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Renormalization of drift and diffusivity in random gradient flows

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Abstract. We investigate the relationship between the effective diffusivity and effective drift of a particle moving in a random medium. The velocity of the particle combines a white noise diffusion process with a local drift term that depends linearly on the gradient of a Gaussian random field with homogeneous statistics. The theoretical analysis is confirmed by numerical simulation.

For the purely isotropic case the simulation, which measures the effective drift directly in a constant gradient background field, confirms the result, previously obtained theoretically, that the effective diffusivity and effective drift are renormalized by the same factor from their local values. For this isotropic case we provide an intuitive explanation, based on a *spatial* average of local drift, for the renormalization of the effective drift parameter relative to its local value.

We also investigate situations in which the isotropy is broken by the tensorial relationship of the local drift to the gradient of the random field. We find that the numerical simulation confirms a relatively simple renormalization group calculation for the effective diffusivity and drift tensors.

1. Introduction

A much studied problem in physics is that of the diffusion of a particle in a random environment. This problem encompasses areas ranging from turbulent diffusion to phase space descriptions of the dynamics of complex disordered systems such as spin glasses. The standard Langevin equation describing such systems is

$$\dot{x} = u + U(x) + w(t) \quad (1)$$

where $w(t)$ is a white noise of zero mean with correlation function

$$\langle w_i(t)w_j(t') \rangle = 2\kappa_{ij}^0 \delta(t - t') \quad (2)$$

and U is a random quenched velocity field with zero mean and u is a constant applied velocity. In this paper we shall concentrate on examples where the asymptotic diffusion is normal, that is we expect

$$\lim_{t \rightarrow \infty} \langle x_i(t)x_j(t) \rangle_c = 2\kappa_{ij}t \quad (3)$$

where the suffix c indicates the cumulant part of the correlator and

$$\lim_{t \rightarrow \infty} \langle x_i(t) \rangle = u_i^c t. \quad (4)$$

The angle brackets indicate an average over the white-noise ensemble, and where appropriate over the ensemble of samples of the random medium. Here κ_{ij} and u_i^e are the bulk diffusivity tensor and bulk drift for the random medium. We shall not examine the case where there is anomalous diffusion; this is of course a very interesting case which has been studied extensively (see for example [1]) with the object of determining the anomalous exponents for the diffusion and is successfully tackled via renormalization group techniques.

A problem of great interest concerns the computation of effective parameters for a diffusion process that combines molecular diffusion with a drift term linearly dependent on the gradient of a random scalar field with spatially homogeneous statistics. In the case where the system, including the statistical properties of the random field, is isotropic, it has been shown, on the basis of plausible but not completely established assumptions, that the effective long-range diffusivity is accurately predicted by a renormalization group calculation (RGC) [2–4]. The result, which is embodied in a very simple formula, is confirmed by numerical simulation to high accuracy. The result is also consistent with the straightforward perturbation expansion to two-loop order but remains accurate beyond the applicability of the expansion to this order [3, 5].

An important parameter relevant to the long-time behaviour of the system, that has not generally been studied, is the value of the effective drift parameter, or tensor, that determines the average drift of particles in an imposed large-scale field gradient. A feature of the isotropic case, respected by the RGC, is that this effective drift coefficient is renormalized relative to its local value by the same factor as the effective diffusivity is renormalized relative to the molecular diffusivity [2–5] in the isotropic case. By including an appropriate constant drift term in the original molecular diffusion process we confirm in this paper, directly by numerical simulation, the equality of the two renormalization factors. We also give an intuitive explanation in terms of spatial averages, of why one should expect that the drift coefficient be renormalized.

We also study the effect of anisotropy on the relationship between bulk drift and diffusivity. Isotropy can break down for three reasons. First, the statistics of the random field may not be isotropic. We have investigated this in a previous paper [6] and shown that, although the predictions of the RGC are still reasonably accurate, there are emerging disparities with the results of the numerical simulation. Such an outcome is to be expected since the results of the RGC were, in this case, shown to differ from straightforward perturbation theory at two-loop order. Second, the molecular diffusion tensor may be non-isotropic and third, the same may be true of the local drift tensor. It is this third possibility that we investigate in this paper by numerical simulation, comparing the results with the predictions of the appropriate RGC. The results actually agree rather well, suggesting that the isotropy of the random field statistics is an important condition for the success of the RGC.

It is convenient for the purpose of discussing anisotropy to consider the most general diffusion equation of the class in which we are interested. It has the form

$$\frac{\partial P}{\partial t} = \partial_i (\kappa_{ij}^0 \partial_j - \lambda_{ij}^0 \partial_j \phi(\mathbf{x}) - u_i) P. \quad (5)$$

Here P is the probability density of a particle moving according to the equation

$$\dot{x}_i = \lambda_{ij}^0 \partial_j \phi(\mathbf{x}) + u_i + w_i(t) \quad (6)$$

where w is the white noise defined in the introduction. A possible physical origin for the drift term is the electric field imposed on a diffusing ion in the presence of randomly positioned charged impurities. In that case ϕ is, up to a normalization, the random electrostatic potential

produced by the impurities. The term u_i represents a constant drift term. In appropriate units we would expect the drift to be given by

$$u_i = \lambda_{ij}^0 g_j \quad (7)$$

where g_i is a uniform (electric) field. If, in the absence of the constant drift term, a system of finite volume is to achieve a currentless Gibbs equilibrium state with a probability density, $P_0(\mathbf{x})$, that satisfies

$$P_0(\mathbf{x}) = N \exp(\beta\phi(\mathbf{x})) \quad (8)$$

with N the normalization factor and β the effective inverse temperature, it is necessary that

$$\kappa_{ij} = \beta\lambda_{ij}. \quad (9)$$

This equality is often referred to as the fluctuation dissipation relation (FDR) [8]. Although such a local fluctuation dissipation relation is necessary if a Gibbs equilibrium state is to be achieved, it does not guarantee this outcome. (Some systems obeying the local FDR may never reach equilibrium and hence may never satisfy the fluctuation dissipation theorem (FDT); this is beyond the scope of our paper but the interested reader may consult [12] for example.)

The special case of equation (5), in which equation (9) holds, is the one that has been studied most, mainly in the isotropic case, precisely because it leads to a Gibbs equilibrium distribution. *A priori* there is no reason why such a relation should apply in a random medium. Indeed if there are forces not derived from a potential, in three dimensions, the random flow will contain an incompressible component and the steady state will have microcurrents. It is interesting to note that in spin glass dynamics the FDR is obeyed but below the critical temperature the FDT is violated; however, if a non-potential term is added to the drift (as part of a Langevin process) the low-temperature phase has been reported to be drastically changed [13], even for small perturbations. Therefore in this paper we shall consider both the cases where the FDR holds and also where it is violated.

The main results of this paper are that when the FDR holds at the level of the bare parameters (i.e. microscopically) then the effective renormalized parameters obtained after averaging over the random field also obey the FDR, at least by the evidence of a perturbative analysis and from our numerical simulations. This is perhaps a more comforting than surprising result. However, we shall also see that for slight, in the perturbative sense, deviations from the FDR, a renormalization group analysis suggests that the effective or bulk parameters are renormalized back towards consistency with the FDR. This suggests that in certain systems where the microscopic dynamics violates the FDR, one may nevertheless measure bulk parameters that do obey the FDR quite closely.

The flow of the effective parameters in the renormalization group analysis between their microscopic and bulk values may be viewed as a progressive coarse graining of the system. Indeed the Langevin equation describing the microscopic dynamics must itself have been derived from the coarse graining of a more physically realistic microscopic dynamics. Hence our results strongly suggest that the effect of coarse graining in the type of system we have examined is to restore the FDR if the microscopic dynamics obeys the FDR sufficiently closely.

2. Dynamics from the Green functions

In the study of diffusions a standard technique is to extract information about the diffusion from the statics—the analysis is quite standard [1,4]. The equation for the static Green

function corresponding to a unit source at \mathbf{x}' is

$$\partial_i(\kappa_{ij}^0 \partial_j - \lambda_{ij}^0 \partial_j \phi(\mathbf{x}) - u_i)G(\mathbf{x}, \mathbf{x}') = -\delta(\mathbf{x} - \mathbf{x}'). \quad (10)$$

The effective Green function obtained after averaging over the random ensemble of flows we denote by $\mathcal{G}(\mathbf{x} - \mathbf{x}')$. It is simpler to study this function in terms of its Fourier transform. It has the form

$$\tilde{\mathcal{G}}(\mathbf{k}) = [\kappa_{mn}^0 k_m k_n - \Sigma(\mathbf{k}) + iu_j W_j(\mathbf{k})]^{-1}. \quad (11)$$

At small \mathbf{k} the irreducible two-point function $\Sigma(\mathbf{k})$ satisfies

$$\Sigma(\mathbf{k}) \sim \sigma_{ij} k_i k_j \quad (12)$$

with the result that the effective long-range diffusivity is

$$\kappa_{ij} = \kappa_{ij}^0 - \sigma_{ij} \quad (13)$$

and

$$W_j(\mathbf{k}) \sim k_i \mu_{ij}. \quad (14)$$

for some coefficient μ_{ij} that we now evaluate. We show below that

$$W_i = [(\lambda^0)^{-1}]_{im} V_m(0, \mathbf{k}) \quad (15)$$

where $V_m(\mathbf{q}, \mathbf{k})$ is the (Fourier transform of the) vertex function that measures the influence of a weak external field on $\mathcal{G}(\mathbf{x}, \mathbf{x}')$. It is calculated below. For small \mathbf{k} we have

$$V_m(0, \mathbf{k}) \sim k_n \lambda_{nm} \quad (16)$$

where λ_{mn} is the effective coupling referred to in the introduction. It follows that for small \mathbf{k}

$$\tilde{\mathcal{G}}(\mathbf{k}) \sim [\kappa_{mn}^0 k_m k_n + ik_m \lambda_{mn} g_n]^{-1}. \quad (17)$$

The interpretation of this result is that the effective drift is

$$u_m^e = \lambda_{mn} g_n. \quad (18)$$

The measurement of the effective drift in a given external field allows us to extract the effective coupling λ_{ij} from the simulation.

For the purposes of simulation we assumed that the random field ϕ is Gaussian, of zero mean and with a two-point correlation function given by

$$\Delta(\mathbf{x} - \mathbf{x}') = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} D(\mathbf{q}) e^{i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')} \quad (19)$$

with

$$D(\mathbf{q}) = \frac{(2\pi)^{\frac{3}{2}}}{k_0^3} e^{-q^2/2k_0^2}. \quad (20)$$

With this normalization

$$\langle (\phi(\mathbf{x}))^2 \rangle = \Delta(0) = 1. \quad (21)$$

We shall also concentrate our study on three-dimensional space.

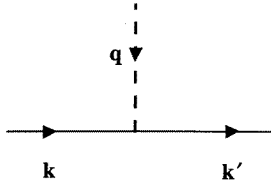


Figure 1. Vertex diagram.

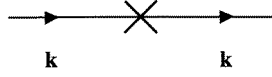


Figure 2. Drift insertion vertex.

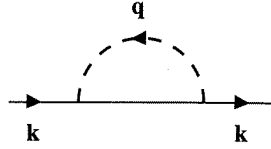


Figure 3. One-loop contribution to Σ .

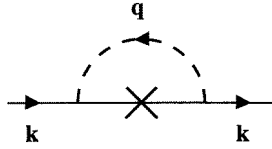


Figure 4. One-loop correction to drift insertion.

3. Graphical rules for perturbation theory

The Feynman rules for the diagrammatic perturbation expansion are essentially the same as in the isotropic case. We have:

- (i) The sum of the inwardly flowing wavevectors at each vertex is zero.
- (ii) Each full line carries a factor of $1/\kappa_{ij}^0 k_i k_j$.
- (iii) Each loop wavevector \mathbf{q} is integrated with a factor $d^3 \mathbf{q}/(2\pi)^3$.
- (iv) Each vertex of the form of figure 1 carries a factor $q_i \lambda_{ij}^0 (\mathbf{k} + \mathbf{q})_j$.
- (v) Each vertex of the form of figure 2 carries a factor $-iu_j k_j$.
- (vi) Each broken curve carries a factor $D(\mathbf{q})$.

4. One-loop contributions

The one-loop contribution to $\Sigma(\mathbf{k})$ is associated with figure 3. It is, according to the Feynman rules,

$$\Sigma^{(1)}(\mathbf{k}) = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} D(\mathbf{q}) \frac{(\mathbf{k} + \mathbf{q})_i \lambda_{ij}^0 q_j k_m \lambda_{mn}^0 q_n}{(\mathbf{k} + \mathbf{q})_r \kappa_{rs}^0 (\mathbf{k} + \mathbf{q})_s}. \quad (22)$$

The one-loop contribution to $u_i W_i(\mathbf{k})$ is associated with figure 4. The Feynman rules imply that it has the form

$$u_i W_i(\mathbf{k}) = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{(\mathbf{k} + \mathbf{q})_i \lambda_{ij}^0 q_j (-iu_j (\mathbf{k} + \mathbf{q})_j) k_m \lambda_{mn}^0 q_n}{((\mathbf{k} + \mathbf{q})_r \kappa_{rs}^0 (\mathbf{k} + \mathbf{q})_s)^2}. \quad (23)$$

If we compare this result with that for the general vertex at one loop associated with figure 5, namely

$$V_i(\mathbf{q}, \mathbf{k}') = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{(\mathbf{k} + \mathbf{q})_j \lambda_{jl}^0 q_l \lambda_{lp}^0 (\mathbf{k}' + \mathbf{q})_p k'_m \lambda_{mn}^0 q_n}{(\mathbf{k} + \mathbf{q})_r \kappa_{rs}^0 (\mathbf{k} + \mathbf{q})_s (\mathbf{k}' + \mathbf{q})_u \kappa_{uv}^0 (\mathbf{k}' + \mathbf{q})_v} \quad (24)$$

we see immediately that

$$V_i(0, \mathbf{k}) = \lambda_{ij}^0 W_j(\mathbf{k}). \quad (25)$$

This result is easily generalized to all orders in perturbation theory. It is equivalent to the relation used in a previous paper [5].

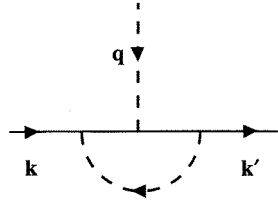


Figure 5. One loop correction to vertex.

5. Spatial averages and mean drift

Some insight into the renormalization of the drift coefficient in the isotropic case ($\lambda_{ij}^{(0)} = \lambda_0 \delta_{ij}$ and $\kappa_{ij}^{(0)} = \kappa_0 \delta_{ij}$) can be obtained by considering a situation in which we allow a large cloud of particles to equilibrate in a large cubical sample with periodic boundary conditions. We then disturb the situation by imposing a uniform background drift field \mathbf{g} causing a mean drift in the particle cloud. The average velocity of the particles is then renormalized relative to the mean local drift because of the lack of uniformity in the background probability distribution adopted by the particles.

In the absence of a background drift field, the particles adopt a density distribution $P_0(\mathbf{x})$ that yields zero particle current. That is

$$\mathbf{J} = (\kappa_0 \nabla - \lambda_0 \nabla \phi(\mathbf{x})) P_0(\mathbf{x}) = 0. \quad (26)$$

The solution of this equation is

$$P_0(\mathbf{x}) = N \exp \left\{ \frac{\lambda_0}{\kappa_0} \phi(\mathbf{x}) \right\} \quad (27)$$

where we will choose N so that $P_0(\mathbf{x})$ can be viewed as a probability distribution, i.e. such that

$$\int_{\text{cube}} d^3 \mathbf{x} P_0(\mathbf{x}) = 1. \quad (28)$$

Here the ratio λ_0/κ_0 may be interpreted as the effective inverse temperature. For a very large cube it is acceptable to enforce this equation as an ensemble average. This allows us to evaluate N as

$$N = \left(V \exp \left\{ \frac{1}{2} \left(\frac{\lambda_0}{\kappa_0} \right)^2 \Delta(0) \right\} \right)^{-1} \quad (29)$$

where V is the volume of the cube.

When an external constant drift \mathbf{g} is applied, the system equilibrates with a new distribution $P_0 + P_1$ that satisfies

$$\nabla \cdot (\kappa_0 \nabla - \lambda_0 \nabla \phi(\mathbf{x}) - \lambda_0 \mathbf{g})(P_0(\mathbf{x}) + P_1(\mathbf{x})) = 0. \quad (30)$$

It turns out that no change of normalization is required. This leads to the solution, correct to $O(\mathbf{g})$, for P_1 ,

$$P_1(\mathbf{x}) = -\lambda_0 \int d^3 \mathbf{x}' G(\mathbf{x}, \mathbf{x}') \nabla P_0(\mathbf{x}') \cdot \mathbf{g} \quad (31)$$

where $G(\mathbf{x}, \mathbf{x}')$ is the Green function for the problem without drift.

At a point \mathbf{x} in a given sample of the medium the velocity of a particle is $\lambda_0(\nabla \phi(\mathbf{x}) + \mathbf{g})$ after averaging over molecular diffusion effects. The drift \mathbf{u} of particles in the steady state

situation with drift can be obtained as a spatial average of this velocity over the large cubical sample:

$$\mathbf{u} = \lambda_0 \int d^3\mathbf{x} (\nabla\phi(\mathbf{x}) + \mathbf{g})(P_0(\mathbf{x}) + P_1(\mathbf{x})). \quad (32)$$

To $O(\mathbf{g})$ we have

$$u_i = \lambda_0 \left[\delta_{ij} - \lambda_0 \int d^3\mathbf{x} d^3\mathbf{x}' (\partial_i\phi(\mathbf{x}))G(\mathbf{x}, \mathbf{x}')\partial_j P_0(\mathbf{x}') \right] g_j. \quad (33)$$

In fact it is reasonable now to take the ensemble average of this quantity, with the result

$$u_i = \lambda_0 \left[\delta_{ij} - \lambda_0 \int d^3\mathbf{x} d^3\mathbf{x}' \langle (\partial_i\phi(\mathbf{x}))G(\mathbf{x}, \mathbf{x}')\partial_j P_0(\mathbf{x}') \rangle \right] g_j. \quad (34)$$

To lowest (non-trivial) order in λ_0 we can replace $G(\mathbf{x}, \mathbf{x}')$ by $G_0(\mathbf{x} - \mathbf{x}')$ and use the identity

$$\langle \phi(\mathbf{x})P_0(\mathbf{x}') \rangle = \frac{\lambda_0}{\kappa_0} \Delta(\mathbf{x} - \mathbf{x}')/V \quad (35)$$

to obtain

$$u_i = \lambda_0 \left[\delta_{ij} - \frac{\lambda_0^2}{\kappa_0} \int d^3\mathbf{x} G_0(\mathbf{x})\partial_i\partial_j'\Delta(\mathbf{x}) \right] g_j. \quad (36)$$

Expressing this in Fourier space we have

$$u_i = \lambda_0 \left[\delta_{ij} - \frac{\lambda_0^2}{\kappa_0^2} \int \frac{d^3\mathbf{q}}{(2\pi)^3} D(q) \frac{q_i q_j}{q^2} \right] g_j. \quad (37)$$

Taking into account the isotropy of the statistical ensemble that we assume in this case, we see that $\mathbf{u} = \lambda\mathbf{g}$ where

$$\lambda = \lambda_0 \left(1 - \frac{1}{3} \frac{\lambda_0^2}{\kappa_0^2} \Delta(0) \right). \quad (38)$$

This is identical with the one-loop perturbation result of previous work [2–5]. A careful analysis of the two-loop diagrams confirms the result to this order. This is, of course, consistent with the RGC result

$$\lambda_e = \lambda_0 \exp \left\{ -\frac{1}{3} \frac{\lambda_0^2}{\kappa_0^2} \Delta(0) \right\} \quad (39)$$

discovered previously. From this point of view, then, the renormalization of the effective drift term comes about because in a steady state the particles adopt, in a given sample, a non-uniform distribution, appropriate to the sample, and the resulting spatial average of the local drift is modified relative to the local ensemble average which yields the local mean value. This should be contrasted with the situation in incompressible flow where the steady state distribution of particles inevitably remains uniform leading to a spatial average that coincides with the ensemble average and no renormalization of the drift coefficient [9, 10].

Table 1. N is the number of modes in a random field. Theoretical values are in brackets.

N	λ_0	g	κ_e	(λ_e/λ_0)
128	1.0	0.05	0.722(2)	0.726(2)
			(0.717)	(0.717)
256	1.5	0.05	0.470(5)	0.474(2)
			(0.472)	(0.472)
256	2.0	0.05	0.269(4)	0.266(11)
			(0.264)	(0.264)
512	2.5	0.05	0.139(5)	0.140(20)
			(0.125)	(0.125)

6. Simulation of drift in the isotropic case

The simulation technique we have used is that described in [4]. Briefly, it is a direct integration of the Langevin equation for the problem implemented using a second-order Runge–Kutta scheme for stochastic differential equations. In table 1 we exhibit the results of measuring both κ_e and λ_e , for an isotropic situation, over a range of values of the disorder parameter λ_0/κ_0 . We assume $\kappa_0 = 1$ and $k_0 = 1$ throughout.

The continuum construction for $\phi(x)$ has been described in previous papers [4–7]. An important point for the present paper is that the random field is constructed from a set of N modes and the integrity of the Gaussian property of the statistics of the random field is dependent on having a sufficiently large value of N .

The results clearly show the equality of the two renormalization parameters for a wide range of disorder parameters. This common value is also equal, as was found in previous work, to the RGC prediction of $\exp\{-\frac{1}{3}\lambda_0^2/\kappa_0^2\}$. There is a slight discrepancy at the higher values of the disorder parameter. We feel that this is a systematic error in the simulation due to the limited number of modes incorporated in the random field. Another possible source of error is that the value of the drift parameter has become so large that $O(g^2)$ effects are influencing the values of the measured quantities. It is also possible that the assumptions behind the renormalization group calculation may no longer be valid at these values of λ_0 . It is interesting to note that, nevertheless, the equality of the two renormalization factors is maintained throughout with particular accuracy. We can be reasonably confident, therefore, of our renormalization group results and the associated Ward identity [5, 6] in this isotropic case.

7. ‘Ward’ identity

In previous work [5] we suggested a Ward identity as an explanation of the proportionality of the renormalization of the vertex and diffusivity matrix. In terms of the bulk parameters this Ward identity simply implied that if $\kappa_{ij}^0 = \beta\lambda_{ij}^0$, then for the effective bulk parameters $\kappa_{ij} = \beta\lambda_{ij}$. The identity was verified to two-loop order in perturbation theory. However, in a slightly different problem (in two dimensions and with a random field where the diffusion turns out to be scale-dependent and hence anomalous) [9, 10], this Ward identity can be shown to hold exactly. Moreover, we have recently, given certain extra assumptions, been able to prove this Ward identity [11]. Here we show that this Ward identity changes form when the bare vertex and diffusivity matrices are no longer proportional to one another, i.e. when the FDR is violated. We will only discuss the change at one-loop order since this is sufficient to demonstrate the breakdown.

From the formulae of the previous section we see that to one-loop order

$$\frac{\partial}{\partial k_i} \Sigma(\mathbf{k}) = [\kappa^0 (\lambda^0)^{-1}]_{ij} V_j(\mathbf{k}, \mathbf{k}) + U_i(\mathbf{k}) \quad (40)$$

where

$$U_i(\mathbf{k}) = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} D(\mathbf{q}) \frac{q_r \lambda_{ri}^0 q_m \lambda_{mn}^0 k_n + q_r \lambda_{rs}^0 (\mathbf{q} + \mathbf{k})_s q_m \lambda_{mi}^0}{(\mathbf{q} + \mathbf{k})_j \kappa_{jl}^0 (\mathbf{q} + \mathbf{k})_l}. \quad (41)$$

For small \mathbf{k} we see that

$$k_i U_i(\mathbf{k}) = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} D(\mathbf{q}) \left\{ \frac{2(q_s \lambda_{rs}^0 k_s)^2}{q_m \kappa_{mn}^0 q_n} - \frac{2q_r \lambda_{rs}^0 q_s q_n \lambda_{mn}^0 k_n q_j \kappa_{jl}^0 k_l}{(q_m \kappa_{mn}^0 q_n)^2} \right\} + O(k^4). \quad (42)$$

It is easy to see that the right-hand side of this equation vanishes to $O(k^4)$ when $\kappa_{ij}^0 \propto \lambda_{ij}^0$. In general, however, it does not vanish. A simple case to consider is one in which the statistics of the $\phi(\mathbf{x})$ -field are isotropic, the diffusivity has the form $\kappa_{ij}^0 = \kappa_0 \delta_{ij}$ but the drift coefficient retains an anisotropic tensorial structure. We can easily evaluate the right-hand side of equation (42) to be

$$k_i U_i(\mathbf{k}) = - \frac{2\Delta(0)}{3\kappa_0} \left\{ \frac{3}{5} k_i [(\lambda^0)^2]_{ij} k_j - \frac{1}{5} \lambda_{mm}^0 k_i \lambda_{ij}^0 k_j \right\} + O(k^4). \quad (43)$$

If we define

$$\bar{\lambda}_{ij}^0 = \lambda_{ij}^0 - \frac{1}{3} \lambda_{mm}^0 \delta_{ij} \quad (44)$$

so that $\bar{\lambda}^0$ is the traceless or quadrupole part of λ^0 then we can recast the above equation in the form

$$k_i U_i(\mathbf{k}) = - \frac{2\Delta(0)}{3\kappa_0} \left\{ \frac{3}{5} k_i [(\bar{\lambda}^0)^2]_{ij} k_j + \frac{1}{5} \lambda_{mm}^0 k_i \bar{\lambda}_{ij}^0 k_j \right\} + O(k^4) \quad (45)$$

that is

$$k_i U_i(\mathbf{k}) = - \frac{2\Delta(0)}{5\kappa_0} k_i [\bar{\lambda}^0 \lambda^0]_{ij} k_j + O(k^4). \quad (46)$$

This form of the result makes it clear that when the traceless part of the drift tensor $\bar{\lambda}^0$ vanishes we return to the situation in which the original Ward identity holds.

For the particular case we are considering the the modified Ward identity implies for small \mathbf{k} the result

$$\frac{\partial}{\partial k_i} \Sigma(\mathbf{k}) = - \frac{\Delta(0)}{15\kappa_0} \{ \lambda_{mm}^0 \lambda_{ij}^0 + 2\lambda_{il}^0 \lambda_{lj}^0 \} k_j - \frac{2\Delta(0)}{3\kappa_0} \left\{ \frac{3}{5} [(\lambda^0)^2]_{ij} k_j - \frac{1}{5} \lambda_{mm}^0 \lambda_{ij}^0 k_j \right\} + O(k^3). \quad (47)$$

On the basis of this calculation we do not expect a simple relationship between the macroscopic diffusivity and the macroscopic drift coefficient. This is confirmed in the next section by a renormalization group calculation.

8. Renormalization group equations

The breakdown of the Ward identity and the absence of any simple relation between the effective diffusivity and drift tensors makes it interesting to examine the consequences of the renormalization group approach to computing the macroscopic parameters. The idea of this approach is to carry out a partial average of the Green function with respect to the components of the random field ϕ in small slices of wavevector space. After we have averaged out all Fourier modes in the random field ϕ with wavevector modulus greater

than some cut-off value Λ , we assume that the problem is identical to the original but with some effective $\kappa_{ij}(\Lambda)$ and an effective $\lambda_{ij}(\Lambda)$. We then compute perturbatively the change in making a further average over Fourier components with wavevector modulus between Λ and $\Lambda - \delta\Lambda$. The changes in κ_{ij} and λ_{ij} may be computed exactly to order $\delta\Lambda$ from the one-loop diagrams in figures 3 and 5 respectively. One then obtains the following differential equations for the (coupled) renormalization group flow of the two tensors. The equations for the diffusivity tensor were written down in [5, 6]. The resulting equations are:

$$\frac{d\kappa_{ij}}{d\Lambda} = \int \frac{d^3\mathbf{q}}{(2\pi)^3} \delta(q - \Lambda) D(q) \frac{(q_m \kappa_{mi} q_n \lambda_{nj} + q_m \kappa_{mj} q_n \lambda_{ni}) q_r \lambda_{rs} q_s - q_m \lambda_{mi} q_n \lambda_{nj} q_r \kappa_{rs} q_s}{(q_r \kappa_{rs} q_s)^2} \quad (48)$$

and

$$\frac{d\lambda_{ij}}{d\Lambda} = \int \frac{d^3\mathbf{q}}{(2\pi)^3} \delta(q - \Lambda) D(q) \frac{q_m \lambda_{mi} q_n \lambda_{nj} q_r \lambda_{rs} q_s}{(q_r \kappa_{rs} q_s)^2}. \quad (49)$$

It is clear from these equations that, as mentioned in a previous paper [6], those solutions satisfying boundary conditions for which $\lambda_{ij}^0 \propto \kappa_{ij}^0$ maintain the the proportionality $\lambda_{ij}(\Lambda) \propto \kappa_{ij}(\Lambda)$ for all Λ with a constant ratio.

It is, of course, easily checked that the isotropic solutions are those of earlier papers, namely

$$\kappa_{ij}(\Lambda) = \kappa_{ij}^S(\Lambda) = \kappa_0 \exp \left\{ -\frac{1}{3} \frac{\lambda_0^2}{\kappa_0^2} \Delta_\Lambda(0) \right\} \delta_{ij} \quad (50)$$

and

$$\lambda_{ij}(\Lambda) = \lambda_{ij}^S(\Lambda) = \lambda_0 \exp \left\{ -\frac{1}{3} \frac{\lambda_0^2}{\kappa_0^2} \Delta_\Lambda(0) \right\} \delta_{ij} \quad (51)$$

where

$$\Delta_\Lambda(0) = \int_{q>\Lambda} \frac{d^3\mathbf{q}}{(2\pi)^3} D(q). \quad (52)$$

We can examine solutions near these isotropic solutions that are perturbed by a small anisotropic change in the local drift tensor. It is no restriction to make this small change traceless. We then have

$$\begin{aligned} \kappa_{ij}(\Lambda) &= \kappa_{ij}^S(\Lambda) + \eta_{ij} \\ \lambda_{ij}(\Lambda) &= \lambda_{ij}^S(\Lambda) + \mu_{ij} \end{aligned} \quad (53)$$

where

$$\begin{aligned} \eta_{ij}(\infty) &= 0 \\ \mu_{ij}(\infty) &= \mu_{ij}^0 \end{aligned} \quad (54)$$

with $\mu_{ii}^0 = 0$. A perturbative analysis of equations (48) and (49) yields

$$\begin{aligned} \frac{d\eta_{ij}}{d\Lambda} &= \frac{\lambda_0}{\kappa_0} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \delta(q - \Lambda) D(q) \left\{ \frac{\lambda_0}{\kappa_0} \frac{2}{3} \eta_{ij} - \frac{3}{15} \frac{\lambda_0}{\kappa_0} (\eta \delta_{ij} + 2\eta_{ij}) + \frac{2}{15} (\mu \delta_{ij} + 2\mu_{ij}) \right\} \\ \frac{d\mu_{ij}}{d\Lambda} &= \frac{\lambda_0^2}{\kappa_0^2} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \delta(q - \Lambda) D(q) \left\{ \frac{2}{3} \mu_{ij} + \frac{1}{15} (\mu \delta_{ij} + 2\mu_{ij}) - \frac{2}{15} \frac{\lambda_0}{\kappa_0} (\eta \delta_{ij} + 2\eta_{ij}) \right\}. \end{aligned} \quad (55)$$

If we introduce a variable $0 < s < 1$ such that

$$s = \int_{q < \Lambda} \frac{d^3 \mathbf{q}}{(2\pi)^3} D(q) \quad (56)$$

and impose the allowed constraint that $\eta = \eta_{ii} = 0$ and $\mu = \mu_{ii} = 0$ we find

$$\begin{aligned} \frac{d\eta_{ij}}{ds} &= \frac{4}{15} \frac{\lambda_0^2}{\kappa_0^2} \eta_{ij} + \frac{4}{15} \frac{\lambda_0}{\kappa_0} \mu_{ij} \\ \frac{d\mu_{ij}}{ds} &= \frac{12}{15} \frac{\lambda_0^2}{\kappa_0^2} \mu_{ij} - \frac{4}{15} \frac{\lambda_0^3}{\kappa_0^3} \eta_{ij}. \end{aligned} \quad (57)$$

These equations are easily integrated and yield the result

$$\begin{aligned} \kappa_{ij} &= \kappa_0 \exp \left\{ -\frac{1}{3} \frac{\lambda_0^2}{\kappa_0^2} \right\} \delta_{ij} - \frac{4}{15} \frac{\lambda_0}{\kappa_0} \exp \left\{ -\frac{8}{15} \frac{\lambda_0^2}{\kappa_0^2} \right\} \mu_{ij}^0 \\ \lambda_{ij} &= \lambda_0 \exp \left\{ -\frac{1}{3} \frac{\lambda_0^2}{\kappa_0^2} \right\} \delta_{ij} + \left(1 - \frac{4}{15} \frac{\lambda_0^2}{\kappa_0^2} \right) \exp \left\{ -\frac{8}{15} \frac{\lambda_0^2}{\kappa_0^2} \right\} \mu_{ij}^0. \end{aligned} \quad (58)$$

It follows that

$$(\lambda \kappa^{-1})_{ij} = \frac{\lambda_0}{\kappa_0} \left(\delta_{ij} + \frac{1}{\lambda_0} \exp \left\{ -\frac{1}{5} \frac{\lambda_0^2}{\kappa_0^2} \right\} \mu_{ij}^0 \right). \quad (59)$$

For this near-isotropic case at least, we see that the proportionality of the macroscopic drift and diffusivity tensors is restored exponentially as the renormalization process takes place. However, we should emphasise here that $\lambda_{ij}(\Lambda)$ is also the effective coupling constant to the random field after we have averaged out the fluctuations in the field ϕ to wave vector modulus Λ . That is, we have effectively been coarse-graining the system. Here we see that the FDR is being exponentially restored upon coarse-graining and that deviations from the FDR appear to be reduced upon coarse-graining. It is a great advantage of the renormalization group method that, in addition to giving fairly accurate quantitative results, it also gives us a physical picture of what is happening in the system when we examine it at different scales. Hence one finds an example of a system which may violate the FDR slightly at one scale but obeys it rather well at large scales. Indeed, most physical models impose the FDR as a prerequisite in order to obtain a model that, on the large scale, obeys Gibbs statistics when in equilibrium. We see here that to obtain a model which is Gibbsian when viewed over suitably large scales it is not strictly necessary to make such an assumption.

9. Numerical simulation in the anisotropic case

We tested the above results from the renormalization group calculation against a simulation for which the asymmetric local drift tensor is diagonal in the coordinate basis with elements

$$\mu^0 = \begin{pmatrix} -\alpha/2 & 0 & 0 \\ 0 & -\alpha/2 & 0 \\ 0 & 0 & \alpha \end{pmatrix}. \quad (60)$$

Because of the axial symmetry of the local drift tensor the same property ensures that the effective diffusion and drift tensors will have the form

$$\kappa_e = \begin{pmatrix} \kappa_{\perp} & 0 & 0 \\ 0 & \kappa_{\perp} & 0 \\ 0 & 0 & \kappa_{\parallel} \end{pmatrix} \quad \text{and} \quad \lambda_e = \begin{pmatrix} \lambda_{\perp} & 0 & 0 \\ 0 & \lambda_{\perp} & 0 \\ 0 & 0 & \lambda_{\parallel} \end{pmatrix}. \quad (61)$$

Table 2. Number of modes in random field is 256. Theoretical values are shown in brackets.

λ_0	α	κ_{\parallel}	κ_{\perp}	λ_{\parallel}	λ_{\perp}
1.0	0.2	0.701(3) (0.685)	0.735(3) (0.732)	0.798(5) (0.803)	0.660(5) (0.674)
1.0	0.1	0.698(3) (0.701)	0.727(2) (0.724)	0.770(6) (0.760)	0.687(5) (0.695)
1.0	-0.1	0.730(5) (0.732)	0.712(2) (0.709)	0.672(5) (0.673)	0.730(5) (0.737)
1.0	-0.2	0.764(4) (0.748)	0.701(3) (0.701)	0.622(6) (0.630)	0.772(7) (0.760)

The results of the numerical simulation for certain values of λ_0 and various values of α are shown in table 2.

The results, with some small discrepancies for the two cases with $|\alpha| = 0.2$, are in good agreement with the predictions of the renormalization group calculations expressed in equations (58). It is not unreasonable that an asymmetry parameter as large as 20% is the limit of applicability of the simple perturbation approach in the previous section. To check the results by simulation in finer detail for smaller values of $|\alpha|$ requires higher statistical accuracy than can easily be achieved. Our simulations typically involved 256 particles in 256 velocity fields and required 100–200 processor hours. Nevertheless, we can conclude with reasonable confidence that the RGC produces an accurate result even in the asymmetric case. It may be that an important condition for the success of the RGC is the isotropy of the random field statistics.

10. Conclusions

In this paper we have confirmed the importance of the role of drift in the set of effective parameters that govern the long-time behaviour of a diffusion process in which a particle moves subject to molecular diffusion and the influence of the gradient of a random scalar field. Another way of expressing this is to say that in addition to the diffusion process itself, it is important to consider the effect on the system of long-range external fields and the strength with which they are coupled to the system. We have exploited this effect by computing and measuring the mean drift in a simulation induced by an external field of constant gradient. The results, however, must also be relevant to all external fields of long range. The conclusion, arrived at in previous work [2–5], and confirmed in this simulation, is the result that the effective drift and diffusivity parameters are renormalized relative to their local values by identical factors in the isotropic case.

We showed how the renormalization of the drift parameter could be interpreted as a result of biased *spatial* averaging effects due to the density distribution adopted by particles passing through the medium represented by the random field under the influence of an external field of constant gradient.

We also examined a situation in which the isotropy is broken by giving the drift tensor an axisymmetric form. We confirm that the Ward identity suggested in previous work as an explanation for the equality of the diffusion and drift renormalization factors is indeed broken in lowest-order perturbation theory. We do not expect a simple relationship between effective diffusion and drift in this case. This is confirmed at a theoretical level by using the renormalization group approach in a near-symmetric situation. The predictions of the

theoretical calculation are verified quite well by the results of a simulation. The implication is that the renormalization group calculation will work reasonably well when the statistics of the random scalar field are isotropic. Given this, we have found that, for the systems we have considered which have only perturbatively small deviations from the FDR at the microscopic level, the coarse-graining induced by averaging out fluctuations of the random field tends to restore the FDR for bulk quantities. It is plausible that the restoration of FDR after coarse-graining happens quite generally, though we have demonstrated it only in a special case. In renormalization group language, we would say that there is a range of theories which have microscopic violations of the FDR that flow towards coarse-grained theories obeying the FDR. It would be very interesting to investigate this situation further and identify systems that violate the FDR at the microscopic level which flow, under the influence of the renormalization group transformation, to bulk systems that do and do not satisfy the FDR, systems that have a variety of ‘fixed points’ with different basins of attraction in the microscopic parameter space.

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