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Stochastic reaction diffusion equations and interacting particle systems

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ABSTRACT. – In this paper after a brief survey of recent progress in the theory of stochastic reaction diffusion equations, we discuss their role in describing deviations from hydrodynamic behaviour in the statistical mechanics of simple models. In this connection we analyse qualitatively the limits of such a description and how this is supplemented by exact calculations.

RÉSUMÉ. – Après une brève description des progrès récents dans la théorie des équations de réaction diffusion stochastiques, nous discutons leur utilisation dans la description des déviations par rapport au comportement hydrodynamique dans la mécanique statistique de modèles simples. Dans ce cadre nous analysons qualitativement les limites d'une telle descriptions et comment elle peut être complémentée par des calculs exacts.

1. In this paper we shall first briefly review some aspects of a theory whose development is very recent: nonlinear partial differential systems of parabolic type perturbed by white noise in time and space. The peculiarity of the subject is that such equations very often do not stand white noise which is a much too singular perturbation. On the other hand important phenomenological equations in physics like the Navier-Stokes equation and all sorts of reaction diffusion equations are examples of parabolic

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systems and additive white noise is a natural modelization of neglected effects and/or background influence in many concrete situations.

A general theory of small fluctuations from thermodynamical equilibrium was proposed long ago by Onsager and Machlup [1] and was developed on the assumption that these were driven by a white noise to be added to the macroscopic evolution equations. Onsager and Machlup considered only finite dimensional situations (no space inhomogeneity) and linear equations (situations close to equilibrium). If now one assumes that the obvious generalization of Onsager-Machlup to the space inhomogeneous case consists in adding a white noise in time and space to the (in general non linear) hydrodynamical macroscopic equations, one is immediately faced with the mathematical difficulties mentioned above.

Actually the first incentive for studying rigorously stochastic parabolic equations came from a different area of physics: quantum field theory. The approach to the construction of Euclidean measures called stochastic quantization indeed requires a serious understanding of such equations. This explains why the methods of constructive quantum field theory provided the tools for the first steps in developing the theory [2] which makes essential use of the concept of renormalization (1). In the next section we shall describe the class of equations which so far have been treated rigorously through an appropriate renormalization procedure. We shall introduce the notion of probabilistic weak solution and briefly discuss its construction. In section 3 we will comment on the scale dependence of fluctuations which is characteristic of our equations and point out some of its consequences.

In the last section we examine a more fundamental question. It has always been an ambition of statistical mechanics to provide a derivation of phenomenological macroscopic equations from the underlying microscopic dynamics. This reductionist program has so far succeeded only for very special discrete models but the insight which emerges is hopefully of much greater generality [4]. The next natural question in connection with these simplified models is a description of the fluctuations with respect to the behaviour imposed by the macroscopic equations. Some progress in this direction has been made recently. We then try to compare the theory of fluctuations for stochastic parabolic equations with results obtained in the context of special microscopic models. Important conclusions will emerge. In general the two descriptions agree only on sufficiently large space scales and for not too large fluctuations.

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(1) *See* also the more abstract setting of Albeverio e Röckner [3] based on the theory of infinite dimensional Dirichlet forms.

2. The general form of stochastic reaction diffusion equations that we shall consider is

$$\partial_t \mathbf{\Phi} = \nu \Delta \mathbf{\Phi} - \mu \mathbf{\Phi} + \mathbf{F} \mathbf{\Phi} + \varepsilon \, \partial_t \mathbf{w}_t \tag{1}$$

with

$$\mathbf{E}(\partial_t w_{ti}(\mathbf{x}) \, \partial_{t'} w_{t'k}(\mathbf{x}')) = \delta(t-t') \, \delta(\mathbf{x}-\mathbf{x}') \, \delta_{ik} \tag{2}$$

$\mathbf{x}$, $\mathbf{x}'$, $\in \mathrm{R}^d$, Φ_i and $\mathrm{F}_i(\mathbf{\Phi})$ are vectors in some finite dimensional space. The $\mathrm{F}_i' s$ are polynomials in $\Phi_i j=1, \ldots, n$ and ε is a parameter describing the intensity of the noise. As it is the system (1), (2) does not make sense if $\mathbf{x}$, $\mathbf{x}'$, $\in \mathrm{R}^d$, $d>1$ due to the singular character of the noise. For $d>1$ white noise generates large fluctuations at small scales in space. If $\mathbf{F}$ is non linear the powers of the fields Φ_i induce high frequency divergences which have to be removed in order to give a meaning to the equation. This is what is called in quantum field theory the problem of ultraviolet stability. The method to solve it when applicable is called renormalization and consists in a redefinition of the physical parameters appearing in the problem. However even after renormalization the equations retain only a formal character due to the appearance of infinite constants.

In order to construct from the renormalized equations a well defined stochastic process, one has to introduce the notion of weak probabilistic solution. This notion exists already in the theory of ordinary stochastic differential equations and applies in those situations where the non linearities are not sufficiently smooth, for example they do not satisfy a Lipschitz condition. The idea consists in the following: even though the equation cannot be solved pathwise, a well defined measure can be associated to it. One way of constructing such a measure is via a regularization of the equation and then a passage to the limit on the associated measure. It is well known that the measure describing the solutions of an ordinary stochastic differential equation can be given explicitely in terms of its Radom-Nykodin derivative with respect to the Wiener measure or some other reference measure. The expression of this density is often referred to as the Cameron-Martin-Girsanov formula. In our case let us take as reference the measure generated by the linear part of (1) that is by the process

$$\partial_t \mathbf{z}_t = (\nu \Delta - \mu) \mathbf{z}_t + \varepsilon \, \partial_t \mathbf{w}_t \tag{3}$$

The formal expression of the density is then

$$\frac{d\mu_{\mathbf{\Phi}}}{d\mu_{\mathbf{z}}} = e^{\xi_{\mathrm{T}}} \tag{4}$$

with

$$\xi_{\mathrm{T}} = \frac{1}{\varepsilon} \int_0^t (:\mathbf{F}(\mathbf{z}_s):, d\mathbf{w}_s) - \frac{1}{2\varepsilon^2} \int_0^t ds \, (:\mathbf{F}(\mathbf{z}_s)):, :\mathbf{F}(\mathbf{z}_s):) \tag{5}$$

The double dots :: indicate the operation of renormalization mentioned above and (.,.) is the scalar product in the space variables. In two space dimensions the divergences are weak (logarithmic), and the renormalization can be accomplished by modifying **F**, which is assumed a polynomial of degree n, with the introduction of monomials of degree lower than n multiplied by infinite constants. Actually in the case of equations (1), (2) one has also to perform an additional smoothing in space of the right hand side of (1) and modify correspondingly the covariance (2). We do not enter into the details of these technical problems for which the reader is referred to [2].

The basic fact is that using the methods of constructive field theory at least in two space dimensions one is able to give a precise meaning to (4), in spite of the infinite renormalizations. In particular correlation functions of the fields

$$E_{\mu_\Phi}(\Phi_{i_1}(\mathbf{x}_1, t_1) \ldots \Phi_{i_n}(\mathbf{x}_n, t_n)) = E_{\mu_z}(e^{\xi_T} z_{i_1}(\mathbf{x}_1, t_1) \ldots z_{i_\mu}(\mathbf{x}_\mu, t_\mu)) \\ T > \max\{t_i\}$$

are well defined distributions in the $\mathbf{x}_i$.

3. In this section we want to point out some peculiarities of the stochastic fields Φ_i, connected with their singular behaviour in the space variables. They are distributions and only when smeared over some region Δ they become good stochastic variables. Therefore as physically meaningful quantities we may take the averages

$$\Phi_{j_\Delta}(t) = \frac{1}{|\Delta|} \int_\Delta d^2 x \, \Phi_j(\mathbf{x}, t) \tag{6}$$

where $|\Delta|$ is the area of Δ. Φ_Δ will possess all moments, however these moments will diverge if Δ shrinnks to a point. Typically for a small Δ

$$E(\Phi_{j_\Delta})^2 \sim \varepsilon^2 C \ln \frac{1}{|\Delta|} \tag{7}$$

This means that even for very small ε the stochastic pertubation will have strong effects on sufficiently small scales. As a consequence the dynamics of the fields will be different at different scales. For example at small scales a stochastic trajectory $\Phi_\Delta(t)$ will hardly reflect the structure of the attractors of the deterministic equation corresponding to $\varepsilon = 0$ and the Lyapunov exponents will depend in general on the chosen Δ. If we want to resolve two points of an attractor separated il some metric by a distance d we have to take a sufficiently large Δ. This in turn leads to some kind of uncertainty relationship in connection with the possibility of studying the spacial dependence of such points [(2)].

In fact all space structure below the scale $|\Delta|^{1/2}$ is lost. In the present two dimensional situation this effect is not very conspicuous due to the weakness of the divergences. The situation would be very different in 3 dimensions where linear divergences are expected. In such a case we would have a relationship of the form

$$|\Delta|^{1/3} d^2 > \varepsilon^2 \mathrm{C} \tag{8}$$

where $|\Delta|$ is the volume of the region Δ and C is a suitable constant; (8) is obtained simply by imposing that the dominant part of $\mathrm{E}(\Phi_{j_\Delta})^2$ be less than d^2. Similar arguments can be developed for the study of the space dependence of any field configuration. Of course the numerical relevance of a relation like (8) has to be analysed in every particular situation.

4. In this section we address an important physical question. To what extent the generalized Onsager-Machlup theory which, as we have emphasized, leads to stochastic PDE, is correct? We begin with a qualitative and simplified description of the problem of hydrodynamic fluctuations for a lattice spin model in d dimensions evolving according to Glauber (spin flip) plus accelerated Kawasaki (simple exchange) dynamics [5]. This means that a function $f(\sigma)$ of a spin configuration σ evolves following the equation

$$\partial_t f = \mathrm{L}_\varepsilon f = \mathrm{L}_\mathrm{G} f + \varepsilon^{-2} \mathrm{L}_\mathrm{E} f \tag{9}$$

with

$$\left.\begin{aligned} \mathrm{L}_\mathrm{G} f &= \sum_{x \in \mathbf{Z}^d} c(x, \sigma)[f(\sigma^x) - f(\sigma)] \\ \mathrm{L}_\mathrm{E} f &= \frac{1}{2} \sum_{|x-y|=1} [f(\sigma^{xy}) - f(\sigma)] \end{aligned}\right\} \tag{10}$$

σ^x is the configuration obtained from σ by flipping the spin at the site x while σ^{xy} is obtained by exchanging the spins at sites x and y. $c(x, \sigma)$ is an appropriate rate function.

The following basic facts were established in [5]. Define the magnetization field and the magnetization fluctuation field

$$\mathrm{X}_t^\varepsilon(\varphi) = \varepsilon^d \sum_{x \in \mathbf{Z}^d} \varphi(\varepsilon x)\, \sigma(x, t) \tag{11}$$

$$\mathrm{Y}_t^\varepsilon(\varphi) = \varepsilon^{d/2} \sum_{x \in \mathbf{Z}^d} \varphi(\varepsilon x)[\sigma(x, t) - \mathrm{E}(\sigma(x, t))] \tag{12}$$

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(2) Under particular boundary condition or in presence of non homogeneous coefficients in the equation the elements of the attractor may exhibit non trivial space dependence.

φ is a test function. Then when $\varepsilon \to 0$.

(*a*) X_t^ε tends in probability to

$$m_t(\varphi) = \int d\mathbf{r}\, \varphi(\mathbf{r})\, m(\mathbf{r}, t)$$

where $m(\mathbf{r}, t)$ is a solution of an equation of the form

$$\partial_t m = \frac{1}{2} \Delta m + F(m) \tag{13}$$

$F(m)$ is typically a local polynomial.

(*b*) Y_t^ε approaches

$$\int dr\, \varphi(\mathbf{r})\, \eta_t(\mathbf{r})$$

where $\eta_t(\mathbf{r})$ is a solution of the linear stochastic equation

$$d\eta_t = \left(\frac{1}{2} \Delta \eta_t + F'(m)\, \eta \right) dt + \alpha_t \tag{14}$$

α_t is a white noise in the time variable and a superposition of *white noise* and *derivatives of white noise* in the space variables.

We make first some heuristic comments. It looks that everything goes as if one could define a local field

$$\xi_t^\varepsilon(\mathbf{r}) = m(\mathbf{r}, t) + \varepsilon^{d/2}\, \eta_t(\mathbf{r}) + \ldots \tag{15}$$

which, using (13) and (14) and eliminating m, satisfies a non linear stochastic differential equation of the form

$$d\xi_t^\varepsilon = \frac{1}{2} \Delta \xi_t^\varepsilon + F(\xi_t^\varepsilon) + \varepsilon^d\, G(\xi_t^\varepsilon, \eta_t) + \ldots + \varepsilon^{d/2}\, \alpha_t \tag{16}$$

This is not really an equation for ξ_t^ε because it still contains η_t. However since η_t is a rapid variable, if compared with ξ_t^ε, we may try to substitute for it its equilibrium expectation values. Then to order $(\varepsilon^{d/2})^2$ we have a closed equation for ξ_t^ε. However if F is non linear this equation has no meaning in any dimension because the derivative of white noise is much too singular. To do better we first smear η_t over some small domain. The new field will satisfy approximately an equation like (14) where only the white noise term survives in α. Similarly for ξ_t^ε. But then something remarkable happens. For $d=2$ and F a polynomial of third degree the term $\varepsilon^2 G$ in (16) evaluated with the equilibrium expectation values for η_t, η_t^2 . . . has exactly the form of the renormalization counterterms necessary to make (16) a meaningful equation in the weak sense described in section 2.

All this is very rough but indicates two important circumstances. A description of the magnetization field in terms of a non linear stochastic parabolic P.D.E. is perhaps possible only if (i) it does not deviate too much from a solution of the hydrodynamic equation, (ii) it is averaged over a suitable scale to eliminate the hard fluctuations induced by the derivative of white noise.

How much of this picture can be substantitated by rigorous arguments? The first results in this direction support the above description and in addition provide the corrections to it when conditions (i) and (ii) are not satisfied. In other words they supplement the Onsager Machlup theory. The rigorous theory is developed by calculating the large fluctuations of the magnetization field when $\varepsilon \to 0$. These are expressed as usual in terms of the action functional

$$\mathrm{I}(m) = -\lim_{\varepsilon \to 0} \varepsilon^d \ln \mathrm{P}(\mathrm{Sup}_t \,|\, \mathrm{X}_t^\varepsilon(\varphi) - m_t(\varphi) \,| < \delta) \tag{17}$$

where m_t is an arbitrary trajectory, $\mathrm{I}(m)$ has been calculated explicitely in a work in collaboration with C. Landim and M. E. Vares [6], developing the approach of [7], for a system strictly related to (9), (10). It is a consequence of our results that for trajectories not too far from a solution of (13) and sufficiently regular at small space scale $\mathrm{I}(m)$ can be written approximately

$$\mathrm{I}(m) = \int_0^t \left\| \partial_s m_s - \frac{1}{2}\Delta m_s - \mathrm{F}(m_s \right\|^2 ds + \mathrm{I}_1\left(\partial_s m - \frac{1}{2}\Delta m - \mathrm{F}(m)\right) \tag{18}$$

where I_1 is a functional which contains powers of its argument higher than 2. The first term in the r.h.s. of (18) is what we may call the Onsager-Machlup approximation and can be interpreted in terms of an underlying stochastic P.D.E. suitably renormalized if $d > 1$ along the lines indicated in section 2. (18) says however that in general the fluctuations have a more complex structure than those generated by adding a white noise to hydrodynamics. As in the Onsager-Machlup approximation the hydrodynamic trajectory remains the most probable trajectory for a fluctuation which relaxes to equilibrium. Work is in progress to clarify the physical consequences of deviation from the Onsager-Machlup theory.

Problems related to those discussed in this section are addressed in a recent paper by G. Eyink [8].

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