Glauber model in a quantum representation

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The Glauber model is reconsidered based on a quantum formulation of the master equation. Unlike the conventional approach the temperature and the Ising energy are included from the beginning by introducing a Heisenberg-like picture of the second quantized operators. This method enables us to get an exact expression for the transition rate of a single flip process $w_i(\sigma_i)$ which is in accordance with the principle of detailed balance. The transition rate differs significantly from the conventional one due to Glauber in the low-temperature regime. Here the behavior is controlled by the Ising energy and not by the microscopic time scale.

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The kinetic Ising model is a very simple but effective model to study nonequilibrium situations. The model is based on the Ising model which describes the interaction of a set of spins with values $\{\sigma_i = \pm 1\}$ at each lattice site i. Starting from an arbitrary initial state, the simplest dynamics consist of a single spin-flip process $\sigma_i \rightarrow -\sigma_i$ which is realized with a certain transition rate $w_i(\sigma_i)$. This rate is included into a master equation, which is an equation of motion for the single-time probability $p(n,t)$. In our case the configuration n consists of the set of all spins in d dimensions. This is usually referred to as the Glauber model [1]. The problem is to find an analytical expression for the transition rate. In order to ensure that the system eventually relaxes to an equilibrium state, one imposes the principle of detailed balance, and the transition rate is chosen in accordance with that principle. One choice is proposed in [2]:

$$w_i^G(\sigma_i) = \frac{1}{2\alpha}\left[1 - \sigma_i \tanh\left(\frac{E_i}{T}\right)\right]. \tag{1}$$

Here the temperature T is given in terms of the Boltzmann constant and E_i is the local energy of the Ising model,

$$E_i = h_i + \sum_{j(i)} J_{ij}\sigma_j, \tag{2}$$

where $j(i)$ means the sum over all nearest neighbors of lattice site i. The local energy arises from the Hamiltonian given by

$$H = -\sum_i h_i\sigma_i - \frac{1}{2}\sum_{i,j} J_{ij}\sigma_i\sigma_j. \tag{3}$$

The quantity h_i is an external field, and the summation in the interacting part goes over all pairs of nearest-neighbor spins. Notice that the choice of the transition rate in Eq. (1) is not unique. Moreover, the interaction energy and the coupling to the heat bath with temperature T are only incorporated into the master equation via the principle of detailed balance. Let us stress that the different choices for the transition probability are discussed in the context of Monte Carlo methods [3]. The goal of the present Brief Report is to include the energy functional and the temperature directly into the master equation from the beginning. With that aim we use a mapping of the master equation onto a dynamic equation in terms of second quantized operators [4–8]; for a recent review see [9].

Let us start from a general master equation written in the form

$$\partial_t p(n,t) = \sum_{n'} [w(n|n')p(n',t) - w(n'|n)p(n,t)] \equiv \sum_{n'} L(n,n')p(n',t). \tag{4}$$

Here $p(n,t)$ is the probability that a certain configuration n is realized at time t and $w(n|n')$ plays the role of the transition probability per unit time from configuration n to n'. In our case the configuration n is given by the orientation of the set of spins. The principle of detailed balance means that the stationary distribution $p_s(n)$ satisfies

$$\frac{p_s(n')}{p_s(n)} = \frac{w(n'|n)}{w(n|n')}. \tag{5}$$

In case the static properties of the system are governed by a Hamiltonian let us make the following ansatz:

$$w(n'|n) = \exp[-\beta H(n')/2]V(n'|n)\exp[\beta H(n)/2]. \tag{6}$$

This ansatz is motivated by the conventional Arrhenius ansatz for transition rates; see also the result obtained in Eq. (13) and the comment made there. Further let us remark that we have assumed the validity of the commutator relation $[H(n),H(n')]=0$. In Eq. (6) the parameter β is an arbitrary one. In case the system is coupled to a heat bath we will identify β with the inverse temperature T in units of the Boltzmann constant. Then the stationary condition Eq. (5) can be rewritten as

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$$\frac{p_s(n')}{p_s(n)} = \frac{V(n'|n)}{V(n|n')}\exp\{\beta[H(n) - H(n')]\}. \tag{7}$$

Inserting Eq. (6) in the master equation (4) we get

$$\partial_t p(n,t) = \sum_{n'} \{\exp[-\beta H(n)/2]V(n|n')\exp[\beta H(n')/2]p(n',t) - \exp[-\beta H(n')/2]V(n'|n)\exp[\beta H(n)/2]p(n,t)\}. \tag{8}$$

Now the further aim is to rewrite Eq. (8) using second quantized operators. Following Refs. [4–6,8,10,11], the probability distribution $p(n,t)$ can be related to a state vector $|F(t)\rangle$ in a Fock space according to $p(n,t)=\langle n|F(t)\rangle$ and $|F(t)\rangle = \Sigma_n p(n,t)|n\rangle$, respectively, where the basic vectors $|n\rangle$ can be expressed by second quantized operators. Using this representation, the underlying master equation can be transformed into an equivalent evolution equation in a Fock space, written in the form

$$\partial_t|F(t)\rangle = \hat{L}|F(t)\rangle. \tag{9}$$

The dynamical matrix elements $L(n,n')$ within the master equation are mapped onto the operator $\hat{L}=\hat{L}(a,a^\dagger)$, where a and $a^\dagger$ are the annihilation and creation operators, respectively. Here the matrix elements of the operator $\hat{L}(a,a^\dagger)$ coincide with the matrix elements $L(n,n')$. Originally, this transformation had been applied for the Bose case with unrestricted occupation numbers [4–6]. Here, we consider the case of restricted occupation numbers [7,8,10,11]. In order to preserve the restriction of the occupation number in the underlying dynamical equations, the commutation rules of the operators a and $a^\dagger$ are chosen as Pauli operators [7,8,13]:

$$[a_i,a_j^\dagger] = \delta_{ij}(1-2a_i^\dagger a_i), \quad [a_i,a_j] = [a_i^\dagger,a_i^\dagger] = 0, \quad a_i^2 = (a_i^\dagger)^2 = 0. \tag{10}$$

The relation to the spin variable is $\sigma_i = 1-2a_i^\dagger a_i$. In case of a single spin-flip process the evolution operator $\hat{L}$ reads

$$\hat{L} = \sum_i [\lambda(1-a_i^\dagger)a_i + \gamma(1-a_i)a_i^\dagger], \tag{11}$$

where λ and γ are the temperature-dependent transition rates; the determination of those is beyond the scope of the present approach. The flip rates are assumed in accordance with the principle of detailed balance manifested in Eq. (5). Obviously, the transition rates should depend on the details of the mutual interaction of the spins. Therefore the evolution operator should be extended by including the temperature and the interaction. In accordance with Eq. (8) we propose the following generalization:

$$\hat{L} = \kappa\sum_i [(1-a_i^\dagger)\exp(-\beta H/2)a_i\exp(\beta H/2) + (1-a_i)\exp(-\beta H/2)a_i^\dagger\exp(\beta H/2)]. \tag{12}$$

Here, κ is a parameter that fixes the time scale of the flip process and H is the Hamiltonian for the underlying interaction given by Eq. (3). Because of the relation between σ_i and the annihilation and creation operators the evolution operator can be rewritten in terms of these operators as

$$\hat{L} = \kappa\sum_i \left[(1-a_i^\dagger)a_i\exp\left(\frac{E_i}{T}\right) + (1-a_i)a_i^\dagger\exp\left(-\frac{E_i}{T}\right)\right] \quad \text{with} \quad E_i = h_i + J(0) - 2\sum_{j(i)} J_{ij}a_j^\dagger a_j, \quad J(0) = \sum_i J_{ij}. \tag{13}$$

Notice that the last relation is derived only by using the algebraic properties of the operators. In case of vanishing mutual interaction, i.e., $J=0$, one observes that the last relation is equivalent to the conventional Arrhenius ansatz. With that aim the comparison of Eqs. (11) and (13) yields the identification $\lambda=\kappa\exp(h/T)$ and $\gamma=\kappa\exp(-h/T)$ according to the Arrhenius ansatz. Our quantum approach yields therefore the possibility of formulating the Arrhenius ansatz in a more formal and mathematical manner.

To proceed further we follow Doi [4] and calculate the average of an arbitrary physical quantity $B(n)$ by using the average of the corresponding operator $B=\Sigma_n|n\rangle B(n)\langle n|$ via [12]

$$\langle B(t)\rangle = \sum_n p(n,t)B(n) = \langle s|B|F(t)\rangle. \tag{14}$$

Here we have used the projection state $\langle s| = \Sigma_n\langle n|$, which is realized only for spin-1/2 fermions in such a simple form. The normalization condition for the probability density is included in the condition $\langle s|F(t)\rangle = 1$ with the consequence [12] that the evolution operator satisfies always the relation $\langle s|L=0$. In the present case the averaged spin variable obeys

$$\frac{1}{2\kappa}\frac{\partial}{\partial t}\langle\sigma_i\rangle = \left\langle \sinh\left(\frac{E_i}{T}\right)\right\rangle - \left\langle \sigma_i\cosh\left(\frac{E_i}{T}\right)\right\rangle. \tag{15}$$

Based upon the conventional master equation Eq. (4) the averaged spin satisfies

$$\frac{\partial}{\partial t}\langle\sigma_i\rangle = -2\langle\sigma_i w_i(\sigma_i)\rangle, \tag{16}$$

where due to Glauber [1] or Suzuki *et al.* [2] the single-transition rate $w_i(\sigma_i)\equiv w(\sigma_1,\ldots,\sigma_i,\ldots,\sigma_N|\sigma_1,\ldots,-\sigma_i,\ldots,\sigma_N)$ is heuristically chosen in Eq. (1). This form of the transition rate is not uniquely determined by the principle of detailed balance. In our approach we can directly find the transition rate by applying the relation

$$\sigma_i\exp\left(-\frac{E_i\sigma_i}{T}\right) = \sigma_i\cosh\left(\frac{E_i}{T}\right) - \sinh\left(\frac{E_i}{T}\right).$$

Using this relation and Eqs. (15) and (16) we get immediately

$$w_i(\sigma_i) = \kappa\exp\left(-\frac{E_i\sigma_i}{T}\right) \equiv \kappa\cosh\left(\frac{E_i}{T}\right)\left[1-\sigma_i\tanh\left(\frac{E_i}{T}\right)\right]. \tag{17}$$

The transition rate is related to the heuristic one by assuming that the time scale α in Eq. (1) is controlled by the spin

configuration as well as the temperature. Now let us discuss the transition rate obtained by Eq. (17) in detail, especially for the case of a vanishing external field. In that case the local energy is reduced to $E_i=\Sigma_{j(i)}J_{ij}\sigma_j$, where the summation is performed over all the z nearest neighbors of the lattice site i. In the high-temperature limit the transition probabilities w_i^G and w_i show the same behavior. In that case the transition rate is obviously only determined by the microscopic time scale α or κ^{-1}. Both probabilities are independent of the spin configuration. In the low-temperature limit $T \ll E_i$ the situation is completely different. Let us first assume that the spin at site i is directed upward, i.e., $\sigma_i=1$. Then one has to distinguish two cases.

(*i*) $E_i<0$. In this realization the majority of nearest-neighbor spins are not adapted to the preferred upward direction of the spin σ_i. In other words, the local spin configuration around σ_i is unfavorable. As a consequence the transition probabilities behave like

$$\lim_{T\to 0} w_i(\sigma_i = 1) = \kappa \exp(|E_i|/T),$$

$$\lim_{T\to 0} w_i^G(\sigma_i = 1) = \frac{1}{\alpha}. \tag{18}$$

While in the Glauber transition rate the microscopic time scale α^{-1} plays the role of a lower cutoff, i.e., spin flips are possible within this time scale, in our realization the transition rate is controlled by the energy E_i of the Ising model. The rate increases drastically and leads to an immediate flip process of the "wrong" spins. The time scale τ_i for a flip is of the order

$$\tau_i \approx \kappa^{-1} \exp(-|E_i|/T).$$

The spins in the energetically unfavorable direction perform the flips with a very high rate in a quite short time interval.

(*ii*) $E_i>0$. In that case the majority of the spins around lattice site i are already adapted and the transition rate tends to zero according to

$$w_i(\sigma_i = 1) = \kappa \exp(-E_i/T). \tag{19}$$

A similar behavior is also observed within the approximation due to Glauber.

In the second case we consider the downward orientation $\sigma_i=-1$. As above we study the two cases of positive and negative local energy E_i. For $E_i<0$ we get in the low-temperature regime

$$\lim_{T\to 0} w_i(\sigma_i = -1) = \kappa \exp(-|E_i|/T) \to 0. \tag{20}$$

The transition rate tends to zero, i.e., all spin flips are suppressed completely. In the opposite case $E_i>0$ the result is

$$\lim_{T\to 0} w_i(\sigma_i = -1) = \kappa \exp(E_i/T), \tag{21}$$

which supports a very high flip rate, whereas the Glauber rate remains simply constant.

Summarizing our Brief Report, we have reconsidered the well-established kinetic Ising model in terms of second quantized operators. The coupling to a heat bath at temperature T and the underlying interaction are included similar to the Heisenberg picture of operators. As a result we get an exact expression for the transition rate which is likewise in accordance with detailed balance. The differences from the conventional Glauber model consists in the low-temperature regime. Here the transition rate is controlled by the Ising energy and not by the microscopic time scale. For low temperatures the transition rate is better adapted to the physical situation in mind.

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