LETTER TO THE EDITOR

Langevin equation for the density of a system of interacting Langevin processes

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Abstract. We present a simple derivation of the stochastic equation obeyed by the density function for a system of Langevin processes interacting via a pairwise potential. The resulting equation is considerably different from the phenomenological equations usually used to describe the dynamics of non-conserved (model A) and conserved (model B) particle systems. The major feature is that the spatial white noise for this system appears not additively but multiplicatively. This simply expresses the fact that the density cannot fluctuate in regions devoid of particles. The steady state for the density function may, however, still be recovered formally as a functional integral over the coursed grained free energy of the system as in models A and B.

Recently there has been a tentative attempt [1] to analyse the liquid–glass transition within the context of the replica approach to disordered systems. A program of implementing replica techniques from disordered systems has had some success in capturing the properties of systems without disorder but which have many metastable states [2–4]. As the glass transition is essentially dynamical, it is useful to have a simple dynamical model for these types of problems. In the literature on liquids there has been a considerable effort to analyse the dynamics of liquid systems. In this letter we present a simple microscopic derivation for the evolution of the density of a system of Langevin processes interacting via pairwise potentials. Rather than working with Fokker–Planck equations in large coordinate spaces and then using projection operator techniques to obtain a hierarchy of equations for the n point density correlation functions, we simply derive a closed functional Langevin equation for the evolution of the density. Using this it is trivial to derive the dynamical BBGKY (e.g. see [5, 6] and references therein) hierarchy of equations. Interestingly, the naive course grained free energy of the system appears quite naturally. However, the equation is not amongst the class of equations used often to describe the approach to equilibrium of systems specified by their free energy as a function of some scalar order parameter [7, 8].

We commence by considering the dynamics of a system of particles in a thermal white noise heat bath. The particles interact via a pairwise potential $V(x)$; this could be a Coulomb type of interaction, a Leonard-Jones type interaction or simply a hard sphere repulsion. Each particle experiences a thermal white noise and moves under the force generated from the potential due to its neighbours. Consequently the ith particle obeys the Langevin equation

$$\frac{\mathrm{d}X_i(t)}{\mathrm{d}t} = \eta_i(t) - \sum_{j=1}^{N} \nabla V(X_i(t) - X_j(t)). \tag{1}$$

To ease notation we have assumed a potential such that $\nabla V(0) = 0$. The noise is uncorrelated in time and the noise acting on a single particle is not correlated with the

noise acting on the others. The components of the noise are also taken to be uncorrelated, hence

$$\langle \eta_i^\mu(t)\eta_j^\nu(t')\rangle = 2T\delta_{ij}\delta^{\mu\nu}\delta(t-t'). \tag{2}$$

Our strategy will be to consider the evolution of the density function for a single particle

$$\rho_i(x,t) = \delta(X_i(t) - x) \tag{3}$$

and we shall then demonstrate how one may write a closed Langevin equation for the global density

$$\rho(x,t) = \sum_{i=1}^N \rho_i(x,t). \tag{4}$$

The derivation follows a well known argument. Consider an arbitrary function f defined on the coordinate space of the system. Using the definition of the density it is a tautology that

$$f(X_i(t)) = \int dx\, \rho_i(x,t) f(x). \tag{5}$$

Expanding the stochastic differential equation using the Ito calculus (for example see [9]) over the next time step δt one obtains

$$\frac{df(X_i)}{dt} = \int dx\, \rho_i(x,t)\left(\nabla f(x)\cdot\eta_i(t) - \nabla f(x)\cdot\left(\sum_{j=1}^N \nabla V(x-X_j(t))\right) + T\nabla^2 f(x)\right). \tag{6}$$

Re-arranging the above integral by integration by parts we obtain

$$\frac{df(X_i)}{dt} = \int dx\, f(x)\left(-\nabla\cdot(\rho_i(x,t)\eta_i(t)) + \nabla\cdot\rho_i(x,y)\left(\sum_{j=1}^N \nabla V(x-X_j(t))\right)\right.$$
$$\left. + T\nabla^2\rho_i(x,t)\right). \tag{7}$$

However, from (5) we may also deduce

$$\frac{df(X_i)}{dt} = \int dx\, \frac{\partial\rho_i(x,t)}{\partial t} f(x). \tag{8}$$

Comparing equations (7) and (8) we find (using the fact that f is an arbitrary function) that

$$\frac{\partial\rho_i(x,t)}{\partial t} = -\nabla\cdot(\rho_i(x,t)\eta_i(t)) + \nabla\cdot\left(\rho_i(x,t)\sum_{j=1}^N \nabla V(x-X_j(t))\right) + T\nabla^2\rho_i(x,t). \tag{9}$$

We emphasize that this argument is standard and the only subtlety is that we have not carried out any thermal averaging at this point. Summing equation (9) over the i and using the definition of the density ρ we obtain

$$\frac{\partial\rho(x,t)}{\partial t} = -\sum_{i=1}^N \nabla\cdot(\rho_i(x,t)\eta_i(t)) + \nabla\cdot\left(\rho(x,t)\int dy\,\rho(y,t)\nabla V(x-y)\right)$$
$$+ T\nabla^2\rho(x,t). \tag{10}$$

This equation is *almost* a closed equation for ρ, the problem is that the noise term appears to contain too much information about the individual ρ_i and hence, in the current form, it

is not a Markovian equation for the evolution of the global density. We define this noise term to be

$$\xi(x, t) = -\sum_{i=1}^{N} \nabla \cdot (\eta_i(t)\rho_i(x, t)). \tag{11}$$

It is clearly still Gaussian and the correlation function is given by

$$\langle \xi(x, t)\xi(y, t')\rangle = 2T\delta(t - t') \sum_{i=1}^{N} \nabla_x \cdot \nabla_y (\rho_i(x, t)\rho_i(y, t)). \tag{12}$$

However, the above term simplifies using a trivial property of the Dirac delta function, explicitly

$$\rho_i(x, t)\rho_i(y, t) = \delta(x - y)\rho_i(x, t) = \delta(x - y)\rho_i(y, t). \tag{13}$$

Using this one finds

$$\langle \xi(x, t)\xi(y, t')\rangle = 2T\delta(t - t')\nabla_x \cdot \nabla_y(\delta(x - y)\rho(x, t)). \tag{14}$$

At this point we shall consider redefining the white noise by introducing a global noise field

$$\xi'(x, t) = \nabla \cdot (\eta(x, t)\rho^{\frac{1}{2}}(x, t)) \tag{15}$$

where η is a global uncorrelated white noise field such that

$$\langle \eta^\mu(x, t)\eta^\nu(y, t')\rangle = 2T\delta(t - t')\delta^{\mu\nu}\delta(x - y). \tag{16}$$

It is easy to see that both Gaussian noises ξ and ξ' have the same correlation functions and are, therefore, statistically identical. We may, therefore, write equation (10) as

$$\frac{\partial \rho(x, t)}{\partial t} = \nabla \cdot (\eta(x, t)\rho^{\frac{1}{2}}(x, t)) + \nabla \cdot \left(\rho(x, t)\int \mathrm{d}y\, \rho(y, t)\nabla V(x - y)\right)$$
$$+ T\nabla^2\rho(x, t). \tag{17}$$

Equation (17) is clearly a closed Langevin equation for the evolution of the particle density of the system. The crucial point is that on insisting on knowing the global property of the white noise field we have gained sufficient information to write down a Markovian evolution equation for ρ. If one were to consider the course grained free energy for the system one would be led to write

$$F = \frac{1}{2}\int \mathrm{d}x\, \mathrm{d}y\, \rho(x)V(x - y)\rho(y) + T\int \mathrm{d}x\, \rho(x)\log\rho(x) \tag{18}$$

up to constant terms in the case of a fixed particle number. Using this as a definition of F it is easy to see that (17) may be written as

$$\frac{\partial \rho(x, t)}{\partial t} = \nabla \cdot \left(\rho(x, t)\nabla\frac{\delta F}{\delta\rho(x)}\bigg|_{\rho(x,t)}\right) + \nabla \cdot (\eta(x, t)\rho^{\frac{1}{2}}(x, t)). \tag{19}$$

Two things are immediately obvious from equation (19): first, particle number is conserved and second, in regions where the system is void of particles the density cannot change and hence stays zero. The above equation is in fact a special case of an equation derived semi-phenomenologically by Kawasaki some 20 years ago in the context of non-polymeric incompressible binary fluids [10]. As is usual in such derivations, the free energy is taken to be of the Ginsburg–Landau type directly, if one sets the velocity field to zero one obtains formally the same equation as (17). The derivation in the case of zero velocity field is brief

enough to be included here for the sake of completeness. One assumes that the density obeys an equation of the form

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot j + \xi(x, t) \tag{20}$$

where j is the current and ξ is the divergence of a random force uncorrelated in time. In the course grained microscopic approach j is simply given by

$$j = -\rho \nabla \frac{\delta F}{\delta \rho} \tag{21}$$

and the fluctuation dissipation theorem (see for example the discussion in [11]) then requires that the noise ξ must have exactly the same correlation function as the noise in (17), hence the result.

Here we briefly recall the two standard models used in dynamical analysis of phase ordering kinetics and other areas [7, 8]. The basic approach here has to been to write down a course grained free energy F for the system and to write for model A (non-conserved dynamics)

$$\frac{\partial \rho}{\partial t} = -\frac{\delta F}{\delta \rho} + \eta(x, t) \tag{22}$$

and for model B (conserved dynamics)

$$\frac{\partial \rho}{\partial t} = \nabla^2 \frac{\delta F}{\delta \rho} + \nabla \cdot \eta(x, t). \tag{23}$$

Here ρ is not necessarily the density and is usually some scalar order parameter for the problem, for example in a binary alloy it would correspond to the difference between the densities of the two particle species and in a spin model it would be the local magnetization. In model B the noise is vector white noise of the type introduced above and in model A it is the scalar counterpart. The models can lead to an equilibrium distribution for ρ of the type that has as its free energy the F one started with, i.e. (formally) the equilibrium functional for ρ is given as

$$P(\rho) = \frac{1}{Z} \exp(-F[\rho]/T) \tag{24}$$

with Z a normalizing factor. One may verify that the functional Fokker–Planck equation for equation (17) also has this as a steady-state solution. In this case it is interesting that the course grained free energy has appeared directly and, in addition, without any appeal to there being a large number of particles in the system, we recall that the term $\int \mathrm{d}x \, \rho(x) \log \rho(x)$ normally occurs after a course graining and then a use of Stirling's formula. In this formulation we have avoided this route, presumably it is the direct use of the Langevin process at the level of microscopic dynamics that has smoothed out the statistics. However, the functional representation of $P[\rho]$ does require additional reference to the underlying physics when it comes to performing what is an *a priori* badly defined functional integral. In the case of both model A and model B (and indeed for the statics) the usual tactic is to resort to an expansion about some fixed background density up to fourth order in the fluctuations; this then yields a dynamical version of Ginsburg–Landau theory. However, we note that, even at the level of this approximation, equation (17) does not become equivalent to models A or B (at this level of approximation one would still be forced to keep terms of third order in the terms multiplying the white noise).

Once we have the full Langevin equation for the density evolution, we may use the standard techniques of stochastic calculus (applied now to functions) in order to obtain

equations for the evolution of functions of the density. Here we shall consider the time dependent correlation function at equal times. We define

$$C(x, y, t) = \langle \rho(x, t)\rho(y, t) \rangle. \tag{25}$$

It is straightforward to see that $C(x, y, t)$ obeys

$$\frac{\partial C(x, y, t)}{\partial t} = -T\nabla^2 \delta(x - y)\langle \rho(x, t) \rangle + \left\langle \nabla \cdot \left(\rho(y, t)\rho(x, t) \int \mathrm{d}z\, \rho(z, t)\nabla V(x - z) \right) \right\rangle$$
$$+ 2T\nabla^2 C(x, y, t) \tag{26}$$

where we have used the symmetry between x and y. Unfortunately, equation (26) is not a closed equation for C. In general, the above may be used to generate a whole hierarchy of equations for the n point functions of the field ρ; in fact this is the dynamical version of the BBGKY hierarchy used in the static problem.

In conclusion, we have presented a very simple derivation of the Langevin equation of the density describing the dynamics of a gas of interacting Langevin processes. In addition, this formalism permits the construction of the BBGKY hierarchy for the dynamical correlation functions in straightforward manner. Rather than being a phenomenological model for the dynamics based around a known course grained free energy, it is directly defined from an albeit simple microscopic model. It has the merit of corresponding to a (at least in the sense of numerical simulations) realizable microscopic dynamics. One rather appealing feature is that the naive course grained free energy of the system appears naturally as the effective potential for the problem.

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