Kinetic induced phase transition

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(March 31, 2017)

Abstract

An Ising model with local Glauber dynamics is studied under the influence of additional kinetic restrictions for the spin-flip rates depending on the orientation of neighboring spins. Even when the static interaction between the spins is completely eliminated and only an external field is taken into account the system offers a phase transition at a finite value of the applied field. The transition is realized due to a competition between the activation processes driven by the field and the dynamical rules for the spin-flips. The result is based on a master equation approach in a quantum formulation.

05.20.Dd, 05.70.Ln, 75.10.Hk, 82.20.Mj
I. INTRODUCTION

The dynamical properties of different models as Ising model, Sherington–Kirkpatrick spin glasses, influence of time dependent external fields have been the subject of continuous interest. Because the conventional Ising model is a static, equilibrium model, a dynamical generalization was first considered by Glauber who introduced the single-spin-flip kinetic Ising model for describing relaxation towards equilibrium. The dynamics is generated by a coupling to a heat bath at a fixed temperature. Hence the rates of the dynamical processes are constrained to satisfy detailed balance. Based on that the static interaction energy of the spins is included in the flip-rates. In this way the equilibrium phase transition inherent for the Ising system in $d > 1$ is also manifested in the dynamical approach such as within the behavior of the relaxation time and the correlation function.

In the present paper we discuss the possibility that the kinetic Ising system undergoes a phase transition although the mutual static interaction between the spins will be neglected completely. The transition is purely mediated by the underlying kinetics. Special attention will be paid to dynamical restrictions for the spin-flip rates instead of including an interaction. As a consequence of such constraints combined with the orientation of the applied field (activation energy) there occurs a competing situation leading to the aforementioned kinetic induced phase transition.

To be specific let us consider a spin system in an external time independent field which is subject to a dynamical process (spin-flip process). However, it is assumed that the flip rates does not depend on the neighboring spin configuration via the static energy between adjacent spins manifested by a Hamiltonian. Alternatively, kinetic restrictions are included independently on their energy. The environment of a fixed spin is oriented in a self-adaptive manner only by the kind of kinetic processes. Formally, this can be achieved by chosing the flip rates depending on the state of the neighboring spins. Furthermore, the flip rates are also determined by the temperature and the activation field. To formulate the master equation under the influence of constraints we use a representation of the underlying kinetic
equation in terms of quantum Pauli–operators. Based on the analogy to quantum mechanics the problem can be studied in a compact form\cite{4,5}, for a recent review see\cite{3,4}. The method allows the inclusion of the above mentioned restrictive conditions in a transparent manner which had been demonstrated for the so called Fredrickson Andersen model\cite{6,7}, see\cite{9}.

II. THE MODEL

Let us use a lattice gas description with the occupation number at a certain lattice site defined by $n_i = 0, 1$. Due to the relation to the spin variable, $S_i = 1 - 2n_i$, an empty site corresponds to an up orientation whereas an occupied site is related to spin-down. The local flip dynamics can be characterized by an evolution operator written in terms of Pauli–operators\cite{9}

$$L_i = \lambda (1 - d_i^\dagger) d_i + \gamma (1 - d_i) d_i^\dagger$$

(1)

The first term gives a nonzero contribution in case of a flip from a spin-down to a spin-up state (or from an occupied to an empty site) with the rate $\lambda$ whereas the second term including the rate $\gamma$ is responsible for the inverse process, i.e. the flip from spin-up to spin-down states. Obviously, the rates $\lambda$ and $\gamma$ can depend on the temperature of a heat bath coupled to the system, on the mutual interaction between the spin degrees of freedom, as well as on the neighboring spin configuration in a kinetic manner discussed below. The coupling to a heat bath is easily realized by the following modification of the evolution operator\cite{9}

$$L = \nu \sum_i \left[ (1 - d_i) \exp(-\beta H/2) d_i^\dagger \exp(\beta H/2) + (1 - d_i^\dagger) \exp(-\beta H/2) d_i \exp(\beta H/2) \right]$$

(2)

The procedure is similar to a ‘thermalized’ Heisenberg picture in quantum mechanics. As the simplest case let us consider a coupling to an activation field of the strength $\varepsilon$

$$H = \sum_i \varepsilon n_i$$

(3)

If $\varepsilon > 0$ for each lattice site the spin-up orientation is preferred. In the opposite case $\varepsilon < 0$ the spin-down state is more favored. The algebraic properties of Pauli–operators can
be used to calculate for instance $\exp(-\beta H/2)d_i^\dagger \exp(\beta H/2) = d_i^\dagger \exp(1/2\beta \varepsilon)$. Comparing eq.(1) and eq.(2) the thermalization leads to temperature dependent activation rates which can be written in the case considered by eq.(3) as

$$\lambda = \nu \exp(\varepsilon/2T) \quad \gamma = \nu \exp(-\varepsilon/2T).$$

(4)

It should be remarked that the transition rate from down to up state is realized at low temperatures with a larger probability than the opposite process (in case $\varepsilon > 0$). For high temperatures, $T \to \infty$, both flip-processes appear with the same probability. Before the model is extended by introducing kinetic restrictions let us demonstrate its applicability.

The evolution operator $L$ obeys the equation

$$\partial_t \ket{F(t)} = L \ket{F(t)}$$

(5)

where the state vector $\ket{F(t)}$ is related to the probability distribution function $P(\vec{n}, t)$ according to $P(\vec{n}, t) = \langle \vec{n} | F(t) \rangle$ with a complete set of basic-vectors $| \vec{n} \rangle$ composed of Pauli–operators. The probability distribution function is assumed to follow a master equation written in the symbolic form

$$\partial_t P(\vec{n}, t) = \hat{L} P(\vec{n}, t).$$

(6)

The evolution operator $L$ in eq.(5) can be mapped onto the operator $\hat{L}$ in the master equation. Such an approach had been introduced by Doi\cite{Doi} using Bose operators\cite{Bose}. A generalization to Pauli–operators had been proposed\cite{Pauli1, Pauli2, Pauli3}, for a recent review see\cite{Review}.

Following\cite{Pauli1, Pauli2, Pauli3} the probability distribution $P(\vec{n}, t)$ is related to a state vector $\ket{F(t)}$ in a Fock-space according to $P(\vec{n}, t) = \langle \vec{n} | F(t) \rangle$ with the basis-vectors $| \vec{n} \rangle$ composed of second quantized operators. A further extension to an $p$–fold occupation number is possible and had been discussed in\cite{Extension}.

The relation between the quantum–like formalism and the probabilistic approach is given by

$$\ket{F(t)} = \sum_{\vec{n}} P(\vec{n}, t) | \vec{n} \rangle.$$  

(7)
As it was shown firstly by Doi\(^2\) the average of an arbitrary physical quantity \(B(\vec{n})\) is defined by the average of the corresponding operator \(B(t)\)

\[
\langle B(t) \rangle = \sum_{\vec{n}_i} P(\vec{n}, t) B(\vec{n}) = \langle s \mid B \mid F(t) \rangle
\]  

(8)

with the state function \(\langle s \mid = \sum \langle \vec{n} \mid\). Using the relation \(\langle s \mid L = 0\) the evolution equation for an operator \(A\) can be written

\[
\partial_t \langle B \rangle = \langle s \mid [B, L] \mid F(t) \rangle.
\]

(9)

It should be stressed that all the dynamical equations covering the classical problem are determined by the commutation rules of the underlying operators and the structure of the evolution operator \(L\). In our case the dynamics of the model is given by spin-flip processes indicating a change of the local occupation number or the spin orientation, respectively.

Based on the above introduced approach the evolution equation for the occupation number operator or the averaged spin for the simple flip process eq.\(2\) is easily derived. We find

\[
u^{-1} \partial \langle n \rangle = -\langle n \rangle e^{\varepsilon/2T} + \langle 1 - n \rangle e^{-\varepsilon/2T}.
\]

(10)

The solution in a spin representation is well known and reads

\[
\langle S(t) \rangle = \tanh(\frac{2\varepsilon}{T}) + S_0 \exp(-t/\tau) \quad \text{with} \quad \tau = \frac{1}{2 \cosh(\frac{2\varepsilon}{T})}.
\]

(11)

The first term represents the stationary state whereas the second one describes the exponential decay with a relaxation time \(\tau\). For low temperatures one finds \(\tau \propto \exp(-\frac{2\varepsilon}{T})\). In the opposite limit the relaxation time shows an algebraic dependence on the activation energy \(\tau \propto \frac{1}{2}(1 - 2(\frac{\varepsilon}{T})^2)\). The results are independent on the sign of the activation energy.

Now we discuss an extension of the model introducing constraints within dynamical rules specified below. It will be demonstrated that in this case the sign of \(\varepsilon\) leads to a complete different behavior of the system. To this aim an anisotropic model is studied where the kind of anisotropy is not originated by the static interaction. Instead of that the flip processes will be modified in the following manner. Whereas the flip process from spin-down
to spin-up orientation should be possible whenever a double occupancy is avoided which is automatically guaranteed by the algebraic properties of the Pauli–operators, the inverse process, spin-up to spin-down flip, should be restricted. Such a flip is only allowed when the neighboring configuration fulfills the condition

$$\frac{1}{2} \sum_{j(i)} (1 + S_j) \leq f$$ (12)

A local spin flip at the lattice site $i$ is only permitted when the number of nearest neighbors denoted by $j(i)$ satisfies the last condition. Here $f$ is a certain but fixed number specified below. Physically the confinement means that flips from up- to down-spin orientations are reduced when the total number of adjacent spins with an spin-up alignment does not exceed the number $f$. Such kinetic restrictions are already introduced by Fredrickson and Andersen within a $f$-spin facilitated kinetic Ising model which is a candidate describing the ultraslow dynamics in the vicinity of a the glass transition.

Here, we analyse an anisotropic version of the model by assuming that only one of the flip rates, $\lambda$ or $\gamma$ are modified which is different from that one discussed for glassy materials. The kinetic restriction manifested by eq.(12) means that a local change from a spin-up state to a spin-down state is not possible when more than $f$ nearest neighbors with respect to a given site are in the up position. Mathematically, the confinement is realized by assuming that the corresponding transition rate, here $\gamma$, will be replaced by $\gamma \rightarrow \gamma n_{r_1} \ldots n_{r_f}$. As the simplest choice let us chose $f = z/2$ where $z$ is the coordination number. This leads to the following evolution operator

$$L = \nu \sum_{ij_1 \ldots j_f} \chi_{i j_1 \ldots j_f} \left[ (1 - d_i) \exp(-\beta H/2) d_i^\dagger \exp(\beta H/2) n_{j_1} \cdots n_{j_f} \right]$$

$$+ \left[ (1 - d_i^\dagger) \exp(-\beta H/2) d_i \exp(\beta H/2) \right]$$ (13)

where $\chi_{i j_1 \ldots j_f}$ is only nonzero when all the indices indicates nearest neighbor sites. Here we consider the case $f = 2$ which corresponds to a cubic lattice in two dimensions. The general results seem to be independent on the special realization. As the main feature of the model there occurs a conflicting situation between the static preferred orientation of the
spins manifested in the sign of the activation energy $\varepsilon$ and the kinetic rules. That case will be discussed in detail in the forthcoming section.

### III. ANISOTROPIC MODEL

Using the algebraic properties of Pauli–operators the evolution equation for the averaged occupation number reads

$$
\partial_t \langle n_j \rangle = \nu \sum_{r,s} \chi_{jrs} \left[ \exp(-\varepsilon_r/2T)\langle (1 - n_j)n_r n_s \rangle - \exp(\varepsilon_j/2T)\langle n_r \rangle \right] \tag{14}
$$

As already demonstrated in the mesoscopic dynamic equations within the classification introduced by Hohenberg and Halperin is rederived in a coarse grained approximation. In the present case the equation is written in the form

$$
\partial_t \langle n_j \rangle = -e^{\varepsilon/2T} z(z - 1) \langle n_j \rangle + e^{-\varepsilon/2T} \sum_{rs} \chi_{jrs} \left[ \langle n_r \rangle \langle n_s \rangle - \langle n_j \rangle \langle n_r \rangle \langle n_s \rangle \right] \tag{15}
$$

It consists of a local part (linear term) and nonlocal terms. After Fourier transformation and introducing the abbreviation $\langle n(\vec{k}, t) \rangle \equiv n_k(t)$ the last equation reads

$$
\nu^{-1} \partial_k n_k(t) = -e^{\varepsilon/T} n_k(t) z(z - 1)
+ e^{-\varepsilon/T} \sum_{p,q} \left[ -\epsilon_{pq} n_{k-p-q}(t)n_p(t)n_q(t) + \epsilon_{k-p} n_{k-p}(t)n_p(t) \right] \tag{16}
$$

Here we have introduced the dispersion relation ($l$ is the lattice constant)

$$
\epsilon_{pq} = 4[\cos p_x l \cos q_x l + \cos p_y l \cos q_y l] + 2[\cos(p_x - q_x)l + \cos(p_y - q_y)l] \tag{17}
$$

The homogeneous stationary state $n_0$ obeys the equation

$$
0 = -\lambda n_0 + \gamma(n_0^2 - n_0^3) \tag{18}
$$

This equation yields three stationary points

$$
n_1 = 0 \quad n_{2/3} = \frac{1}{2} \left[ 1 \pm \sqrt{1 - 4\rho} \right] \quad \text{with} \quad \rho = \frac{\lambda}{\gamma} = \exp(\varepsilon/T). \tag{19}
$$

Making the conventional ansatz $n(k, t) = n_0 \delta(\vec{k}) + m(\vec{k}, t)$ we get
\[ \partial_t m(\vec{k}, t) = -\Lambda(\vec{k}) m(\vec{k}, t) \quad \text{with} \]
\[ \Lambda(\vec{k}, t) = \lambda \epsilon_{00} + \gamma [(2\epsilon_{k_0} + \epsilon_{00})n_0^2 - 2\epsilon_{k_0}n_0] \quad (20) \]

From the linear stability analysis we conclude that the spin-up orientation \( n_1 = 0 \) is always stable independently on the sign of the activation energy \( \epsilon \). For the nonzero solutions the function \( \Lambda(\vec{k}) \) introduced in eq. (20) can be written in the form

\[ \Lambda(\vec{k}) = \Lambda(0) + \lambda \epsilon_{00}(2 - \cos(k_x l) + \cos(k_y l)) \]

\[ \text{with} \quad \Lambda(0) = \epsilon_{00} \gamma (n_0 - 2\rho) \quad (21) \]

Obviously, the sign of gap \( \Lambda(0) \) in eq. (21) is responsible for the stability. Whenever \( \epsilon > 0 \) the both nonzero solutions \( n_2 \) and \( n_3 \) are unstable. Hence, we find that in this kind of an anisotropic model the up orientated spin state is the single stable one. The result is expected because the static field (activation energy) favors the spin-up state, \( \epsilon > 0 \), and the dynamic rules support the same orientation with a larger probability as the opposite one. The result is independently on the temperature and the strength of the activation energy.

The situation is complete different analysing the case \( \epsilon < 0 \). The static energy would favor the down orientation of the spins due to the sign of the field. In contrast to that the dynamical rules tend to avoid such a state because states with a down-spin orientation are reduced by the kinetic restrictions. As the result of the competition between both processes there appears a critical temperature \( T_c = \frac{|\epsilon|}{ln 4} \). Above this temperature only the state \( n_1 = 0 \) is a stable one. For \( T < T_c \) both states \( n_1 \) and \( n_2 \) are stable, where \( n_2 \) can be rewritten

\[ n_2 = \frac{1}{2} \left[ 1 + \sqrt{1 - \exp(-|\epsilon| (T^{-1} - T_c^{-1}))} \right] \quad (22) \]

The situation described in the case \( \epsilon < 0 \) is remarkable. For high temperature the spin-up state is realized. Whereas the flip rates in this case are of the same order the static term would favor a spin-down state. Due to the kinetic restrictions such a state is not realized, or with other words the dynamic rules with the above introduced constraints work much stronger than the activation field. The phase transition is exclusively induced by the
kinetics. For very low temperatures the flip-rate to an up state (promoted by $\lambda$) is very small compared with the rate for the opposite process. Insofar, the kinetics favor the occurrence of the spin-down orientation. From this point of view one should expect that for $T < T_c$ only the state $n_2 \neq 0$ is realized. This intuitive result can be confirmed by comparing the energy of both states. Starting from eq.(15) we find an energy function $F$ which reads

$$F = \frac{\lambda}{2}n^2 - \frac{\gamma}{3}n^3 + \frac{\gamma}{4}n^4$$

(23)

where we have considered only the homogeneous case which seems to be sufficiently. The function $F$ plays the role of the free energy. However, it should be stressed that $F$ is not simply a Ginzburg-Landau functional because different to that one the prefactor of the quadratic part does not change its sign at the phase transition temperature ($\lambda > 0$) reflecting the fact that the system does not possess a phase transition in equilibrium. Now let us calculate the energy difference $\Delta F = F(n_2) - F(n = 0)$ with the result

$$\Delta F < 0 \quad \text{for} \quad T < T_0 = \frac{|\varepsilon|}{\ln(4.5)}$$

$$\Delta F > 0 \quad \text{for} \quad T > T_0$$

(24)

From here we conclude, that the solution $n_1 = 0$, spin-up orientation, is energetically preferred within the interval $T_0 < T < T_c$ whereas for $T < T_0$ the nonzero solution $n_2$ is stable and is related to the lowest energy. The situation is comparable with a first order phase transition, but as already stressed, the transition is originated by the kinetic restrictions and it is not driven by the energy.

The above introduced model can be easily extended by considering other restrictions. For instance the flip process spin-down to spin-up can be reduced when $f = 2$ neighbors are in the down position. In our approximation it means that the transition rate $\lambda$ is replaced by $\lambda(1 - n)^2$. The result does not change when simultaneously one substitutes $\lambda$ by $\gamma$ and $\varepsilon$ by $-\varepsilon$. Another extension can be realized when both flip processes are confined for instance by assuming $\lambda \to \lambda(1 - n)^2$ and $\gamma \to \gamma n^2$. When the activation energy is


positive, \( \varepsilon > 0 \), one finds three stable equilibrium solutions \( n_1 = 0, n_2 = 1, n_3 = \frac{\lambda}{\lambda + \gamma} \) with \( F(n_1) < F(n_2) < F(n_3) \). In the opposite case of a negative activation field \( \varepsilon < 0 \) we get two stable solutions \( n_1 = 0 \) and \( n_2 = 1 \) with \( F(n_2) < F(n_1) \). A third solution \( n_3 = \frac{\lambda}{\lambda + \gamma} \) is only stable for \( T > T_c \). Moreover, other realization for constraints does not lead to significant changes.

**IV. CONCLUSIONS**

In the present paper we have considered a system with competing forms of interactions. Whereas the static energy is simply the energy for spins in a field which does not lead to an equilibrium phase transition the dynamical rules for the thermal activated flip processes are supplemented by additional restrictions. These restrictions are self organized by the orientation of neighboring spins with respect to a given one. Whenever the field and the kinematics favor the same spin orientation a phase transition is suppressed. In the opposite case, when orientation preferred by the static activation field will be restricted or even when a certain order is prevented by the dynamics the system offers a phase transition. There appear two stable solutions below a critical temperature \( T_c \) where this temperature is purely determined by the field and not by quantities included in an energy functional of Ginzburg-Landau type. To be specific, we have analysed the case that a down-orientation (occupation number \( n = 0 \)) is supported by the orientation of the field \( \varepsilon \). The flip-rate \( \lambda \) responsibly for a spin-flip from down-to up-orientation is purely given by the activation process. However the inverse process, a spin-flip from up- to down-orientation (rate \( \gamma \)) is additional constrained by the dynamical alignment of neighboring spins. In particular, the mentioned flip process is strongly restricted when more than a half of the neighboring spins of a fixed one is already in an up-position. This conflicting situation leads to the phase transition at \( T_c \). For low temperatures the relation \( \gamma \gg \lambda \) is valid. The flip process, spin-up to spin-down, is realized with a much higher rate as the inverse process. Because the restrictions favors an up-orientation we find for a finite temperature that the state \( n \simeq 1 \) is the stable one. This state
is always realized for $T < T_0$. However, there exists a second stable solution with spin-up orientation but with a higher energy. On that manner this state is only a metastable one. At $T_0$ both states are simultaneously stable and coexist with the same energy. For $T > T_0$ the up-orientation is favored with a lower energy. When $T > T_c$ only the up-orientation is stable, that means the restrictive dynamics determines the behavior of the model.

It seems to be for the first time that such a kinetic mediated phase transition is discussed. As a further step we should take into account fluctuations to observe the detailed behavior in the vicinity of the branching point.
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