The relaxation to equilibrium in one-dimensional Potts models

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Abstract

A brief overview is given of the studies of relaxation to equilibrium in one-dimensional kinetic Potts models with only nearest neighbour couplings at low temperatures, both for spin-conserving and nonconserving dynamics. For ferromagnetic couplings, the model shows coarsening, with typical size of domains increasing as a power of time. For antiferromagnetic couplings, the state of the system in the limit of large times need not be frozen, as the system keeps jumping between the large number of degenerate ground states. A large variety of relaxational behaviour is seen. Some new results for the $q = 3$ antiferromagnetic Potts model, under Glauber and Kawasaki dynamics, are briefly summarized.

Keywords: Relaxation to equilibrium, kinetic Potts models, Ising model, Markovian evolution of one-dimensional Potts models.

1. Introduction

It is over 50 years since the celebrated solution of the Ising model in two dimensions was found by Onsager. Since then, the number of exactly soluble models in equilibrium statistical mechanics has grown, and is now quite large (see Baxter[1], for example). However, only a very small fraction of these can be solved exactly for $d > 2$. (The case $d = \infty$ is exceptional, as then fluctuations become small, and the mean-field approximation becomes exact).

The number of problems which can be solved analytically in non-equilibrium statistical mechanics is much smaller. Furthermore, the thermodynamic arrow of time introduces anisotropies which further complicate the problem. Thus, it is not very surprising that the vast majority of theoretical papers on relaxation in non-equilibrium systems have dealt with one-dimensional problems.

However, my reason for discussing stochastic evolution in one-dimensional models here is not just that the questions are easier to answer in one dimension. In fact, one can see a very large class of different types of relaxations even in the one-dimensional problems. I shall confine myself to Markovian evolution of one-dimensional Potts models with only nearest neighbour coupling, and no external field. Introduction of external field makes the problem much harder, and the exact solution is not known even for Ising chains.

I shall show that depending on whether the coupling is ferro- or antiferro-magnetic, and the dynamics (spin flip or spin exchange) one gets a very wide class of relaxation behaviors.

We consider q-state Potts spins σ_i, $i = 1$ to L, each taking values 0, 1,... $(q-1)$. The Hamiltonian of the system is the simple nearest-neighbour coupling.

$$H = -J\sum_i \delta(\sigma_i, \sigma_{i+1}).$$

We consider time evolution of this system from an initial disordered state. In Glauber dynamics, single spins can flip ($\sigma_i \rightarrow \sigma_i'$) with a rate (which satisfies the detailed balance condition)

$$\Gamma_{\sigma_i \rightarrow \sigma_i'} = \tfrac{1}{2}\left[1 - \tanh\frac{\beta \Delta E}{2}\right]$$

where ΔE is the difference between the final and the initial configurations when spin σ_i is flipped to σ_i'. For one-dimensional systems, correlations in the steady state are large only for temperature close to zero, and we study this dynamics for large inverse temperatures β.

In Kawasaki dynamics[2] adjacent spins can get exchanged, with a rate which is

$$\Gamma[...\sigma_i = a, \sigma_{i+1} = b... \rightarrow \{...\sigma_i = b, \sigma_{i,a} = a,...\}] = \tfrac{1}{2}\left[1 - \tanh\frac{\beta \Delta E}{2}\right].$$

2. The ferromagnetic Potts models

The stochastic evolution of ferromagnetic Ising chain with single spin flip dynamics in the absence of external filed was shown by Glauber to be exactly soluble long ago[3]. Unfortunately, significant extensions of this solution to other q, longer-range interactions, have not been possible so far. However, the general qualitative behaviour of the evolution is quite well understood.

We consider first the Glauber dynamics for the Ising case $q = 2$. Imagine a sudden quench from a high-temperature initial configuration to zero temperature. After a finite amount of time has elapsed, the system would still have a finite density of kinks (domain walls). Under the single spin flip dynamics, these kinks undergo diffusive motion. If two domain walls come to adjacent sites, they can annihilate each other, reducing the number of domains by 2. This corresponds to the diffusion-limited annihilation reaction

$$A + A \rightarrow \phi.$$
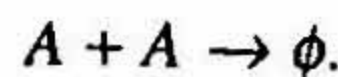
If at time t, the typical separation between domain walls is $L(t)$, then for a finite fraction of these to annihilate and disappear, they have to move a distance of order L, which required a time of order L^2. This implies that

$$L(t) \sim t^{1/2}$$

the average energy per spin scales as $L^{-1}(t)$, and goes down as $t^{-1/2}$. Glauber's solution also showed that spin–spin autocorrelation function shows a $t^{-1/2}$ decay.

The same argument holds for general q. For higher q, when two kinks merge, they may not annihilate completely, but give rise to single kink (this occurs roughly with probability $\frac{q-2}{q-1}$). Thus the reaction–diffusion processes corresponding to general q are

$$A + A \rightarrow A$$
$$A + A \rightarrow \phi.$$
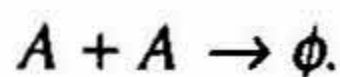
Also, spin–spin autocorrelation function would show the same $t^{-1/2}$ decay.

Even though the dynamics of the ferromagnetic Potts model with spin-flip dynamics is thus easily analyzed in terms of annihilating diffusing random walkers, and thus corresponds to the classical dynamical scaling exponent $z = 2$, the problem is not devoid of surprises. This is illustrated by the recent result of Derrida et al.[4], where the authors studied the fraction of spin which never flip in a zero temperature quench from totally disordered initial state. These authors prove that the fraction decreases as a nontrivial power $t^{-\theta(q)}$, where $\theta(q)$ is a q-dependent exponent given by

$$\theta(q) = -\frac{1}{8} + \frac{2}{\pi^2}\left[\cos^{-1}\left(\frac{q-2}{2\sqrt{q}}\right)\right]^2.$$

Note that the exponent $\theta(q = 3)$ is an irrational number. It is remarkable that this irrational exponent occurs even in such a simple model.

Let us now discuss the low-temperature dynamics of ferromagnetic Potts model under the spin-exchange (Kawasaki) dynamics. In this case, if we have a strictly zero temperature dynamics, then the system quickly relaxes into one of many metastable states such as

aaabbbccccbbbddddddcccccccc.... .

So long as each domain of parallel spins has more than two sites, it is easy to see that these are no lower energy states which can be reached by a single pair exchange. Further relaxation occurs by activation dynamics. We exchange a pair at the boundary of two domains, say, at the boundary of domains of type d and c. This costs extra energy $2J$, and creates a single isolated 'atom' d in the sea of c's, and also an isolated c in the sea of d's. These single atoms can move by pair exchanges without any additional energy cost (only one can move, the jump by either one of the isolated atoms renders the other immobile). The typical time for activation is $\exp(2J/kT)$. Once an excited 'atom' is formed, it does a diffusive motion. The motion ends when it hits a boundary of a domain in the same state as itself. The distance between the two domains in the same state is of the same order as the typical size of a domain. If the typical size of a domain is $L(t)$ at time t, then the diffusing particle is reabsorbed at the same boundary with probability $(1-1L(t))$, and at the other boundary with probability $1/L(t)$. The net result is transfer of one particle from one cluster to a nearby cluster of the same Potts state by an 'evaporation and recondensation' process. We need on an average such random transfers of order $L^2(t)$, so that the net transfer is $\sqrt{L^2(t)} \cong L(t)$ which changes the typical size of a region by a finite factor. This argument gives

$$L(t) \sim \left(e^{-\frac{2J}{kT}}\right) t^{1/3}, \text{ for } \exp(6J/kT) \ll t \ll \exp(9J/kT).$$

Thus the energy density $E(t) \sim t^{-1/3}$. The analogue of the exponent $\theta(q)$ has not yet been determined for the Kawasaki dynamics.

3. The antiferromagnetic case

The antiferromagnetic $q = 2$ Potts model (Ising case) is different from $q \geq 3$ in that for $q = 2$, the ground state is only two-fold generate, while for $q \geq 3$, the ground state has a high degeneracy, the number of states increasing as $(q-1)^L$ for a chain of length L.

Consider first the Ising case. In this case, by a unitary transformation corresponding to flipping all the spins on the odd sites, the Hamiltonian gets converted into that of a ferromagnetic Ising model. Thus the behaviour of energy at time t, and spin–spin autocorrelation functions is the same as for the ferromagnetic Ising model.

Thus, in the zero-temperature quench from totally disordered state described in the previous section, with the Glauber dynamics, the energy per site decreases also as $t^{-1/2}$. The average size of ordered domains increases as

$$L(t) \sim t^{1/2}$$

the spin–spin autocorrelation function decreases as

$$\langle S(0)S(t) \rangle \sim t^{-1/2}.$$

The probability that a spin is not flipped up to time t decreases as $t^{-3/8}$ as in the ferromagnetic Ising case.

Now, consider the antiferromagnetic Ising chain with Kawasaki dynamics. Again, we start with a totally disordered initial state (infinite temperature), and suddenly quench to zero temperature. After some time, a typical state would be

$$...abababbabababbbababaabababab... .$$

Here the domain walls are underlined. These undergo diffusive motion. Two walls of the same type cannot come closer than two units. If two diffusing walls of different types come nearer to each other, they annihilate each other by the reaction

$$aabb \rightarrow abab.$$
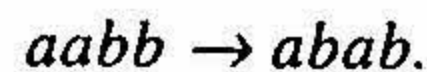
Thus the dynamics of this process is the same as the diffusion-limited reaction

$$A + B \rightarrow \phi.$$
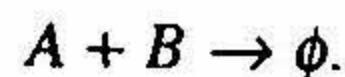
There is a large body of work on these reactions[5,6]. The basic result is that the energy density varies as $t^{-1/4}$. The typical size of a domain

$$L(t) \sim t^{1/4}.$$

This result is understood as follows: If we start with a totally disordered state, diffusive dynamics leads to smoothening over length scales of order $t^{1/2}$. Thus all pairs of type a- and type-b kinks within this scale would meet each other and annihilate. However, any access of a- or b-type kinks survives. The excess of a type kinks on averging are $t^{1/2}$ sites would be typically of the order $t^{1/4}$. And thus their typical density of kinks decreases with time as $t^{1/4}$. As the density of kinks is the same as the energy density, we get

$$E(t) \sim t^{-1/4}$$

typical distance between kinks and the H increases as $t^{1/4}$.

Now let us discuss the case $q \geq 3$. Let us consider the Glauber dynamics first. Then whatever the state of two neighbouring spins, there exists at least one state [in general $(q-2)$ states] which corresponds to the local minima of energy. As there is a finite rate to go into any of these states, we see that starting from a disordered state, the energy relaxation is exponential in time

$$E(t)-E_0 \leq \exp[-At]$$

where E_0 is the ground state energy and A is some constant. Thus the system approaches ground state with an exponential rate. However, in this case, the ground state has infinite degeneracy, and at long times, the system shows no tendency to reach a dead state, as it keeps moving between different ground states. If $(q \geq 4)$, then each spin keeps flipping at finite rate, and the initial state correlation function $\langle \delta_{\sigma_i(0)}; \sigma_i(t) \rangle$ and autocorrelation function in the steady state both decay exponentially in time.

For $q \geq 4$, with Kawasaki dynamics also, the situation is quite simple. As the number of spins of each of q species is separately conserved, if the fractional number of atoms of one species is larger than half, the minimum energy configuration cannot be reached. However, the density of pairs of spins which can be flipped without increasing the energy in a typical state is finite and thus the spins keep diffusing. This implies that in the steady state, the autocorrelation function is diffusive

$$\langle \delta_{\sigma_i(t)}, \sigma_i(t+\tau) \rangle \sim \tau^{-1/2}, \text{ for large } \tau.$$

The case $q = 3$ requires special care. For a chain of size L, there are 3.2^{L-1} ground states, the long time dynamics involves transitions between these states. Let us denote the three states of spin at a site by integer 0, 1 and 2. Define $\delta_i = q_{i+1}-q_i$ (mod 3). Then in the groundstates δ_i's take values ± 1.

Consider the Glauber dynamics first. Then a spin can flip only if spins on both sites of it are in the same state. In terms of δ_i, this corresponds to interchanging a pair $[+ 1,-1]$ by $[-1, + 1]$. The quantity $\Sigma_i \delta_i$ is the total winding number of the state, and is conserved by the dynamics. Thus the state space breaks up into L mutually disconnected sectors. If the system is started from a high-energy state, it will relax to one of these sectors, and would not be able to go to other ground states. Thus the motion is not ergodic.

Let us now calculate the spin–spin autocorrelation function in a typical sector. In the steady state define.

$$e(t) = \left\langle e^{i\pi \frac{2}{3}(q_i(t)-q_i(0))} \right\rangle.$$

Expressed in terms of δ_i, this becomes the expectation value of exponential of the sum of δ_i's. Now, the dynamics of δ_i's is diffusion of hardcore particles on a line. In this case,

it is very well known that the density field satisfies linear diffusion equation[7] and the variance of number of particles to the left of i, increases as $t^{1/2}$. This shows that for this case we have

$$C(t) \sim \exp(-At^{1/2}).$$

Finally, let us consider the Kawasaki dynamics for the antiferro $q = 3$ Potts model. For this case, the only spin exchanges which do not increase energy are

$$0120 \leftrightarrow 0210, \ 1201 \leftrightarrow 1021 \ \text{and} \ 2102 \leftrightarrow 2012.$$

In terms of the variables δ_i, the dynamics corresponds to

$$111 \leftrightarrow -1-1-1$$

at any three adjacent sites in the same state δ, we flip them together at a fixed rate. This is the trimer deposition evaporation model recently introduced by Barma et al[8]. This dynamics has been studied by us recently. It is found that there is a strong breaking of ergodicity, and the number of disjoint sectors is exponential in the size of the lattice. The system has an infinite of conservation laws, which are most simply represented as a conservation law of an object called the 'irreducible string'. The longtime behaviour of relaxation depends on the sector, and many different behaviours are seen[10]. We refer the reader to the original papers for details. However, the most common behaviour of autocorrelation function of δ's in this case is found to be

$$\langle \delta_i(t)\delta_i(t + \tau) \rangle \sim \tau^{-1/4} \ \text{for} \ t \gg \tau \gg 1.$$

which corresponds to a four-point correlation function terms of the original spin variables q.

4. Conclusion

Thus we see that even the one-dimensional Potts model, which has a rather trivial equilibrium behaviour displays a variety of relaxations, in the dynamical case. The possible behaviours are summarized in Fig.1. One can expect some more surprises if we study the Potts model with next nearest neighbour-couplings also. These are known to give a rather complicated phase diagram even in equilibrium statistical mechanics (in the mean field theory). Extension of this approach to other values of q is an interesting problem. For example, $q = 1$ is known to be related to the percolation problem, $q = 0$ is the spanning trees/resistor network problem by the well-known work of Fortuin and Kasteleyn. Can one define a 'Glauber' or 'Kawasaki' dynamics for these cases? What about noninteger values of q? Clearly, cluster-flip algorithms do not qualify, as they are nonlocal. An important question is effect of external magnetic fields. The critical slowing down in the presence of complex values of magnetic field is related to the statistics of branched polymers, and is of interest[11]. If the magnetic field is time-dependent, we have a simple model to study the hysteresis in ferromagnets, which has been subject of much interest lately[12, 13]. Another important question is the relaxation behaviour in higher dimensions. It is hoped that this paper will induce the reader to think about these and related problems.
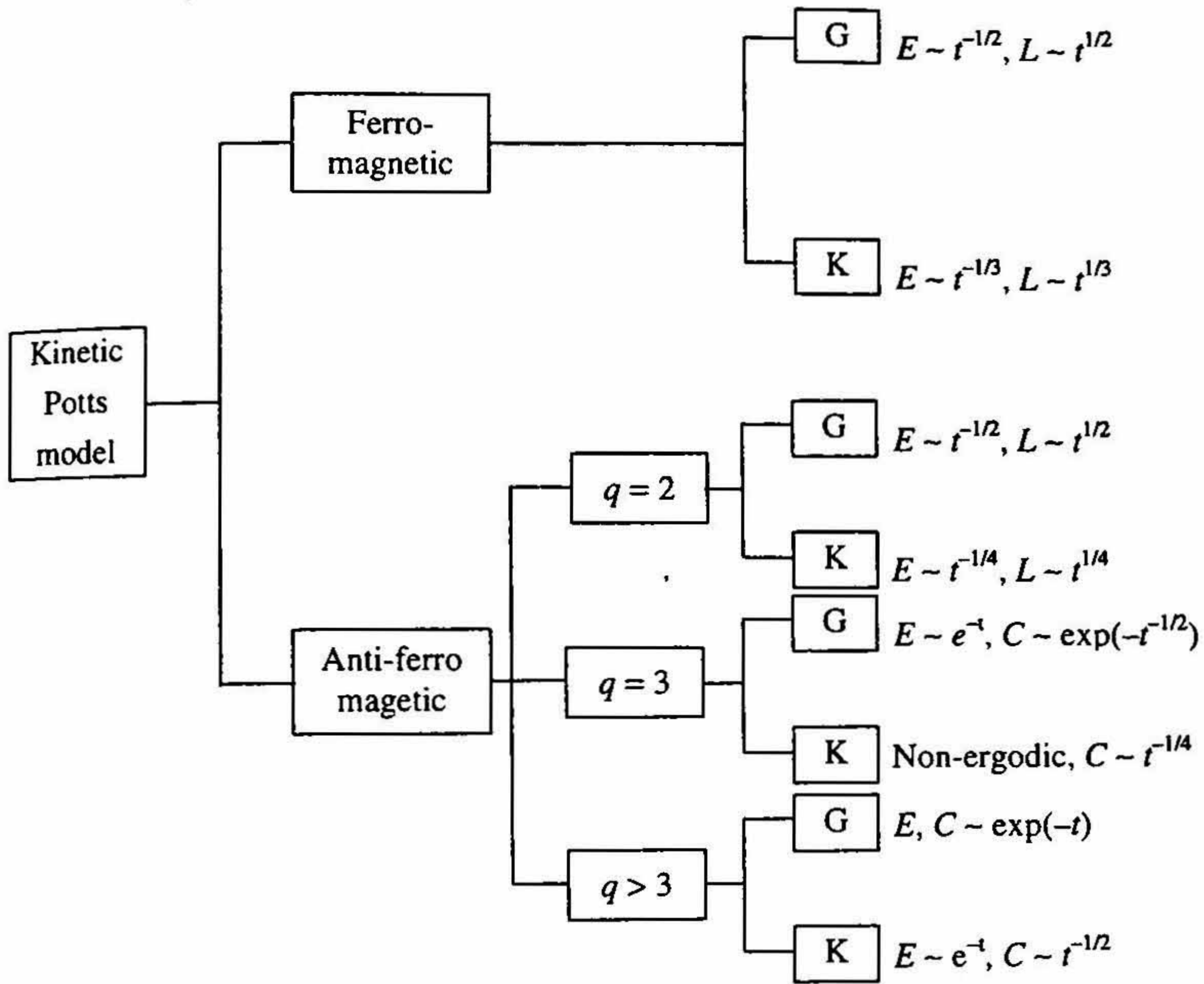
FIG. 1. Different types of relaxation behavior in the one-dimensional kinetic Potts models.

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