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LETTER TO THE EDITOR

Langevin and Fokker–Planck equations for kinetic growth and aggregation processes

Yonathan Shapir

Physics Department, Brookhaven National Laboratory, Upton, New York 11973, USA

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Abstract. A theoretic approach to account for the intrinsic fluctuations of kinetic growth and aggregation processes in their equations of motion is presented. Langevin equations, with multiplicative noise terms, are derived for continuous variants of the Eden models and for the transparent diffusion-limited aggregation. The related Fokker-Planck equations are derived as well. Fluctuations are irrelevant for the Eden models but are probably relevant for the diffusion-limited aggregation. The possible use of the stochastic equations to regularise their effects in this latter case is briefly discussed.

Different models of aggregating clusters and kinetic growth have attracted much attention recently. This interest was primarily stimulated by the introduction of the Witten-Sander model (Witten and Sander 1981, 1983) for the diffusion-limited aggregation (DLA). The clusters which are grown according to this process in numerical simulations (Witten and Sander 1981, 1983; see Family and Landau (1984) for many references) have a self-similar structure with a non-trivial fractal dimension $\bar{d}$ smaller than the dimensionality of the embedding space, d. The first real-space renormalisation calculation (Gould *et al* 1983) led to the conclusion that their fractal dimension is different from that of branched-polymers configurations (Lubensky and Isaacson 1978, Parisi and Sourlas 1981, Shapir 1983). More theoretical works were based on mean-field equations of motion (Nauenberg *et al* 1983, Ball *et al* unpublished). Their spherically symmetric solutions with $\bar{d}=d-1$ were argued to be unstable (Nauenberg 1983). From the beginning it was realised that these mean-field equations are not sufficient because they overlook the intrinsic fluctuations of the process which are essential to the formation of the fractal structure. Extensive numerical investigations (Witten 1985, Witten and Kantor unpublished†) have been conducted to answer the question of what type of noise should be added to the mean-field equations in order to grow DLA types of clusters. A different theoretical approach which witnesses recent important progress is based on Hamiltonian and field-theoretic formulations (Parisi and Zhang 1985, Shapir and Zhang 1985, Peliti 1985). In the present work I provide the missing link between these two approaches. Some years ago Martin, Siggia and Rose (1973, hereafter referred to as MSR) showed how to obtain a generating function from the stochastic equation. Here I follow the reverse procedure: from the new field theories I deduce the Langevin and Fokker-Planck equations of different growth and aggregating processes. In particular, the exact form of multiplicative noise terms are derived. These novel stochastic formulations will be very useful to computer simulations and

† I am thankful to these authors for communicating their results privately.

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may also provide a new approach to regularisation and renormalisation as discussed briefly in the following.

It is instructive to begin with the Eden (1961) mechanism which has attracted much attention by itself recently. In infinite number of dimensions (Parisi and Zhang 1984) and on the Cayley tree (Vannimenus *et al* 1984) it coincides with the DLA model. Here we shall address other variants of this model, namely the transparent and the saturated Eden models.

In the transparent model the time evolution of a connected cluster which consists of $n_i(t)$ particles at each site i and a given time t, is according to the following rule: each one of the particles on the nearest-neighbour sites may give birth to a new particle with probability α per unit time. Let us denote by

$$N_i(t) = \sum_{j\mathrm{NN}i} n_j(t) \tag{1}$$

the total number of particles on the neighbouring sites to site i. The average change in $n_i(t)$

$$\Delta n_i(t) = n_i(t+\Delta t) - n_i(t) \tag{2}$$

is

$$\overline{\Delta n}(t) = \alpha N(t)\Delta t. \tag{3}$$

In the mean-field equation $N_i(t)$ is also replaced by its average. If we define by $\rho(\boldsymbol{r}, t)$ the local density of particles, the time derivative of its average $\bar{\rho}(\boldsymbol{r}, t)$ in the mean-field approximation is

$$\dot{\bar{\rho}}(\boldsymbol{r}, t) = \lambda(1 + a^2\nabla^2)\bar{\rho}(\boldsymbol{r}, t). \tag{4}$$

In this mean-field equation λ is a constant proportional to α and to the coordination number, which has also been absorbed into the effective lattice spacing a. Starting with the initial conditions:

$$\rho(\boldsymbol{r}, t) = \rho_0\delta(\boldsymbol{r})\delta(t) \tag{5}$$

the mean-field solution is (Parisi and Zhang 1985):

$$\bar{\rho}(\boldsymbol{r}, t) = \frac{\rho_0}{(4\pi\lambda a^2 t)^{d/2}} \exp\left(\lambda t - \frac{|\boldsymbol{r}|^2}{4\lambda a^2 t}\right). \tag{6}$$

A simple physical motivation to the way the fluctuations are introduced is as follows: the birth of the new particles are an independent event. Therefore, the mean square deviation in $\Delta n_i(t)$ will be proportional in the continuum limit to its average:

$$\overline{\Delta n_i^2(t)} - \overline{\Delta n_i(t)}^2 \xrightarrow[\Delta t\to 0]{} \overline{2\Delta n_i(t)} \tag{7}$$

(the choice of the coefficient 2 will be explained in the following). The Langevin equation for the fluctuating density may thus be:

$$\dot{\rho}(\boldsymbol{r}, t) = \lambda(1 + a^2\nabla^2)\rho(\boldsymbol{r}, t) + [2\lambda(1 + a^2\nabla^2)\rho(\boldsymbol{r}, t)]^{1/2}\xi(\boldsymbol{r}, t) \tag{8}$$

where $\xi(\boldsymbol{r}, t)$ is a Gaussian white noise which obeys

$$\langle\xi(\boldsymbol{r}, t)\rangle = 0 \qquad \text{and} \qquad \langle\xi(\boldsymbol{r}, t)\xi(\boldsymbol{r}', t') = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta(t - t'). \tag{9}$$

To prove that this conjecture is correct I first construct the MSR generating function by the introduction of an auxiliary field $\hat{\rho}(\boldsymbol{r}, t)$ and the corresponding sources $h(\boldsymbol{r}, t)$

and $\hat{h}(\boldsymbol{r}, t)$ and average over the noise to obtain

$$Z(h(\boldsymbol{r}, t), \hat{h}(\boldsymbol{r}, t)) = \mathcal{N} \int \mathrm{d}\hat{\rho}\, \mathrm{d}\rho \exp\left(\int_0^\infty \mathrm{d}t \int_{-\infty}^{\infty} \mathrm{d}^d x \, (\mathcal{L}[\hat{\rho}, \rho] + \hat{h}\hat{\rho} + h\rho) \right) \tag{10}$$

(the explicit dependence of the fields on the coordinates has been dropped). One may still discard the determinant which cancels equal-time loops (despite the multiplicative noise) with an adequate choice of the discrete lattice to start with. The effective instantaneous and local Liouvillian is:

$$\mathcal{L}[\hat{\rho}, \rho] = -\hat{\rho}\dot{\rho} + \hat{\rho}\lambda(1 + a^2\nabla^2)\rho + \lambda\hat{\rho}^2(1 + a^2\nabla^2)\rho. \tag{11}$$

Exactly the same Liouvillian is derived by the use of the Fock-space formalism (Doi 1976, Grassberger and Scheunert 1980) to an ensemble of identical particles $P(i)$ which undergo the reaction:

$$P(i) \xrightarrow{\alpha} P(i) + P(j) \tag{12}$$

where i and j are (nearest-neighbour) NN sites. This confirms the validity of (8).

It is straightforward to derive a BBGKY type of hierarchy of equations for different moments of ρ and $\dot{\rho}$ just from averaging products of the equations of motion, for example for $\langle \dot{\rho}(\boldsymbol{r}, t)\dot{\rho}(\boldsymbol{r}', t')\rangle$ we find

$$\langle \dot{\rho}(\boldsymbol{r}, t)\dot{\rho}(\boldsymbol{r}', t')\rangle = \langle \dot{\rho}(\boldsymbol{r}, t)\rangle\langle \dot{\rho}(\boldsymbol{r}', t'\rangle + \langle 2\dot{\rho}(\boldsymbol{r}, t)\rangle\delta(\boldsymbol{r} - \boldsymbol{r}')\delta(t - t') \tag{13}$$

etc. The probability distribution

$$W(y(\boldsymbol{r}, t), t) = \langle \delta[y(\boldsymbol{r}, t) - \rho(\boldsymbol{r}, t)]\rangle_\xi \tag{14}$$

follows the Fokker–Planck equation in the Itô sense (see, e.g., Jouvet and Phythian 1980):

$$\frac{\partial W}{\partial t} = \int \mathrm{d}^d r\, \lambda \left(\frac{\partial^2}{\partial y^2} - \frac{\partial}{\partial y} \right) [(1 + a^2\nabla^2) y W]. \tag{15}$$

As expected, the solution to this equation does not tend towards a normalisable equilibrium distribution.

An alternative stochastic equation may be formulated with a pair of complex white-noise variables one additive and one multiplicative:

$$\dot{\rho}(\boldsymbol{r}, t) = \lambda(1 + a^2\nabla^2)\rho(\boldsymbol{r}, t)[1 + \eta(\boldsymbol{r}, t)] + \eta^\dagger(\boldsymbol{r}, t) \tag{16}$$

with the distribution:

$$P(\eta^\dagger, \eta) = \frac{1}{2\pi} \exp\left(-\int \mathrm{d}^d r \int \mathrm{d}t \, (\eta^\dagger(\boldsymbol{r}, t)\eta(\boldsymbol{r}, t)) \right) \tag{17}$$

which yields the same Liouvillian (11) if the functional integration is restricted to the real axis $\operatorname{Im} \rho = \operatorname{Im} \hat{\rho} = 0$.

In principle one could multiply the noise by a small coefficient and introduce it perturbatively. However, it is easy to check the irrelevance of the noise in the present case: not only $\lambda > 0$ and the system is in the supercritical regime where MFT should hold but the diagrams generated by the Liouvillian (11) are tree-like and therefore this noise does not induce any harmful fluctuations.

The situation is somewhat different in the saturated Eden model. It is defined as the transparent version discussed above but with a bounded number of particles on each site. This is implemented by adding the reaction (12) which creates particles with probability α, the reaction

$$2P(i) \xrightarrow{\beta} P(i) \tag{18}$$

which annihilates them with probability $\beta \ll \alpha$. Due to this process the Liouvillian acquires a new term of the form: $-(\beta/2)(\hat{\rho}+1)\hat{\rho}\rho^2$. The noise changes accordingly and the Langevin equation which follows is

$$\dot{\rho}(\boldsymbol{r}, t) = \lambda(1+a^2\nabla^2)\rho(\boldsymbol{r}, t) - (\beta/2)\rho^2(\boldsymbol{r}, t) + [2\lambda(1+a^2\nabla^2)\rho(\boldsymbol{r}, t) - \beta\rho^2(\boldsymbol{r}, t)]^{1/2}\xi(\boldsymbol{r}, t). \tag{19}$$

The mean-field solution to this equation without noise was discussed by Parisi and Zhang (1985). The diagrammatic expansion for the correlation functions does contain loops but since $\lambda > 0$ this process is supercritical and mean-field theory is expected to describe it correctly, at least as long as the bulk properties are concerned. The cluster, therefore, will grow compact with $\bar{d} = d$ (Eden 1961) and the fluctuations will only affect its surface (Racz and Plischke 1983, 1985).

We now turn to the transparent DLA. In this version of the Witten-Sander model the cluster is formed by $n_i(t)$ particles $P(i)$ at each site at a given time. The whole cluster is immersed in a sea of diffusing particles $D(i)$. They are injected continuously from infinity and are transformed into cluster particles according to the reaction:

$$P(i) + D(j) \xrightarrow{\alpha} P(i) + P(j) \tag{20}$$

where i and j are nearest-neighbour sites. As explained very clearly by Peliti (1985) the Fock-space method is readily made for this model. Let us introduce the fields $\phi(\boldsymbol{r}, t)(\hat{\phi}(\boldsymbol{r}, t))$ to represent the density field (and its conjugate field) of the diffusing particles. The effective Liouvillian (Peliti 1985) takes the form (C is the diffusion constant):

$$\mathscr{L}[\rho, \hat{\rho}, \phi, \hat{\phi}] = -\hat{\rho}\dot{\rho} - \hat{\phi}\dot{\phi} + C\hat{\phi}\nabla^2\phi + \lambda(\hat{\rho} - \hat{\phi})\phi(1+a^2\nabla^2)\rho[1+(1+a^2\nabla^2)\hat{\rho}]. \tag{21}$$

The simplest corresponding Langevin equations are

$$\dot{\phi}(\boldsymbol{r}, t) = C\nabla^2\phi(\boldsymbol{r}, t) - \lambda\phi(\boldsymbol{r}, t)(1+a^2\nabla^2)\rho(\boldsymbol{r}, t)[1+\eta(\boldsymbol{r}, t)] \tag{22a}$$

$$\dot{\rho}(\boldsymbol{r}, t) = \lambda\phi(\boldsymbol{r}, t)(1+a^2\nabla^2)\rho(\boldsymbol{r}, t)[1+\eta(\boldsymbol{r}, t)] + (1+a^2\nabla^2)\eta^\dagger(\boldsymbol{r}, t) \tag{22b}$$

where $\eta(\boldsymbol{r}, t)$ and $\eta^\dagger(\boldsymbol{r}, t)$ are a pair of conjugate complex white-noise variables with the distribution given by (17).

If we neglect terms proportional to $\nabla^2\hat{\rho}$ (for simplicity and anyway they are probably irrelevant) we may derive the following (Itô sense) Fokker-Planck equation for the transparent DLA

$$\frac{\partial W}{\partial t} = \int \mathrm{d}^d r \left(\frac{\partial}{\partial \phi_s} - \frac{\partial}{\partial \rho_s} + \frac{\partial^2}{\partial \rho_s^2} - \frac{2\partial^2}{\partial \rho_s \partial \phi_s}\right)[\lambda(1+a^2\nabla^2)\phi_s(1+a^2\nabla^2)\rho_s W] + \frac{\partial}{\partial \phi_s}(C\nabla^2\phi_s W) \tag{23}$$

for the probability distribution $W(\rho_s(\boldsymbol{r}, t), \phi_s(\boldsymbol{r}, t), t)$ of the solutions $\rho_s(\boldsymbol{r}, t)$ and $\phi_s(\boldsymbol{r}, t)$ to the Langevin equations (22).

The effects of the saturation may be introduced as before. Moreover, the discrete character of the noise may also be included in the field theory through terms which are quartic (or higher) in the auxiliary fields $\hat{\rho}$ and $\hat{\phi}$. There is no *a priori* reason for these terms to be irrelevant and the possibility that the transparent DLA discussed here and the opaque Witten–Sander (1983) model belong to two different universality classes cannot be excluded (Witten 1985, Witten and Kantor, unpublished). Since the spherically symmetric mean-field solutions are unstable we still lack a systematic perturbative scheme to approach the details of these questions. In particular it may imply that the renormalised equations of motion are qualitatively different from the microscopic ones. Clearly one has to look for non-perturbative methods. Such a method was suggested recently in the context of the stochastic static random-fields problem (Shapir 1984). In that approach the stochastic variables themselves are renormalised according to the response of the system to the perturbation. A similar self-consistent regularisation method may be the adequate one for the DLA model as well. The values of the exponents will then be selected as those which satisfy the self-consistent condition.

To conclude, stochastic Langevin and Fokker–Planck equations for different growth and aggregating processes have been derived. This may be an important step forward in providing a theoretical framework to these most challenging models which, so far, have been approached mostly by numerical simulations. The fluctuations are irrelevant in the Eden mechanism but are pertinent to the aggregation processes of diffusing particles and an original renormalisation scheme, which may be based on the stochastic equations, will be required to extract their universal features.

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