On the Ising spin model

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Contents

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where E_0 … “intermolecular forces”; E_1 … “spin–external field interaction”.

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- 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.

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

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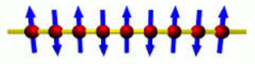

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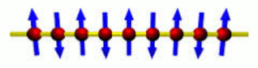

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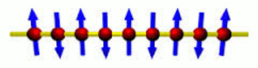

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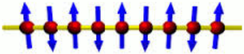

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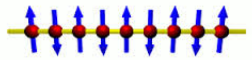

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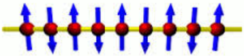

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- However, for the model, it is assumed we know the rate of probability transitions (probability of change of configuration per unit time).
- We may, for example, introduce a tendency for a particular spin σ_n to correlate with its neighboring spins by assuming the rate depends appropriately on the momentary spin values of the other particles.

Master equation

General form:

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

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Parameter γ - correspondence with the Ising model

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- With the Glauber's choice for the rates one finds
$$\frac{p_n(\ldots,-\sigma_n,\ldots)}{p_n(\ldots,\sigma_n,\ldots)} = \frac{w_n(\ldots,\sigma_n,\ldots)}{w_n(\ldots,-\sigma_n,\ldots)} = \frac{1-\frac{1}{2}\gamma\sigma_n(\sigma_{n-1}+\sigma_{n+1})}{1+\frac{1}{2}\gamma\sigma_n(\sigma_{n-1}+\sigma_{n+1})}.$$

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

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

Quantities of interest 1/2

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

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

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- 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.

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

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- 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

- 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

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

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

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- 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

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

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

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- We arrive at the solution

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

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

Chebyshev polynomials

- Recall Chebyshev polynomials of the second kind are defined as

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

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

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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

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- Fourier transform:

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

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- 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

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

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

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

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

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

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

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

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- 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

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- 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:

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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

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

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

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

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

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

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- 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.

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Solution for the spin correlations

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

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- 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.

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

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Generalizations - spin systems in a magnetic field

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- 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 $H = H(t)$,

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

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Generalization - multi-temperature Ising models

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- 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.,

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

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Thank you!