# Rigorous Derivation of Reaction-Diffusion Equations with Fluctuations

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We study interacting particle (spin) systems on a lattice under the combined influence of Glauber (spin flip) and simple exchange (Kawasaki) dynamics. We prove that when the conserving exchanges occur on a microscopically fast scale the macroscopic density (magnetization) evolves according to an autonomous nonlinear diffusion-reaction equation. Microscopic fluctuations about the deterministic macroscopic evolution are found explicitly. They grow, with time, to become infinite, when the deterministic solution is unstable.

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In this note we show how to derive rigorous nonlinear diffusion-reaction–type equations[1] for the macroscopic evolution of microscopically simple model systems particles on a lattice with stochastic microscopic dynamics.[2] These types of equations are often used to describe chemically reacting systems, population genetics, etc.[1] Our analysis contains some of the essential elements involved in the transition from microscopic to macroscopic evolution equations in general systems: the suitable rescaling of space and time.[3] By such rescalings one takes account of the central fact that there are a very large number of atoms in each drop of macroscopic fluid and that there is a big spread between microscopic and macroscopic time scales. This brings in the "law of large numbers" which is crucial for obtaining deterministic autonomous macroscopic equations for quantities which fluctuate on the microscopic scale.

The simplicity of our model systems permits us to obtain also these fluctuations around the deterministic solutions directly from the microscopic dynamics. These fluctuations form a Gaussian field with an amplitude of $O(\epsilon^{d/2})$ around stable solutions of the macroscopic equations but grow exponentially or like a power around unstable solutions.

In the simplest case these solutions are spatially uniform stationary solutions of the nonlinear equation, some of which are stable and others unstable. They can be interpreted (in some cases) as coexisting stationary states of our microscopic lattice system, even before we take the limit $\epsilon \to 0$. N.B.: These stationary states are generally *not* equilibrium Gibbs states with *any* finite-range (or rapidly decaying) potential. They are nonequilibrium stationary states which can have phase transition even in one dimension.

The study of such stationary nonequilibrium microscopic states is in itself a problem of great interest and was one motivation for undertaking the present work.[4] Another motivation is our hope that the analysis of the microscopic fluctuations about the deterministic macroscopic equations will add to our understanding of the instabilities and pattern formation associated with nonlinear evolution equations.[5] This may be particularly so in cases where stochastic lattice models are invented to simulate physically important and mathematically intractable nonlinear equations, e.g., those describing the motion of an interface between two fluids.[6]

Our system is a simple cubic lattice in $d$ dimensions, at each site of which there is a spin $\boldsymbol{\sigma}(\mathbf{x}) = \pm 1$, $\boldsymbol{\sigma} = \{\boldsymbol{\sigma}(\mathbf{x}) | \mathbf{x} \in Z^d\}$. (Equivalently we can think of occupied and empty sites or of two chemical species.) We consider two mechanisms by which a configuration of the lattice $\sigma$ changes with time: a Glauber dynamics in which a spin flips at a site $\mathbf{x}$, $\boldsymbol{\sigma} \to \boldsymbol{\sigma}^{\mathbf{x}}$, with a rate $c(\mathbf{x};\boldsymbol{\sigma})$, and a Kawasaki dynamics in which unequal spins at neighboring sites exchange, $\boldsymbol{\sigma} + \boldsymbol{\sigma}^{\mathbf{x},\mathbf{y}}$, with a constant rate.

There are very few restrictions on $c(\mathbf{x};\boldsymbol{\sigma})$. For concreteness it is useful to think of a Glauber dynamics which satisfies detailed balance for the Gibbs state of a one-dimensional Ising model with nearest-neighbor interactions $J$ at reciprocal temperature $\beta$,

$$c(\mathbf{x};\boldsymbol{\sigma}) = \{1 - \gamma\sigma(x)[\sigma(x+1) + \sigma(x-1)] + \gamma^2\sigma(x+1)\sigma(x-1), \tag{1}$$

where $\gamma = \tanh\beta J$.

The exchange process, on the other hand, being independent of the spin configuration on neighboring sites, acts *as if* the system were at an infinite temperature, $\beta = 0$. We shall furthermore assume that this exchange rate is very fast compared to the flip rate, i.e., the magnetization-conserving dynamics will take place, in the language of the introductory paragraphs, on a microscopic time scale. This change in scales will be denoted by $\epsilon^{-2}$, with $\epsilon << 1$.

The "equation of motion" for $f(\boldsymbol{\sigma},t)$, the expected value at time $t$ of a function $f$, when the spin configuration

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at $t=0$ is $\sigma$, is a sum of a Glauber and a simple exchange Kawasaki term,

$$\frac{df(\sigma,t)}{dt}=\sum_{\mathbf{x}\in Z^d} c(\mathbf{x};\sigma)[f(\sigma^{\mathbf{x}},t)-f(\sigma,t)]+\epsilon^{-2}\sum_{|\mathbf{x}-\mathbf{y}|=1}[f(\sigma^{\mathbf{x},\mathbf{y}},t)-f(\sigma,t)]=L_G f+\epsilon^{-2}L_K f. \tag{2}$$

We shall now define the macroscopic magnetization density by rescaling space by $\epsilon^{-1}$. (The relation between space and time rescalings depends on the microscopic dynamics.[3]) Let $\Lambda^\delta$ be a cubical box with sides of length $\sigma$, $\Lambda_{\mathbf{r}}^\delta$, centered on $\mathbf{r}\in R^d$. The magnetization density on this scale is

$$m^\epsilon(\mathbf{r},t;\sigma)=S_t^\epsilon[\epsilon^d\sum_{\epsilon\mathbf{x}\in\Lambda_{\mathbf{r}}^\delta}\sigma(\mathbf{x})], \tag{3}$$

where $S_t^\epsilon=\exp[L_G+\epsilon^{-2}L_K]t$. $m^\epsilon(\mathbf{r},t;\ )$ is a random variable whose probability distribution depends on the initial probability distribution of the system. We shall assume the latter to have good cluster properties and that as $\epsilon\to 0$, $\epsilon^{-d}|\langle\sigma(\mathbf{x})\rangle_0-m_0(\epsilon\mathbf{x})|\to 0$, where $m_0(\mathbf{r})$ is a smooth function of $\mathbf{r}$, $\mathbf{r}\in R^d$, $|m_0(\mathbf{r})|\le 1$, and $\langle\ \rangle_0$ denotes expectations with respect to the initial distribution.

In the limit $\epsilon\to 0$ there is a true separation between the microscopic and macroscopic scales and $m_0(\mathbf{r})$ becomes the macroscopic magnetization at $t=0$. We now expect that the exchanges which become infinitely fast on the macroscopic time scale when $\epsilon\to 0$ will cause the spins in the box $\Lambda_{\mathbf{r}}^\delta$ to be distributed independently (with a product measure) at the instantaneous value of the magnetization $m^\epsilon(\mathbf{r},t;\sigma)$. This magnetization will change because of fluxes through boundaries of $\Lambda_{\mathbf{r}}^\delta$ and spin flips which try to make the spins correlated. On the other hand $\Lambda_{\mathbf{r}}^\delta\to\infty$ so $m^\epsilon(\mathbf{r},t;\ )$ should become a deterministic variable $m(\mathbf{r},t)$ (fluctuations should go to zero), and its time evolution be determined by use of this product measure to evaluate the changes it undergoes. This is exactly what happens:

Our results form two theorms.

*Theorem 1.*—In the limit $\epsilon\to 0$, $m^\epsilon(\mathbf{r},t;\sigma)\to\int_{\Lambda_{\mathbf{r}}^\delta}m(\mathbf{r}',t)d^3r^1$, a deterministic (nonfluctuating) function of $\mathbf{r}$ and $t$, with the density $m(r,t)$ satisfying the equation

$$\partial m(\mathbf{r},t)/\partial t=\nabla^2 m+F(m(\mathbf{r},t)) \tag{4}$$

with the initial condition $m(\mathbf{r},0)=m_0(\mathbf{r})$.

$F(m)=-\langle 2\sigma(0)c(0;\sigma)\rangle_{\nu_m}$ is a polynomial in $m$—the average being taken with respect to the to the Bernoulli (product) measure $\nu_m$, $\langle\sigma(\mathbf{x})\rangle_{\nu_m}=m$ for all $\mathbf{x}$. This is the same as the infinite-temperature equilibrium state with magnetization per site $m$. $F(m(\mathbf{r},t))$ is in fact equal to the almost sure value of $\lim_{\epsilon\to 0}L_G m^\epsilon(\mathbf{r},t;\sigma)$ in the Bernoulli measure $\nu_{m(\mathbf{r},t)}$ which is what we expected. For example in (1), we have

$$\frac{\partial m(r,t)}{\partial t}=\frac{\partial^2 m}{\partial r^2}+2(2\gamma-1)m-2\gamma^2 m^3. \tag{5}$$

To see the microscopic fluctuations in the magnetization—corresponding to the deviations of the probability distribution at time $t$ from a product measure—we must magnify them in an appropriate way. This is given by the next theorem.

*Theorem 2.*—Let

$$\phi^\epsilon(\mathbf{r},t;\sigma)=\epsilon^{-d/2}[m^\epsilon(\mathbf{r},t;\sigma)-m(\mathbf{r},t)];$$

then

$$\phi^\epsilon(\mathbf{r},t;\sigma)\underset{\epsilon\to 0}{\to}\int\phi(\mathbf{r},t),$$

a random Gaussian field satisfying the following Ornstein-Uhlenbeck–type stochastic equation:

$$\frac{\partial\phi(\mathbf{r},t)}{\partial t}=\nabla^2\phi+2F'(m(\mathbf{r},t))\phi+\frac{dW(\mathbf{r},t)}{dt}, \tag{6}$$

where $W(\mathbf{r},t)$ is a Brownian motion or Wiener process ($dW/dt$ is "white" noise) with the covariance

$$\langle W(\mathbf{r},t)W(\mathbf{r}',t')\rangle=\min(t,t')[-(1-m^2)\nabla^2\delta(\mathbf{r}-\mathbf{r}')-\nabla(1-m^2)\nabla\delta(\mathbf{r}-\mathbf{r}')+4f(m)\delta(\mathbf{r}-\mathbf{r}')], \tag{7}$$

where $f(m)=\langle c(0;\sigma)\rangle_{\nu_m}[=1-\gamma(2-\gamma)m^2$, for example (1)].

The equal-time correlations of the fluctuation field $\phi$,

$$c(\mathbf{r},\mathbf{r}';t)=\langle\phi(\mathbf{r},t)\phi(\mathbf{r}',t)\rangle,$$

satisfy the following equations:

$$c(\mathbf{r},\mathbf{r}';t)=[1-m^2(\mathbf{r},t)]\delta(\mathbf{r}-\mathbf{r}')+\tilde{c}(\mathbf{r},\mathbf{r}';t), \tag{8}$$

$$\partial\tilde{c}(\mathbf{r},r';t)/\partial t=\Delta\tilde{c}_t+2F'(m)\tilde{c}_t-2\delta(r-r')[(\nabla m)^2-F'(m)(1-m^2)+mF(m)-2f(m)], \tag{9}$$

$$\tilde{c}(\mathbf{r},\mathbf{r}',0)=0.$$

The roof of these theorems uses a dual branching process; cf. Liggett,[2] Sect. 3, for a clear presentation of duality. This reduces the study of a Markov process on an uncountable state space ($\{-1,1\}^Z$ in our case) to the study of its simpler dual process, a Markov chain on a countable state space. We can then obtain estimates on the correlations built up by the Glauber dynamics in a macroscopic region, scale $\epsilon^{-1}$, in a macroscopic time, scale $\epsilon^{-2}$. The details of the proofs are rather long and will be presented elsewhere.[7] For the case when there are no flips our results reduce to those of De Masi *et al.*[3]

We shall discuss the behavior of the macroscopic magnetization and its fluctuations in terms of the one-dimensional example in (5). The general case should be very similar although less is known about the solutions of the diffusion-reaction equation in $d>1$.

Equation (5) has for a given $m(r,0)=m_0(r)$, $|m_0|\leqslant 1$, a unique solution $m(r,t)$ for $t\geqslant 0$, with $|m(q,t)|\leqslant 1$.[1] The general time-dependent solutions can be rather complicated. The analysis of their stability, particularly for the "propagating" ones, is a subject of great current interest in terms of "pattern selection."[4] We shall only discuss here the simplest case, when $m(r,t)=\overline{m}(\gamma)$ is independent of $r$ and $t$.

We note first that for $\gamma<0$, corresponding to antiferromagnetic interactions, $\overline{m}(\gamma)=0$ is the unique translationally invariant stationary solution—and it is stable. For the more interesting ferromagnetic case, $\gamma>0$, the solution $\overline{m}=0$ is unique for $\gamma<\gamma_c=\frac{1}{2}$. For $\gamma>\gamma_c$ there are three solutions: $\overline{m}=0$, and $\overline{m}=\pm m^*=\pm(2\gamma-1)^{1/2}/\gamma$ corresponding to the magnetized state. The latter solutions are stable while the $\overline{m}=0$ solution is unstable. The value $\gamma_c$ clearly corresponds to a mean-field–type critical point—its origin lying in the decorrelations among the spins induced by the fast exchanges.

The instability of the $\overline{m}=0$ state, for $\gamma>\gamma_c$, is reflected in the unbounded growth of the fluctuations about this state obtained from the solution of (9). For the example (1) the equation for the covariance with initial condition $m_0=0$ is

$$\partial\tilde{c}_t/\partial t=\Delta\tilde{c}_t-4(1-2\gamma)\tilde{c}_t+8\gamma\delta(r-r'),$$

$$\tilde{c}(r,r';0)=0,$$

and the solution is

$$\tilde{c}_t(r,r')=8\gamma\int_0^t ds\,(4\pi s)^{-1/2}\exp[(r-r')^2/4s]\exp[-4(1-2\gamma)s].$$

For $\gamma>\gamma_c$, $\tilde{c}_t\to\infty$ as $t\to\infty$, the growth being like $\sqrt{t}$ for $\gamma_c$ and exponential for $\gamma>\gamma_c$, while for $\gamma<\gamma_c$,

$$\tilde{c}_t(r,r')\to\frac{\gamma/2}{\gamma_c-\gamma}\exp[-2(1-2\gamma)^{1/2}|r-r'|]$$

so that the Gaussian field $\phi$ approaches a stationary state with exponentially decaying covariances (on the macroscopic scale).

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