0)$$

- Matrix form of the equation for the time evolution of the magnetization ($\alpha = 1$):

$$\dot{q}(t) = -M\,q(t)$$

where

$$M = \begin{pmatrix} 1 & -\gamma/2 & 0 & \dots & 0 \\ -\gamma/2 & 1 & -\gamma/2 & \dots & 0 \\ 0 & -\gamma/2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \qquad q(t) = \begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix}$$

- The solution reads:

$$q(t) = \exp(-tM)q(0)$$

- Matrix M is hermitian (Jacobi) operator with simple spectrum, hence

$$M = \sum_n \lambda_n \langle V_n, \cdot \rangle V_n$$

where $\lambda_1, \dots, \lambda_N$ are eigenvalues of M and $V_1, \dots, V_N$ are corresponding eigenvectors.

- Matrix form of the equation for the time evolution of the magnetization ($\alpha = 1$):

$$\dot{q}(t) = -M\, q(t)$$

where

$$M = \begin{pmatrix} 1 & -\gamma/2 & 0 & \dots & 0 \\ -\gamma/2 & 1 & -\gamma/2 & \dots & 0 \\ 0 & -\gamma/2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{pmatrix}, \qquad q(t) = \begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix}$$

- The solution reads:

$$q(t) = \exp(-tM)q(0)$$

- Matrix M is hermitian (Jacobi) operator with simple spectrum, hence

$$M = \sum_n \lambda_n \langle V_n, \cdot \rangle V_n$$

where $\lambda_1, \dots, \lambda_N$ are eigenvalues of M and $V_1, \dots, V_N$ are corresponding eigenvectors.

- We arrive at the solution

$$q(t) = \sum_n e^{-t\lambda_n} \langle V_n, q(0) \rangle V_n.$$

- Recall Chebyshev polynomials of the second kind are defined as

$$U_n(\cos\phi) = \frac{\sin\left((n+1)\phi\right)}{\sin\phi}, \quad n = 0, 1, 2, \ldots$$

- Recall Chebyshev polynomials of the second kind are defined as

$$U_n(\cos\phi) = \frac{\sin((n+1)\phi)}{\sin\phi}, \quad n = 0, 1, 2, \ldots$$

- U_n satisfies a system of second order difference equations:

$$U_{n-1}(x) - 2xU_n(x) + U_{n+1}(x) = 0, \qquad U_0(x) = 1, \quad U_1(x) = 2x.$$

- Recall Chebyshev polynomials of the second kind are defined as

$$U_n(\cos\phi) = \frac{\sin((n+1)\phi)}{\sin\phi}, \quad n = 0, 1, 2, \ldots$$

- U_n satisfies a system of second order difference equations:

$$U_{n-1}(x) - 2xU_n(x) + U_{n+1}(x) = 0, \qquad U_0(x) = 1, \quad U_1(x) = 2x.$$

- $U_n(x)$ is a polynomial of degree n with zeros

$$x_k^{(n)} = \cos\left(\frac{k\pi}{n+1}\right), \quad k = 1, \ldots, n.$$

Chebyshev polynomials

- Recall Chebyshev polynomials of the second kind are defined as

$$U_n(\cos\phi) = \frac{\sin\left((n+1)\phi\right)}{\sin\phi}, \quad n = 0, 1, 2, \ldots$$

- U_n satisfies a system of second order difference equations:

$$U_{n-1}(x) - 2xU_n(x) + U_{n+1}(x) = 0, \qquad U_0(x) = 1, \quad U_1(x) = 2x.$$

- $U_n(x)$ is a polynomial of degree n with zeros

$$x_k^{(n)} = \cos\left(\frac{k\pi}{n+1}\right), \quad k = 1, \ldots, n.$$

- From this one easily deduces that $MV_n = \lambda_n V_n$ (with $(V_n)_1 = 1$) iff

$$\lambda_n = \frac{1}{\gamma}\left(1 - \cos\left(\frac{n\pi}{N+1}\right)\right) \quad \text{and} \quad V_n = \left(U_0(\lambda_n), U_1(\lambda_n), \ldots, U_{N-1}(\lambda_n)\right)^T$$

for $n = 1, \ldots, N$.

- Recall Chebyshev polynomials of the second kind are defined as

$$U_n(\cos\phi) = \frac{\sin((n+1)\phi)}{\sin\phi}, \quad n = 0, 1, 2, \dots$$

- U_n satisfies a system of second order difference equations:

$$U_{n-1}(x) - 2xU_n(x) + U_{n+1}(x) = 0, \qquad U_0(x) = 1, \quad U_1(x) = 2x.$$

- $U_n(x)$ is a polynomial of degree n with zeros

$$x_k^{(n)} = \cos\left(\frac{k\pi}{n+1}\right), \quad k = 1, \dots, n.$$

- From this one easily deduces that $MV_n = \lambda_n V_n$ (with $(V_n)_1 = 1$) iff

$$\lambda_n = \frac{1}{\gamma}\left(1 - \cos\left(\frac{n\pi}{N+1}\right)\right) \quad \text{and} \quad V_n = (U_0(\lambda_n), U_1(\lambda_n), \dots, U_{N-1}(\lambda_n))^T$$

  for $n = 1, \dots, N$.
- These formulas yield a precise expression for the time evolution of the magnetization vector $q(t)$.

Approximation for $N \gg 1$ - an infinite chain

- Since the number of particles N of the system is usually assumed to be large, one can consider an approximation of the model with $N \to \infty$ - an infinite chain.

Approximation for $N \gg 1$ - an infinite chain

- Since the number of particles N of the system is usually assumed to be large, one can consider an approximation of the model with $N \to \infty$ - an infinite chain.
- It is convenient, in this case, to alter slightly the scheme of numbering the spins by labeling a particular spin as zeroth and designating those to one side with positive integers and those to the other side with negative integers.

- Since the number of particles N of the system is usually assumed to be large, one can consider an approximation of the model with $N \to \infty$ - an infinite chain.
- It is convenient, in this case, to alter slightly the scheme of numbering the spins by labeling a particular spin as zeroth and designating those to one side with positive integers and those to the other side with negative integers.
- In this scheme, we may take as the equation of motion for magnetization $q(t)$ in the same form as before

$$\dot{q}(t) = -M\, q(t).$$

However, now M is corresponding (infinite) Jacobi matrix acting on $\ell^2(\mathbb{Z})$:

$$M = \begin{pmatrix} \ddots & \ddots & \ddots & & & \\ & -\gamma/2 & 1 & -\gamma/2 & & \\ & & -\gamma/2 & 1 & -\gamma/2 & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

- Since the number of particles N of the system is usually assumed to be large, one can consider an approximation of the model with $N \to \infty$ - an infinite chain.
- It is convenient, in this case, to alter slightly the scheme of numbering the spins by labeling a particular spin as zeroth and designating those to one side with positive integers and those to the other side with negative integers.
- In this scheme, we may take as the equation of motion for magnetization $q(t)$ in the same form as before

$$\dot{q}(t) = -M\, q(t).$$

However, now M is corresponding (infinite) Jacobi matrix acting on $\ell^2(\mathbb{Z})$:

$$M = \begin{pmatrix} \ddots & \ddots & \ddots & & & \\ & -\gamma/2 & 1 & -\gamma/2 & & \\ & & -\gamma/2 & 1 & -\gamma/2 & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

- The solution reads

$$q(t) = \exp(-tM)q(0) = \int_{\mathbb{R}} e^{-t\lambda} dE_M(\lambda) q(0)$$

where E_M is the spectral projection of self-adjoint operator M.

- Since the number of particles N of the system is usually assumed to be large, one can consider an approximation of the model with $N \to \infty$ - an infinite chain.
- It is convenient, in this case, to alter slightly the scheme of numbering the spins by labeling a particular spin as zeroth and designating those to one side with positive integers and those to the other side with negative integers.
- In this scheme, we may take as the equation of motion for magnetization $q(t)$ in the same form as before

$$\dot{q}(t) = -M\, q(t).$$

However, now M is corresponding (infinite) Jacobi matrix acting on $\ell^2(\mathbb{Z})$:

$$M = \begin{pmatrix} \ddots & \ddots & \ddots & & & \\ & -\gamma/2 & 1 & -\gamma/2 & & \\ & & -\gamma/2 & 1 & -\gamma/2 & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

- The solution reads

$$q(t) = \exp(-tM)q(0) = \int_{\mathbb{R}} e^{-t\lambda} dE_M(\lambda)q(0)$$

where E_M is the spectral projection of self-adjoint operator M.
- Thus, the spectral analysis of M is essential.

Diagonalization of discrete Laplacian

- Consider T operator acting on $\ell^2(\mathbb{Z})$ as

$$(T\psi)_n = -\psi_{n-1} + 2\psi_n - \psi_{n+1}, \quad n \in \mathbb{Z}.$$

Diagonalization of discrete Laplacian

- Consider T operator acting on $\ell^2(\mathbb{Z})$ as

$$(T\psi)_n = -\psi_{n-1} + 2\psi_n - \psi_{n+1}, \quad n \in \mathbb{Z}.$$

- T is bounded self-adjoint operator which is explicitly diagonalizable.

Diagonalization of discrete Laplacian

- Consider T operator acting on $\ell^2(\mathbb{Z})$ as

$$(T\psi)_n = -\psi_{n-1} + 2\psi_n - \psi_{n+1}, \quad n \in \mathbb{Z}.$$

- T is bounded self-adjoint operator which is explicitly diagonalizable.
- Fourier transform:

$$U : \ell^2(\mathbb{Z}) \to L^2\left((0, 2\pi], \frac{d\varphi}{2\pi}\right) : \psi \mapsto (U\psi)(\varphi) = \sum_{n \in \mathbb{Z}} \psi_n e^{in\varphi}$$

- Consider T operator acting on $\ell^2(\mathbb{Z})$ as

$$(T\psi)_n = -\psi_{n-1} + 2\psi_n - \psi_{n+1}, \quad n \in \mathbb{Z}.$$

- T is bounded self-adjoint operator which is explicitly diagonalizable.
- Fourier transform:

$$U : \ell^2(\mathbb{Z}) \to L^2\left((0, 2\pi], \frac{d\varphi}{2\pi}\right) : \psi \mapsto (U\psi)(\varphi) = \sum_{n\in\mathbb{Z}} \psi_n e^{in\varphi}$$

- The inverse is clearly

$$(U^{-1}f)_n = \int_0^{2\pi} e^{-in\varphi} f(\varphi) \frac{d\varphi}{2\pi}.$$

- Consider T operator acting on $\ell^2(\mathbb{Z})$ as

$$(T\psi)_n = -\psi_{n-1} + 2\psi_n - \psi_{n+1}, \quad n \in \mathbb{Z}.$$

- T is bounded self-adjoint operator which is explicitly diagonalizable.
- Fourier transform:

$$U : \ell^2(\mathbb{Z}) \to L^2\left((0, 2\pi], \frac{d\varphi}{2\pi}\right) : \psi \mapsto (U\psi)(\varphi) = \sum_{n\in\mathbb{Z}} \psi_n e^{in\varphi}$$

- The inverse is clearly

$$(U^{-1}f)_n = \int_0^{2\pi} e^{-in\varphi} f(\varphi) \frac{d\varphi}{2\pi}.$$

- It is a matter of straightforward computation to verify

$$\left(UTU^{-1}f\right)(\varphi) = 2\left(1 - \cos(\varphi)\right) f(\varphi).$$

The spectral measure of T

- Let $\psi, \chi \in \ell^2(\mathbb{Z})$ and $f \in C([0,4])$ are arbitrary. Denote
$$d\mu_{\psi,\chi}(\lambda) = d\langle \psi, E_T(\lambda)\chi \rangle.$$

- Let $\psi, \chi \in \ell^2(\mathbb{Z})$ and $f \in C([0,4])$ are arbitrary. Denote

$$d\mu_{\psi,\chi}(\lambda) = d\langle \psi, E_T(\lambda)\chi \rangle.$$

- Then

$$\int_0^4 f(\lambda) d\mu_{\psi,\chi}(\lambda) = \langle \psi, f(T)\chi \rangle_{\ell^2} = \langle U\psi, \underbrace{(Uf(T)U^{-1})}_{=f(2(1-\cos\varphi))} U\chi \rangle_{L^2}$$

The spectral measure of T

- Let $\psi, \chi \in \ell^2(\mathbb{Z})$ and $f \in C([0,4])$ are arbitrary. Denote

$$d\mu_{\psi,\chi}(\lambda) = d\langle \psi, E_T(\lambda)\chi \rangle.$$

- Then

$$\int_0^4 f(\lambda) d\mu_{\psi,\chi}(\lambda) = \langle \psi, f(T)\chi \rangle_{\ell^2} = \langle U\psi, \underbrace{\left(Uf(T)U^{-1}\right)}_{=f(2(1-\cos\varphi))} U\chi \rangle_{L^2}$$

$$= \int_0^{2\pi} \overline{U\psi}(\varphi) U\chi(\varphi) f\left(2(1-\cos\varphi)\right) \frac{d\varphi}{2\pi} = \int_0^{\pi} + \int_{\pi}^{2\pi} \ldots \text{subst. } x = 2(1-\cos\varphi)$$

- Let $\psi, \chi \in \ell^2(\mathbb{Z})$ and $f \in C([0,4])$ are arbitrary. Denote

$$d\mu_{\psi,\chi}(\lambda) = d\langle \psi, E_T(\lambda)\chi\rangle.$$

- Then

$$\int_0^4 f(\lambda) d\mu_{\psi,\chi}(\lambda) = \langle \psi, f(T)\chi\rangle_{\ell^2} = \langle U\psi, \underbrace{(Uf(T)U^{-1})}_{=f(2(1-\cos\varphi))} U\chi\rangle_{L^2}$$

$$= \int_0^{2\pi} \overline{U\psi}(\varphi) U\chi(\varphi) f\left(2(1-\cos\varphi)\right) \frac{d\varphi}{2\pi} = \int_0^{\pi} + \int_{\pi}^{2\pi} \ldots \text{subst. } x = 2(1-\cos\varphi)$$

- $$\int_0^4 f(\lambda) d\mu_{\psi,\chi}(\lambda) = \frac{1}{2\pi}\int_0^4 f(x)\Bigg[(\overline{U\psi})\left(\arccos\left(\frac{2-x}{2}\right)\right)(U\chi)\left(\arccos\left(\frac{2-x}{2}\right)\right) + (\overline{U\psi})\left(2\pi - \arccos\left(\frac{2-x}{2}\right)\right)(U\chi)\left(2\pi - \arccos\left(\frac{2-x}{2}\right)\right)\Bigg]\frac{dx}{\sqrt{4x-x^2}}$$

Matrix elements of the spectral measure of T

- Put $\psi = e_m$, $\chi = e_n$ then we get

$$\frac{d\mu_{m,n}(x)}{dx} = \frac{1}{\pi\sqrt{4x - x^2}} \underbrace{\cos\left[(n-m)\arccos\left(\frac{2-x}{2}\right)\right]}_{=T_{|n-m|}\left(\frac{2-x}{2}\right)} \quad \text{on} \quad [0,4].$$

- Put $\psi = e_m$, $\chi = e_n$ then we get

$$\frac{d\mu_{m,n}(x)}{dx} = \frac{1}{\pi\sqrt{4x - x^2}} \underbrace{\cos\left[(n-m)\arccos\left(\frac{2-x}{2}\right)\right]}_{=T_{|n-m|}\left(\frac{2-x}{2}\right)} \quad \text{on} \quad [0,4].$$

- Recall $q(t) = \exp(-tM)q(0)$ and we have the relation

$$M = \frac{\gamma}{2}\left(T - 2\left(1 - \frac{1}{\gamma}\right)I\right)$$

Matrix elements of the spectral measure of T

- Put $\psi = e_m$, $\chi = e_n$ then we get

$$\frac{d\mu_{m,n}(x)}{dx} = \frac{1}{\pi\sqrt{4x - x^2}} \underbrace{\cos\left[(n-m)\arccos\left(\frac{2-x}{2}\right)\right]}_{=T_{|n-m|}\left(\frac{2-x}{2}\right)} \quad \text{on} \quad [0,4].$$

- Recall $q(t) = \exp(-tM)q(0)$ and we have the relation

$$M = \frac{\gamma}{2}\left(T - 2\left(1 - \frac{1}{\gamma}\right)I\right)$$

- Thus,

$$q_n(t) = \sum_m \langle e_n, \exp(-tM)e_m\rangle q_m(0) = \sum_m \int_0^4 \exp\left(-\frac{\gamma t}{2}\left(\lambda - 2(1-\gamma^{-1})\right)\right) d\mu_{m,n}(\lambda)$$

Matrix elements of the spectral measure of T

- Put $\psi = e_m$, $\chi = e_n$ then we get

$$\frac{d\mu_{m,n}(x)}{dx} = \frac{1}{\pi\sqrt{4x - x^2}} \underbrace{\cos\left[(n-m)\arccos\left(\frac{2-x}{2}\right)\right]}_{=T_{|n-m|}\left(\frac{2-x}{2}\right)} \quad \text{on} \quad [0,4].$$

- Recall $q(t) = \exp(-tM)q(0)$ and we have the relation

$$M = \frac{\gamma}{2}\left(T - 2\left(1 - \frac{1}{\gamma}\right)I\right)$$

- Thus,

$$q_n(t) = \sum_m \langle e_n, \exp(-tM)e_m\rangle q_m(0) = \sum_m \int_0^4 \exp\left(-\frac{\gamma t}{2}\left(\lambda - 2(1-\gamma^{-1})\right)\right) d\mu_{m,n}(\lambda)$$

- Substitute $x = (2-\lambda)/2$, then

$$q_n(t) = \frac{1}{\pi}\sum_m q_m(0)e^{-t}\int_{-1}^{1} e^{\gamma t x}T_{|n-m|}(x)\frac{dx}{\sqrt{1-x^2}}$$

Chebyshev expansion of the exponential and final formula

- $\forall x \in [-1, 1]$ and $\forall z \in \mathbb{C}$ it holds [A&S 9.6.34]

$$e^{zx} = I_0(z)T_0(x) + 2\sum_{n\geq 1} I_n(z)T_n(x).$$

where I_n stands for the modified Bessel function of the first kind: $I_n(z) = i^{-n}J_n(iz)$.

Chebyshev expansion of the exponential and final formula

- $\forall x \in [-1, 1]$ and $\forall z \in \mathbb{C}$ it holds [A&S 9.6.34]

$$e^{zx} = I_0(z)T_0(x) + 2\sum_{n\geq 1} I_n(z)T_n(x).$$

  where I_n stands for the modified Bessel function of the first kind: $I_n(z) = i^{-n}J_n(iz)$.

- From this and orthogonality of $\{T_n(x)\}$ one deduces

$$\int_{-1}^{1} e^{zx}\,T_n(x)\frac{dx}{\sqrt{1-x^2}} = \pi I_n(z), \quad n = 0, 1, 2, \ldots.$$

Chebyshev expansion of the exponential and final formula

- $\forall x \in [-1, 1]$ and $\forall z \in \mathbb{C}$ it holds [A&S 9.6.34]

$$e^{zx} = I_0(z)T_0(x) + 2\sum_{n\geq 1} I_n(z)T_n(x).$$

  where I_n stands for the modified Bessel function of the first kind: $I_n(z) = i^{-n}J_n(iz)$.

- From this and orthogonality of $\{T_n(x)\}$ one deduces

$$\int_{-1}^{1} e^{zx}T_n(x)\frac{dx}{\sqrt{1-x^2}} = \pi I_n(z), \quad n = 0, 1, 2, \ldots.$$

- Hence, we arrived at the final formula for time evolution of the magnetization vector:

$$q_n(t) = \sum_m q_m(0)e^{-t}I_{|n-m|}(\gamma t)$$

Remark 1 - induced transient polarization

Assume the case in which all of the spin expectations $q_n(0)$ vanish except for the one:

$$q_n(0) = \delta_{n,0}.$$

Remark 1 - induced transient polarization

Assume the case in which all of the spin expectations $q_n(0)$ vanish except for the one:

$$q_n(0) = \delta_{n,0}.$$

Then we have a simple formula

$$q_n(t) = e^{-t} I_{|n|}(\gamma t).$$

Remark 1 - induced transient polarization

Assume the case in which all of the spin expectations $q_n(0)$ vanish except for the one:

$$q_n(0) = \delta_{n,0}.$$

Then we have a simple formula

$$q_n(t) = e^{-t} I_{|n|}(\gamma t).$$

Known properties of modified Bessel function then yields:

Remark 1 - induced transient polarization

Assume the case in which all of the spin expectations $q_n(0)$ vanish except for the one:

$$q_n(0) = \delta_{n,0}.$$

Then we have a simple formula

$$q_n(t) = e^{-t} I_{|n|}(\gamma t).$$

Known properties of modified Bessel function then yields:

1. First functions q_n rise as

$$q_n(t) \sim \frac{1}{|n|!} \left(\frac{\gamma t}{2}\right)^{|n|} e^{-t}, \quad t \ll \frac{|n|}{\gamma}.$$

Remark 1 - induced transient polarization

Assume the case in which all of the spin expectations $q_n(0)$ vanish except for the one:

$$q_n(0) = \delta_{n,0}.$$

Then we have a simple formula

$$q_n(t) = e^{-t} I_{|n|}(\gamma t).$$

Known properties of modified Bessel function then yields:

1. First functions q_n rise as

$$q_n(t) \sim \frac{1}{|n|!}\left(\frac{\gamma t}{2}\right)^{|n|} e^{-t}, \quad t \ll \frac{|n|}{\gamma}.$$

2. They then reach a maximum at time

$$t \sim \frac{|n|}{\sqrt{1-\gamma^2}}.$$

Remark 1 - induced transient polarization

Assume the case in which all of the spin expectations $q_n(0)$ vanish except for the one:

$$q_n(0) = \delta_{n,0}.$$

Then we have a simple formula

$$q_n(t) = e^{-t} I_{|n|}(\gamma t).$$

Known properties of modified Bessel function then yields:

1. First functions q_n rise as
$$q_n(t) \sim \frac{1}{|n|!}\left(\frac{\gamma t}{2}\right)^{|n|} e^{-t}, \quad t \ll \frac{|n|}{\gamma}.$$
2. They then reach a maximum at time
$$t \sim \frac{|n|}{\sqrt{1-\gamma^2}}.$$
3. Finally, for much larger times, they decrease as
$$q_n(t) \sim \frac{1}{\sqrt{2\pi\gamma t}} e^{-(1-\gamma)t}.$$

Remark 2 - absence of permanent magnetization

- If we put $x = 1$ in the previously mentioned identity we find

$$e^z = I_0(z) + 2\sum_{n\geq 1} I_n(z),$$

for $T_n(1) = 1$.

Remark 2 - absence of permanent magnetization

- If we put $x = 1$ in the previously mentioned identity we find

$$e^{z} = I_0(z) + 2\sum_{n\geq 1} I_n(z),$$

for $T_n(1) = 1$.

- Using this formula and assuming some convergence conditions one deduces

$$\sum_{n} q_n(t) = e^{-(1-\gamma)t} \sum_{n} q_n(0).$$

- If we put $x = 1$ in the previously mentioned identity we find

$$e^{z} = I_{0}(z) + 2\sum_{n\geq 1} I_{n}(z),$$

for $T_n(1) = 1$.

- Using this formula and assuming some convergence conditions one deduces

$$\sum_{n} q_{n}(t) = e^{-(1-\gamma)t} \sum_{n} q_{n}(0).$$

- A similar phenomena can be shown in the case of finite chain ($N < \infty$). It tells us that the total magnetization always decreases exponentially.

Remark 2 - absence of permanent magnetization

- If we put $x = 1$ in the previously mentioned identity we find

$$e^{z} = I_0(z) + 2\sum_{n\geq 1} I_n(z),$$

  for $T_n(1) = 1$.
- Using this formula and assuming some convergence conditions one deduces

$$\sum_{n} q_n(t) = e^{-(1-\gamma)t}\sum_{n} q_n(0).$$

- A similar phenomena can be shown in the case of finite chain ($N < \infty$). It tells us that the total magnetization always decreases exponentially.
- This result corresponds to the known absence of permanent magnetization in the linear Ising model.

Contents

Solution for the spin correlations

- Similarly as in the case of magnetization, one can multiply the master equation by the product $\sigma_j\sigma_k$ ($j \neq k$) and sum over the σ variables.

- Similarly as in the case of magnetization, one can multiply the master equation by the product $\sigma_j \sigma_k$ ($j \neq k$) and sum over the σ variables.
- Taking into account the Glauber expression for w_n, the resulting equation reads

$$\frac{d}{dt} r_{j,k}(t) = -2 r_{j,k}(t) + \frac{1}{2}\gamma \left(r_{j,k-1}(t) + r_{j,k+1}(t) + r_{j-1,k}(t) + r_{j+1,k}(t) \right), \quad k \neq j.$$

For $j = k$ we have the identity $r_{k,k}(t) = 1$.

- Similarly as in the case of magnetization, one can multiply the master equation by the product $\sigma_j\sigma_k$ ($j \neq k$) and sum over the σ variables.
- Taking into account the Glauber expression for w_n, the resulting equation reads

$$\frac{d}{dt}r_{j,k}(t) = -2r_{j,k}(t) + \frac{1}{2}\gamma\left(r_{j,k-1}(t) + r_{j,k+1}(t) + r_{j-1,k}(t) + r_{j+1,k}(t)\right), \quad k \neq j.$$

For $j = k$ we have the identity $r_{k,k}(t) = 1$.

- The derivation of the general solution is not so straightforward as before. Nevertheless, it can be derived in terms of modified Bessel functions again:

$$r_{j,k}(t) = \eta^{j-k} + e^{-2t}\sum_{n>m}\left[r_{n,m}(0) - \eta^{n-m}\right]\left(I_{j-n}(\gamma t)I_{k-m}(\gamma t) - I_{j-m}(\gamma t)I_{k-n}(\gamma t)\right),$$

for $j \geq k$, where

$$\eta = \tanh\left(J/kT\right)$$

is the so called short-range order parameter of the Ising model.

Contents

Generalizations - spin systems in a magnetic field

- The Ising model in a magnetic field ($H \neq 0$) is described via Hamiltonian

$$-J\sum_{m}\sigma_{m}\sigma_{m+1} - H\sum_{n}\sigma_{n}.$$

Generalizations - spin systems in a magnetic field

- The Ising model in a magnetic field ($H \neq 0$) is described via Hamiltonian

$$-J\sum_{m}\sigma_m\sigma_{m+1} - H\sum_{n}\sigma_n.$$

- Glauber introduced the formula for the transition rates

$$w_n(\sigma) = \frac{1}{2}\left(1 - \beta\sigma_n + \frac{1}{2}\gamma(\beta - \sigma_n)(\sigma_{n-1} + \sigma_{n+1})\right).$$

The new parameter β correspond to the magnetic field $\beta = \tanh\left(H/kT\right)$

- The Ising model in a magnetic field ($H \neq 0$) is described via Hamiltonian

$$-J\sum_{m}\sigma_m\sigma_{m+1} - H\sum_{n}\sigma_n.$$

- Glauber introduced the formula for the transition rates

$$w_n(\sigma) = \frac{1}{2}\left(1 - \beta\sigma_n + \frac{1}{2}\gamma(\beta - \sigma_n)(\sigma_{n-1} + \sigma_{n+1})\right).$$

  The new parameter β correspond to the magnetic field $\beta = \tanh(H/kT)$

- The evolution equation for magnetization is more complicated since it is an inhomogenous system combining functions q_n with pair-correlations $r_{n-1,n}$ and $r_{n,n+1}$.

Generalizations - spin systems in a magnetic field

- The Ising model in a magnetic field ($H \neq 0$) is described via Hamiltonian

$$-J\sum_{m}\sigma_m\sigma_{m+1} - H\sum_{n}\sigma_n.$$

- Glauber introduced the formula for the transition rates

$$w_n(\sigma) = \frac{1}{2}\left(1 - \beta\sigma_n + \frac{1}{2}\gamma(\beta - \sigma_n)(\sigma_{n-1} + \sigma_{n+1})\right).$$

  The new parameter β correspond to the magnetic field $\beta = \tanh(H/kT)$

- The evolution equation for magnetization is more complicated since it is an inhomogenous system combining functions q_n with pair-correlations $r_{n-1,n}$ and $r_{n,n+1}$.
- Nevertheless, the general solution for magnetization has been found even in the case of time dependent magnetic field $H = H(t)$,

$$q_n(t) = e^{-t}\sum_{k} q_k(0)I_{n-k}(\gamma t) + \frac{1}{kT}\frac{1-\eta^2}{1+\eta^2}\int_0^t e^{-(1-\gamma)(t-s)}H(s)ds.$$

Generalization - multi-temperature Ising models

- It is possible to think of a model with a spin chain whose every particle is associated with its own heat reservoir of temperature T_n.

Generalization - multi-temperature Ising models

- It is possible to think of a model with a spin chain whose every particle is associated with its own heat reservoir of temperature T_n.
- This model is described by the same way as before. Only the factor γ from the Glauber's expression for rates depends on the index:

$$\gamma_n = \tanh\left(2J/kT_n\right).$$

Generalization - multi-temperature Ising models

- It is possible to think of a model with a spin chain whose every particle is associated with its own heat reservoir of temperature T_n.
- This model is described by the same way as before. Only the factor γ from the Glauber's expression for rates depends on the index:

$$\gamma_n = \tanh\left(2J/kT_n\right).$$

- Some attention has been paid to two-temperature kinetic Ising models, see [Racz, Zia 94], [Mobilia, Schmittmann, Zia 05], [Mazilu, Williams 09], and others.

- It is possible to think of a model with a spin chain whose every particle is associated with its own heat reservoir of temperature T_n.
- This model is described by the same way as before. Only the factor γ from the Glauber's expression for rates depends on the index:

$$\gamma_n = \tanh\left(2J/kT_n\right).$$

- Some attention has been paid to two-temperature kinetic Ising models, see [Racz, Zia 94], [Mobilia, Schmittmann, Zia 05], [Mazilu, Williams 09], and others.
- The two-temperature model represent the simplest generalization beyond the completely uniform system. However, there are other possibilities for modifications which are interesting and perhaps physically relevant, e.g.,

$$T_n \sim \frac{\alpha}{n}.$$

References

1. E. Ising, Z. Physik **31**, (1925)
2. L. Onsager, Phys. Rev. **65**, (1944)
3. R. J. Glauber, J. Math. Phys. **4**, (1965)
4. R. J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Academic Press, 1982
5. Z. Racz, R. K. P. Zia, Phys. Rev. E **49**, (1994)
6. M. Mobilia, B. Schmittmann, R. K. P. Zia, Phys. Rev. E **71**, (2005)
7. I. Mazilu, H. T. Williams, Phys. Rev. E **80**, (2009)

1. E. Ising, Z. Physik **31**, (1925)
2. L. Onsager, Phys. Rev. **65**, (1944)
3. R. J. Glauber, J. Math. Phys. **4**, (1965)
4. R. J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Academic Press, 1982
5. Z. Racz, R. K. P. Zia, Phys. Rev. E **49**, (1994)
6. M. Mobilia, B. Schmittmann, R. K. P. Zia, Phys. Rev. E **71**, (2005)
7. I. Mazilu, H. T. Williams, Phys. Rev. E **80**, (2009)

Thank you!