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Diffusion of active tracers in fluctuating fields

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Abstract

The problem of a particle diffusion in a fluctuating scalar field is studied. In contrast to most studies of advection diffusion in random fields, ours analyzes the case where the particle position is also coupled to the dynamics of the field. Physical realizations of this problem are numerous and range from the diffusion of proteins in fluctuating membranes to the diffusion of localized magnetic fields in spin systems. We present exact results for the diffusion constant of particles diffusing in dynamical Gaussian fields in the adiabatic limit, where the field evolution is much faster than the particle diffusion. In addition we compute the diffusion constant perturbatively, in the weak coupling limit, when the interaction of the particle with the field is small, using a Kubo-type relation. Finally we construct a simple toy model which can be solved exactly, and which extrapolates between the adiabatic limit, for fields with rapid dynamics, and the limit where the field is quenched or frozen.

1. Introduction

The diffusion of passive particles in complex and random velocity fields has been extensively studied in statistical mechanics and fluid mechanics. In most of these studies one is interested in the dispersion of tracer particles which are advected by the complex or random field but which do not affect the field itself-it is for this reason they are called passive [1, 2]. These systems can be studied in the case of incompressible velocity fields (relevant for problems of turbulent dispersion in fluid mechanics) and the case where the velocity field is derived from a gradient (relevant to statistical mechanics and dynamical transitions related to the glass transition). As well as diffusion in time dependent fields, the problem of diffusion in quenched random fields has also been extensively studied [3]. Assuming that the advecting velocity field has zero mean, the passive tracer particle may diffuse normally as $\langle \mathbf{x}^2(t) \rangle \sim t$ but in certain circumstances the particle diffuses anormally $\langle \mathbf{x}^2(t) \rangle \sim t^{2\nu}$ with $\nu \neq 1/2$. In the case where $\nu < 1/2$ the diffusion is called subdiffusive and when $\nu > 1/2$ the diffusion is called superdiffusive [4]. Other interesting phenomena arise when one considers the diffusion of an ensemble of non-interacting (among themselves) tracers. Here, depending on the statistics of the advecting field, clustering phenomena may arise [2].

In this paper we will consider a problem where the tracer particle's position is coupled to the evolution of a scalar field. This means that the particle is advected by the field but also that the dynamics of the field is affected by the particle position. We take the dynamics of the field to be over damped stochastic dynamics. An interesting question arises as to how the diffusion of the particle depends on the field's dynamics, for instance one could have the same Hamiltonian for the system but in one case the field may evolve according to model A (non-conserved order parameter) dynamics and in the other by model B (conserved order parameter) dynamics or indeed Brownian hydrodynamics [5]. We will first concentrate our study on the case where the field dynamics is much more rapid than the local diffusion of the tracer particle. In this limit we will show that the diffusion of the particle is always slowed down by coupling the field. This is in contrast to the case where the effect of the tracer on the particle is ignored and where in this limit it can be shown that the diffusion of the particle is speeded up. We then consider a perturbative calculation of the effective diffusion constant where the coupling between the field and particle position is weak. This computation is based on a Kubo-like relation for the effective diffusion constant, in addition this relation shows explicitly that the diffusion constant of the particle is reduced when its position is coupled to the fluctuating field.

A concrete example of this problem is the diffusion of a protein on a membrane. The protein's position can be coupled to the height fluctuations of the membrane, for instance by tending to impose a local mean curvature [6]. Alternatively the

protein's position could be coupled to the local composition of the membrane; this could be because the protein has an affinity for a particular lipid type in a multicomponent lipid membrane or because it imposes a local tilt on the lipid hydrocarbon tails [7]. These two types of couplings lead to membrane mediated interactions between proteins but they will also modify the dynamics of a protein in the membrane. Indeed the question of what determines a protein's diffusion constant in a lipid bilayer is biologically very important. The problem was first addressed by Saffmann and Delbrück [8] based on a two-dimensional fluid model. However experimental studies [9] suggest that this simple fluid model may not explain the experimental data on protein and peptide diffusion constants as a function of their size. A number of studies have subsequently shown that protein coupling to membrane composition and height can substantially modify the protein's We should note that height diffusion constant [10–16]. fluctuations can modify the effective observed diffusion constant of a protein in a membrane even when there is no coupling between the fluctuations and protein position. This is because the protein diffuses in the plane of the membrane but the diffusion is observed on the projected area; this, geometric effect, leads to an apparent reduction of the diffusion constant [17, 18].

2. The model

Consider the dynamics of a Langevin particle, whose position is denoted by $\mathbf{x}(t)$, diffusing with a linear coupling to a fluctuating free field. The overall Hamiltonian for the system is

$$H = \frac{1}{2} \int \phi(\mathbf{x}) \Delta \phi(\mathbf{x}) \, d\mathbf{x} - hK\phi(\mathbf{x}(t)) \tag{1}$$

where we will take Δ and K to be self-adjoint operators. For two operators $A(\mathbf{x}, \mathbf{x}')$ and $B(\mathbf{x}, \mathbf{x}')$, their composition as operators is $AB(\mathbf{x}, \mathbf{x}') = \int d\mathbf{x}'' A(\mathbf{x}, \mathbf{x}'') B(\mathbf{x}'', \mathbf{x}')$ and applying the operator $A(\mathbf{x}, \mathbf{x}')$ to the function $f(\mathbf{x})$ gives the function $Af(\mathbf{x}) = \int d\mathbf{x}' A(\mathbf{x}, \mathbf{x}') f(\mathbf{x}')$. If the operator A is translation invariant we will also write $A(\mathbf{x}, \mathbf{x}') = A(\mathbf{x} - \mathbf{x}')$; this is the case of all the operators used here.

The above Hamiltonian applies to many systems. For example if we take $\Delta = -\nabla^2 + m^2$ and K = 1, this is a model for a point magnetic field of magnitude h diffusing in a Gaussian ferromagnetic model. If $\Delta = \kappa_b \nabla^4 - \sigma \nabla^2$ and $K = -\nabla^2$, the Hamiltonian is the Helfrich one for the height fluctuations of a lipid membrane where ϕ represents the height and the choice of K is due to the fact the particle is coupled to the local membrane curvature [19]. Here we are interested in the diffusion of the particle in the field. However to study the dynamics of diffusion we must also define the dynamics of the field. Here we will take for the field dynamics the general dissipative dynamics form

$$\frac{\partial \phi(\mathbf{x})}{\partial t} = -\kappa_{\phi} R \frac{\delta H}{\delta \phi(\mathbf{x})} + \sqrt{\kappa_{\phi}} \xi(\mathbf{x}, t) \tag{2}$$

where R is a self-adjoint dynamical operator and ξ is a Gaussian noise of zero mean which is uncorrelated in time. For instance, $R = \delta(\mathbf{x} - \mathbf{x}')$ corresponds to model A

conserved dynamics and $R = -\nabla^2 \delta(\mathbf{x} - \mathbf{x}')$ corresponds to model B dynamics [5]. If one is considering the case where ϕ represents the height fluctuations of a membrane then using Brownian hydrodynamics the Fourier transform of R, \tilde{R} is given by $\tilde{R}(\mathbf{k}) = 1/4\eta |\mathbf{k}|$, where η is the viscosity of the solvent surrounding the membrane [17]. The field dynamics is taken so as to respect detailed balance, so that the Gibbs–Boltzmann distribution is found for the equilibrium measure of the field and the particle position. This means that the correlation function of the noise respects the fluctuation dissipation relation

$$\langle \xi(\mathbf{x}, t)\xi(\mathbf{x}', t')\rangle = 2TR(\mathbf{x} - \mathbf{x}')\delta(t - t'), \tag{3}$$

where T is the temperature of the system. The dynamics of the particle is given by

$$\frac{\partial x_i(t)}{\partial t} = -\kappa \frac{\partial H}{\partial x_i} + \sqrt{\kappa} \eta_i(t), \tag{4}$$

where the noise terms is Gaussian noise with mean zero and correlation function

$$\langle \eta_i(t)\eta_i(t')\rangle = 2T\delta_{ij}\delta(t-t').$$
 (5)

The coefficients κ and κ_ϕ can be used to set the relative time scale between the dynamics of the field fluctuations and that of the tracer movement. In the absence of a coupling between the field and the particle, the particle diffuses normally and within the notation set up here the mean squared displacement at large times behaves as

$$\langle \mathbf{x}^2(t) \rangle \sim 2dT\kappa t = 2dDt,$$
 (6)

where d is the spatial dimension and $D = T\kappa$ is the bare diffusion constant. For the specific choice of Hamiltonians considered here we thus have the equations of motion

$$\frac{\partial \phi(\mathbf{x})}{\partial t} = -\kappa_{\phi} R \Delta \phi(\mathbf{x}) + h \kappa_{\phi} R K(x - \mathbf{x}(t)) + \sqrt{\kappa_{\phi}} \xi(\mathbf{x}, t)$$
 (7)

and

$$\frac{\partial x_i(t)}{\partial t} = h\kappa \nabla K \phi(\mathbf{x}(t)) + \sqrt{\kappa} \eta_i(t). \tag{8}$$

In the limit where it is defined we will be interested in the effective diffusion constant for the tracer defined via

$$\langle \mathbf{x}^2(t) \rangle \sim 2dT \kappa_{\rm e} t = 2dD_{\rm e} t,$$
 (9)

where $D_{\rm e}$ is the effective late time diffusion constant.

We note that, as mentioned above, equation (8) has been extensively studied in the case where the field ϕ evolves independently of the particle position. This problem is referred to as the advection diffusion of a passive scalar (the concentration of the particle) in a fluctuating field ϕ . This is obtained in the limit where one sets h=0 in equation (7) but keeps $h\neq 0$ in equation (8). It was suggested that this limit can be used to approximate the diffusion of the tracer particle in [10, 12]. In this case it is found that the effect of the field fluctuations can be to increase the diffusivity of the tracer particle with respect to that obtained when it is

not coupled to the fluctuating field (h=0). However the numerical simulations of [13] where the effect of the particle position on the field is taken into account suggests that the diffusion is reduced with respect to the case h=0 and in [16] the authors of [10, 12] revisited the problem and numerically and analytically confirmed the findings of [13]. The adiabatic results obtained here show that in this limit the diffusivity is always diminished with respect to the case h=0 and we argue that this is the limit where the diffusivity should be the most rapid. We also will show via a Kubo-type formula that active coupling to the fluctuating field should always reduce the value of the diffusion constant.

3. The adiabatic limit

We will now analyze the dynamics of this system in the limit $\kappa_{\phi}\gg\kappa$, i.e. where the field dynamics is much quicker than that of the particle. The basic idea is that one can eliminate the field variable in a mathematically controlled manner to yield an effective diffusion equation for the particle where the field no longer appears implicitly. This sort of procedure can be carried out at the level of the Fokker–Planck equation using projection operator methods [20]. However in the case here as we have a dynamical variable ϕ with an infinite number of degrees of freedom we will use an alternative method based on direct analysis of the Langevin equations [21, 22].

First we assume that at t = 0 the field $\phi = 0$ everywhere as at late times, when the field is equilibrated, this condition on the initial field configuration is unimportant. However in cases where the field stays out of equilibrium, for example where it coarsens, the initial condition will be important. Integrating the equation of motion for the field then gives

$$\phi(\mathbf{x}) = \int_0^t \mathrm{d}s \, \exp(-\kappa_\phi(t-s)R\Delta)[h\kappa_\phi RK(\mathbf{x} - \mathbf{x}(s)) + \sqrt{\kappa_\phi}\xi(\mathbf{x}, s)]. \tag{10}$$

Now if κ_{ϕ} is large and the operator $R\Delta$ is positive, the above integral is dominated by the region where s is close to t. We make the simple change of variables u=t-s in the above to find

$$\phi(\mathbf{x}) = \int_0^t du \, \exp(-\kappa_\phi u R \Delta) [h \kappa_\phi R K (\mathbf{x} - \mathbf{x}(t - u)) + \sqrt{\kappa_\phi} \xi(\mathbf{x}, t - u)]. \tag{11}$$

A Taylor expansion about u = 0 of the terms of the form $\mathbf{x}(t - u)$ yields,

$$\phi(\mathbf{x}) = \int_{0}^{t} du + \exp(-\kappa_{\phi} u R \Delta) \left[h \kappa_{\phi} R K(\mathbf{x} - \mathbf{x}(t)) + h \kappa_{\phi} u \right] \times \frac{dx_{j}(t)}{dt} \nabla_{j} R K(\mathbf{x} - \mathbf{x}(t)) + \sqrt{\kappa_{\phi}} \xi(\mathbf{x}, t) + O\left(\frac{1}{\kappa_{\phi}^{\frac{3}{2}}}\right)$$

$$= h \Delta^{-1} K(\mathbf{x} - \mathbf{x}(t)) + \frac{h}{\kappa_{\phi}} \frac{dx_{j}(t)}{dt} (R \Delta)^{-2} \nabla_{j} R K(\mathbf{x} - \mathbf{x}(t)) + \sqrt{\frac{1}{\kappa_{\phi}}} (R \Delta)^{-1} \xi(\mathbf{x}, t),$$

$$(12)$$

as each power of u in the Taylor expansion yields a factor of $1/\kappa_{\phi}$ on performing the integral over u. There are also

operator terms of the form $\exp(-t\kappa_{\phi}R\Delta)$ coming from the upper limit of the integration at u=t, however as we assume that $R\Delta$ is positive these terms can be neglected at large times t. This assumption is physically equivalent to assuming that the field in the absence of the particle can equilibrate in a finite time. If this is not the case then there is a possibility that the diffusion can become anomalous due to growing length scales in the field. Indeed we will see that the diffusion constant for localized fields in Gaussian ferromagnets can vanish if the field's equilibrium correlation length diverges.

We must now compute $\nabla K \phi(\mathbf{x}(t))$ from the above. We may write the first term of equation (12) using its Fourier representation as

$$hK\Delta^{-1}K(\mathbf{x} - \mathbf{x}(t)) = \frac{h}{(2\pi)^d} \int d\mathbf{k} \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)} \exp(i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}(t)))$$
(13)

and the second term is given by

$$\frac{\mathrm{d}x_{j}(t)}{\mathrm{d}t}K(R\Delta)^{-2}\nabla_{j}RK(\mathbf{x} - \mathbf{x}(t)) = \frac{\mathrm{d}x_{j}(t)}{\mathrm{d}t}\frac{h}{\kappa_{\phi}(2\pi)^{d}}$$

$$\times \int \mathrm{d}\mathbf{k}\,\mathrm{i}k_{j}\frac{\tilde{K}^{2}(k)}{\tilde{\Delta}(k)^{2}\tilde{R}(k)}\exp(\mathrm{i}\mathbf{k}\cdot(\mathbf{x} - \mathbf{x}(t))). \tag{14}$$

The results now give that to the order of approximation in $1/\kappa_\phi$ used above we have

$$\nabla_{i}K\phi(\mathbf{x}(t)) = \frac{h}{(2\pi)^{d}} \int d\mathbf{k} \, \mathrm{i}k_{i} \frac{\tilde{K}^{2}(k)}{\tilde{\Delta}(k)} - \frac{\mathrm{d}x_{j}(t)}{\mathrm{d}t} \frac{h}{\kappa_{\phi}(2\pi)^{d}}$$

$$\times \int d\mathbf{k} \, k_{j}k_{i} \frac{\tilde{K}^{2}(k)}{\tilde{\Delta}(k)^{2}\tilde{R}(k)} + \sqrt{\frac{1}{\kappa_{\phi}}} \nabla_{i}K(R\Delta)^{-1}\xi(\mathbf{x}, t).$$
(15)

The first term is zero by isotropy and we can also write

$$\int d\mathbf{k} \, k_j k_i \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)} = \frac{\delta_{ij}}{d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)}.$$
 (16)

We may thus write the effective Langevin equation for $\mathbf{x}(t)$ as

$$\left(1 + \frac{h^2 \kappa}{\kappa_{\phi} d (2\pi)^d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)} \right) \frac{dx_i(t)}{dt}$$

$$= h \kappa \sqrt{\frac{1}{\kappa_{\phi}}} \nabla_i K (R\Delta)^{-1} \xi(\mathbf{x}(t), t) + \sqrt{\kappa} \eta_i(t). \tag{17}$$

Let us remark here that if we had not taken into account the effect of the particle position on the field and had simply considered the effect of the field on the particle, the case of passive diffusion, we would have arrived at the effective diffusion equation

$$\frac{\mathrm{d}x_i(t)}{\mathrm{d}t} = h\kappa \sqrt{\frac{1}{\kappa_{\phi}}} \nabla_i K(R\Delta)^{-1} \xi(\mathbf{x}(t), t) + \sqrt{\kappa} \eta_i(t). \quad (18)$$

The effective diffusion constant for the process of equation (17) κ_e is simply related to that of equation (18), which we will denote by κ^* , via

$$\frac{\kappa_{\rm e}}{\kappa^*} = \left[1 + \frac{h^2 \kappa}{\kappa_{\phi} d(2\pi)^d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)} \right]^{-2}. \tag{19}$$

If we write equation (18) as

$$\frac{\mathrm{d}x_i(t)}{\mathrm{d}t} = \zeta_i(\mathbf{x}(t), t),\tag{20}$$

we see that the correlation function for the noise is given by

 $\langle \zeta_i(\mathbf{x}(t), t) \zeta_i(\mathbf{x}(t'), t') \rangle = 2T \delta(t - t') \delta_{ij} \kappa$

$$\times \left[1 + \frac{h^2 \kappa}{\kappa_{\phi} d(2\pi)^d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)} \right], \tag{21}$$

which immediately yields

$$\frac{\kappa^*}{\kappa} = 1 + \frac{h^2 \kappa}{\kappa_{\phi} d(2\pi)^d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)} \tag{22}$$

and

$$\frac{\kappa_{\rm e}}{\kappa} = \left[1 + \frac{h^2 \kappa}{\kappa_{\phi} d (2\pi)^d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)} \right]^{-1}. \tag{23}$$

We thus see that if the particle diffuses passively in the field, the diffusion constant (κ^*) is increased by its advection by the field. However in the active case, when the coupling is taken into account, the diffusion constant is reduced. Moreover to first order in κ/κ_{ϕ} we find that the change in the two different diffusion constants with respect to their bare values is the same in magnitude but of opposite sign. It is interesting to note that there is no temperature dependence on the renormalization of $\kappa_{\rm e}$ due to the interaction with the field. This means that $D_{\rm e}$ retains a simple linear dependence on T within the adiabatic approximation.

Note that the integrals occurring in the above can be ultra-violet divergent. This may be the case for certain local operators K, for example $K(\mathbf{x} - \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}')$. When numerically simulating the system in this case one can just introduce an ultra-violet cut-off in the simulation, i.e. a maximal Fourier mode. The result given here shows that a naive application of the Stokes–Einstein relationship works for the effective diffusion constant $D_{\rm e}$. Define by D the diffusion constant without a coupling to the field. For a particle moving at constant velocity the frictional force, opposing the motion, is given by

$$f_0 = \lambda_0 v. \tag{24}$$

However, the friction is related to the mobility via

$$v = \mu_0 f_0. \tag{25}$$

Stokes-Einstein tells us that, when it is valid (see later discussion),

$$D = \mu_0 T, \tag{26}$$

and using the fact that $D = T\kappa$ we have that $\lambda_0 = 1/\kappa$.

Now in presence of the coupling one can compute the average frictional force f_{ϕ} due to the fluctuation field [14, 15] and one finds that

$$f_{\phi} = \lambda_{\phi} v \tag{27}$$

where λ_{ϕ} is given by

$$\lambda_{\phi} = \frac{h^2}{\kappa_{\phi} d(2\pi)^d} \int d\mathbf{k} \, k^2 \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)}. \tag{28}$$

The total frictional force is thus given by

$$f = f_0 + f_\phi = (\lambda_0 + \lambda_\phi)v. \tag{29}$$

This gives via the Stokes-Einstein relation

$$D_{e} = \mu_{e}T = \frac{T}{\lambda_{0} + \lambda_{\phi}}$$

$$= \frac{D}{\left[1 + \frac{h^{2}D\beta}{\kappa_{d}(2\pi)^{d}} \int d\mathbf{k} \, k^{2} \frac{\tilde{K}^{2}(k)}{\tilde{\lambda}(k)^{2} \tilde{E}(k)}\right]},$$
(30)

where $\beta = 1/T$, which is equivalent to the result equation (23). We also note that all the terms in the integrand of equation (23) are positive and thus we have within the adiabatic approximation that $D_{\rm e} < D$. The application of the Stokes-Einstein relation that we have just made is clearly not exact. To compute the diffusion constant using the Stokes-Einstein relation one must compute the average value of the velocity vat constant applied force [3]. This is a much harder problem than computing the average force at constant velocity. In a previous paper [15] we argued that the Stokes-Einstein relation as applied above should be valid when the fluctuations of the force are small, and thus the force is near to constant in the statistical sense. The fact that the average force is large means that the friction is large and thus the diffusion constant is small. Here we see that the adiabatic limit reproduces the approximate application of the Stokes-Einstein relation given above. This result can be explained by examining the expression given for the autocorrelation function of the force fluctuations given in [14]; here one sees in the adiabatic limit that fluctuations of the force become uncorrelated in time and their amplitude becomes small.

3.1. Examples

We will now consider a number of special cases of our principle result equation (23) which we will write as

$$\frac{\kappa_{\rm e}}{\kappa} = \left[1 + \frac{h^2 S_d \kappa Q}{\kappa_{\phi} d (2\pi)^d}\right]^{-1}.$$
 (31)

with

$$Q = \int dk \, k^{d+1} \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)^2 \tilde{R}(k)},\tag{32}$$

and where S_d is the area of a sphere of radius 1 in d dimensions.

Considering now a localized magnetic field diffusing in a ferromagnet within the Gaussian approximation, we take

$$\tilde{\Delta}(k) = k^2 + m^2. \tag{33}$$

We assume a magnetic field with a localized Gaussian profile and thus

$$\tilde{K}(k) = \exp\left(-\frac{k^2 a^2}{2}\right). \tag{34}$$

With this we find

$$Q = m^{d-2} \int_0^\infty dq \frac{q^{d+1}}{(q^2+1)^2} \exp(-q^2 m^2 a^2)$$
 (35)

for model A dynamics and

$$Q = m^{d-4} \int_0^\infty \mathrm{d}q \frac{q^{d-1}}{(q^2+1)^2} \exp(-q^2 m^2 a^2)$$
 (36)

for model B dynamics.

In certain cases one can take the limit $a \to 0$ in the above and thus obtain results that are only weakly dependent on the cut-off. However these cases depend strongly on the mass of the field theory and the result can be divergent when the theory is critical, i.e. when m = 0. These cases are the following

• Model A: $d \leq 1$

$$Q = \frac{\pi}{4m}, \qquad d = 1. \tag{37}$$

• Model B: $d \leq 3$

Q =
$$\frac{\pi}{4m^3}$$
, $d = 1$
= $\frac{1}{2m^2}$, $d = 2$
= $\frac{\pi}{4m}$, $d = 3$. (38)

We thus see that as the mass of the scalar field is decreased or its correlation length $\xi=1/m$ increases the diffusion constant of the active tracer particle is decreased. In the limit where $h\gg 1$ the magnetic tracer will be surrounded by a polarized region where the field ϕ has the same sign as the tracer field. The size of the polarized region will be of order ξ and the modification to the diffusion constant above presumably reflects the effective mobility of this polarization cloud. It is also interesting to note the different dependence on m between model A and B in one dimension.

Cases where the results have a strong dependence on the cut-off have been extensively discussed in [15]. A notable example among these cases is that of a protein, which is linearly coupled to the local membrane curvature. However if the protein is linearly coupled to the membrane height profile the corrections to the diffusion constant in the adiabatic limit are independent of the cut-off. Such a linear coupling could be induced by holding a membrane protein in an optical trap or due to its interaction with an actin cytoskeleton or similar polymer network. Here the Helfrich Hamiltonian for lipid membranes gives [19]

$$\tilde{\Delta} = \kappa_{\rm b} k^4 + \sigma k^2,\tag{39}$$

where κ_b is the bending rigidity and σ the surface tension. The dynamical operator for membrane dynamics is given by

$$\tilde{R} = \frac{1}{4nk},\tag{40}$$

where η is the viscosity of the surrounding fluid [17], defining R this way means that we set $\kappa_{\phi}=1$ in equation (31) and the adiabatic limit corresponds to small η . Using these forms in equation (32) then yields the correction to the diffusion constant

$$Q = \frac{\pi \eta}{\kappa_{\rm h}^{\frac{1}{2}} \sigma^{\frac{3}{2}}}.\tag{41}$$

We note that this correction diverges in the limit where the surface tension σ vanishes. The corresponds to the point where the static correlation length of membrane height fluctuations $\xi = \sqrt{\frac{\kappa}{\sigma}}$ diverges.

4. Weak coupling limit

In this section we use a formally Kubo-like expression for the effective diffusion constant; the expression can formally be computed to $O(h^2)$ in the particle-field coupling parameter, thus giving an expression for $D_{\rm e}$ which is exact to this order. To obtain the Kubo formula we integrate equation (8) to obtain

$$\mathbf{x}(t) - \mathbf{x}(0) = h\kappa \int_0^t \nabla K \phi(\mathbf{x}(s)) ds + \sqrt{2T\kappa} \mathbf{B}(t)$$
 (42)

where \mathbf{B}_t is a standard d-dimensional Brownian motion with

$$\langle B_i(t)B_j(s)\rangle = \delta_{ij}\min\{t,s\}. \tag{43}$$

In the above we assume that at t=0 the system is in equilibrium (i.e. we assume that the volume of the system is finite, and \mathbf{x}_0 and the initial field configuration ϕ are chosen from the equilibrium distribution (see [3] for more details)). Now subtracting the first term of the right-hand side of equation (42) from both sides, squaring the resulting equation and taking the average yields

$$\langle (\mathbf{x}(t) - \mathbf{x}(0))^2 \rangle + h^2 \kappa^2 \left\langle \left(\int_0^t \nabla K \phi(\mathbf{x}(s)) \, \mathrm{d}s \right)^2 \right\rangle = 2T d\kappa t,$$
(44)

where the cross term on the right-hand side is zero due to the Onsager relations [3]. We can thus define a time dependent diffusion constant via

$$\langle (\mathbf{x}(t) - \mathbf{x}(0))^2 \rangle = 2dD_{e}(t)t = 2dT\kappa_{e}(t)$$

$$= 2Td\kappa t - h^2 \left\langle \left(\kappa \int_0^t \nabla K\phi(\mathbf{x}(s)) \, \mathrm{d}s\right)^2 \right\rangle$$
(45)

where the late time limit of these two quantities are the effective values $\lim_{t\to\infty} D_{\rm e}(t)$, $\kappa_{\rm e}(t)=D_{\rm e}$, $\kappa_{\rm e}$. We may therefore write

$$\frac{D_{\rm e}}{D} = 1 - \frac{h^2 \beta^2 D}{2d} \lim_{t \to \infty} \left\langle \frac{1}{t} \left(\int_0^t \nabla K \phi(\mathbf{x}(s)) \mathrm{d}s \right)^2 \right\rangle. \tag{46}$$

From this exact formula we see that the value of the diffusion constant is reduced by the interaction with the field. This expression may now be evaluated to $O(h^2)$ by replacing $\mathbf{x}(t)$ by the pure Brownian motion $\sqrt{2D}\mathbf{B}_t$ of the particle without interaction of the field and using the correlation function for the free field without interaction with the particle which can be written as

$$\langle \phi_0(\mathbf{x}, t) \phi_0(\mathbf{y}, s) \rangle = T \int \frac{d\mathbf{k}}{(2\pi)^d} \tilde{\Delta}^{-1}(k)$$

$$\times \exp(-\kappa_{\phi} | t - s| \tilde{R}(k) \tilde{\Delta}(k)) \exp(i\mathbf{k} \cdot (\mathbf{x} - \mathbf{y})). \tag{47}$$

After a straight forward computation using the fact that $\mathbf{B}(t)$ and ϕ_0 are independent we obtain

$$\frac{D_{\rm e}}{D} = 1 - \frac{h^2 \beta D}{d} \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{k^2 \tilde{K}^2(k)}{\tilde{\Delta}(k) (\kappa_{\phi} \tilde{R}(k) \tilde{\Delta}(k) + Dk^2)} + O(h^4).$$
(48)

Note that in the adiabatic limit this result is clearly equivalent to equation (30) to $O(h^2)$. In terms of the variables κ equation (48) reads

$$\frac{\kappa_{\rm e}}{\kappa} = 1 - \frac{h^2 \kappa}{d} \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^d} \frac{k^2 \tilde{K}^2(k)}{\tilde{\Delta}(k) (\kappa_{\phi} \tilde{R}(k) \tilde{\Delta}(k) + T \kappa k^2)} + O(h^4); \tag{49}$$

note therefore in contrast to the purely adiabatic result equation (23) that there is a temperature dependent renormalization of $\kappa_{\rm e}$. Another interesting thing to note is that in this perturbative result we can recover the case where the field is frozen, i.e. the other extreme to the adiabatic limit where $\kappa_{\phi}=0$. Here the field is quenched and has correlation function $T\Delta^{-1}$. This quenched result agrees with the first order perturbation result for quenched random fields [3].

4.1. Examples

Once again we will consider the Gaussian ferromagnet under model A and model B dynamics and compare the results with those of section 3.1. In order to facilitate the comparison we will write equation (49) as

$$\frac{\kappa_{\rm e}}{\kappa} = 1 - \frac{h^2 S_d \kappa}{\kappa_{\phi} d (2\pi)^d} Q \tag{50}$$

which has the same form in perturbation theory as equation (31) but where Q is given by

$$Q = \int dk \, k^{d+1} \frac{\tilde{K}^2(k)}{\tilde{\Delta}(k)(\tilde{\Delta}(k)\tilde{R}(k) + \frac{T_K}{K_0}k^2)}.$$
 (51)

We see that the expression for Q in equation (51) is the same as that in the adiabatic limit in the two limiting cases, $\kappa/\kappa_{\phi} \to 0$ and when $T \to 0$. We will again consider the cases where the diffusion constant is finite, as the cut-off is taken to infinity, and compare the corrections to the diffusion constant in the adiabatic and weak coupling limits.

• Model A. $d \leq 1$

$$Q = \frac{\kappa_{\phi}\pi}{2T\kappa m} \left[1 - \frac{1}{(1 + \frac{T\kappa}{\kappa_{\phi}})^{\frac{1}{2}}} \right], \qquad d = 1. \quad (52)$$

Here we thus find that the diffusion constant diverges as 1/m when $m \to 0$ as is the case in the adiabatic approximation.

• Model B. $d \leq 3$

$$Q = \frac{\pi \kappa_{\phi}}{2T\kappa m} \left[1 - \frac{1}{\left(1 + \frac{T\kappa}{\kappa_{\phi}m^2}\right)^{\frac{1}{2}}} \right], \qquad d = 1$$

$$= \frac{\kappa_{\phi}}{2\kappa T} \ln\left(1 + \frac{T\kappa}{\kappa_{\phi}m^2}\right), \qquad d = 2$$

$$= \frac{\pi \kappa_{\phi}}{2T\kappa} \left[\left(m^2 + \frac{T\kappa}{\kappa_{\phi}}\right)^{\frac{1}{2}} - m \right], \qquad d = 3.$$
(53)

Here we see comparing with the results of section 3.1 that divergence in 1/m is reduced due to the temperature dependent term. In one and two dimensions the divergence is reduced but in three dimensions it is completely eliminated.

In the case of a two-dimensional membrane with a linear coupling to the height profile, the correction to the diffusion is, as in the adiabatic approximation, cut-off independent. Here we find that for $\sigma \kappa_b < 4\eta^2 T^2 \kappa^2$

$$Q = \frac{\eta \pi}{\sigma (\sigma \kappa_{\rm b} - 4\eta^2 T^2 \kappa^2)^{\frac{1}{2}}} \times \left[1 - \frac{2}{\pi} \tan^{-1} \left(\frac{2\eta T \kappa}{(\sigma \kappa_{\rm b} - 4\eta^2 T^2 \kappa^2)^{\frac{1}{2}}} \right) \right], \tag{54}$$

and we easily see how the adiabatic result in recovered in the limit $\eta T \kappa / \kappa_{\phi} \rightarrow 0$. When $\sigma \kappa_{b} > 4 \eta^{2} T^{2} \kappa^{2}$ the result can be written as

$$Q = \frac{\eta}{\sigma (4\eta^2 T^2 \kappa^2 - \sigma \kappa_b)^{\frac{1}{2}}} \times \ln \left[\frac{4(\eta T \kappa + (\eta^2 T^2 \kappa^2 - \frac{\sigma \kappa_b}{4})^{\frac{1}{2}})^2}{\kappa_b \sigma} \right].$$
 (55)

In the limit of high temperatures this result can be written as

$$Q \approx \frac{1}{2\sigma T\kappa} \ln \left(\frac{16\eta^2 T^2 \kappa^2}{\kappa_b \sigma} \right),\tag{56}$$

and we see that the correction to the diffusion has a relatively weak logarithmic dependence on the viscosity of the fluid surrounding the membrane η , and the bending rigidity κ_b .

5. A toy model

In the general class of models studied above we have been able to obtain partial results on the effective diffusion constant of an active tracer in two distinct limits: the adiabatic limit and the weak coupling limit. Here we present a simple toy model whose behavior can be thoroughly analyzed. We consider a tracer particle **x** coupled to another diffusion process **y** via the Hamiltonian defined by

$$H(\mathbf{x}, \mathbf{v}) = V(\mathbf{x} - \mathbf{v}), \tag{57}$$

where V is a function such that there exists a vector (or set of vectors) **a** such that, $V(\mathbf{x}) = V(\mathbf{x} + \mathbf{a})$ in the algebraic or statistical sense. For example we could take $V(\mathbf{x})$ to be a periodic function or one that is statistically invariant by translation. The coupled diffusion equations for \mathbf{x} and \mathbf{y} are given by

$$\frac{\partial x_i}{\partial t} = -\kappa_x \frac{\partial V(\mathbf{x} - \mathbf{y})}{\partial x_i} + \sqrt{\kappa_x} \eta_{x_i}$$
 (58)

$$\frac{\partial y_i}{\partial t} = \kappa_y \frac{\partial V(\mathbf{x} - \mathbf{y})}{\partial x_i} + \sqrt{\kappa_y} \eta_{y_i},\tag{59}$$

where the noise variables above are white noise at temperature T as defined earlier. In the case where the variable \mathbf{y} is frozen (or equivalently $\kappa_y = 0$), as the function V is translationally invariant and if it is bounded, we expect the process \mathbf{x} will have an effective quenched diffusion constant defined by

$$\langle \mathbf{x}_{t}^{2} \rangle \sim 2dD_{e}^{(q)}t = 2dT\kappa_{e}^{(q)}t, \tag{60}$$

and which is independent of the choice of \mathbf{y} by the translational invariance of V. We note that it is possible to compute $D_{\rm e}$ exactly in a number of special cases [3]. In order to see the effect of the dynamics of \mathbf{y} on the process \mathbf{x} we define the new variables

$$\mathbf{u} = \mathbf{x} - \mathbf{y} \tag{61}$$

$$\mathbf{v} = \kappa_{\mathbf{v}} \mathbf{x} + \kappa_{\mathbf{x}} \mathbf{y},\tag{62}$$

and it is then easy to see that these new dynamical variables obey

$$\frac{\partial u_i}{\partial t} = -(\kappa_x + \kappa_y) \frac{\partial V(\mathbf{u})}{\partial u_i} + \sqrt{\kappa_x} \eta_{x_i} - \sqrt{\kappa_y} \eta_{y_i}$$
 (63)

$$\frac{\partial v_i}{\partial t} = \kappa_y \sqrt{\kappa_x} \eta_{x_i} + \kappa_x \sqrt{\kappa_y} \eta_{y_i}. \tag{64}$$

Furthermore one can easily see that the noises in these two equations are independent and thus the processes \mathbf{u} and \mathbf{v} are independent. The process \mathbf{u} is simply a time rescaled form of the quenched problem and \mathbf{v} is a free Brownian motion. The mean squared displacement of the two processes can thus be computed easily and are given by

$$\langle \mathbf{u}_t^2 \rangle \sim 2dT \kappa_e^{(q)} \frac{\kappa_x + \kappa_y}{\kappa_x} t$$
 (65)

$$\langle \mathbf{v}_t^2 \rangle \sim 2dT \kappa_x \kappa_y (\kappa_x + \kappa_y) t.$$
 (66)

Finally using the independence of \mathbf{u} and \mathbf{v} we find that

$$\langle \mathbf{x}_t^2 \rangle \sim 2dT \kappa_x \left(\frac{\kappa_e^{(q)} + \kappa_y}{\kappa_x + \kappa_y} \right) t,$$
 (67)

which gives the effective diffusion constant of \mathbf{x} as

$$\frac{D_{\rm e}}{T} = \kappa_{\rm e} = \kappa_x \left(\frac{\kappa_{\rm e}^{(q)} + \kappa_y}{\kappa_x + \kappa_y} \right). \tag{68}$$

We see that in the quenched limit $\kappa_y=0$ we obtain that $\kappa_e=\kappa_e^{(q)}$ as we should. In addition it is clear that κ_e is an increasing function of κ_y , the quenched case being a lower bound for the effective diffusion constant. Another interesting fact about the expression equation (68) is that there are a number of models where the quenched diffusion constant vanishes, signaling the transition from a regime of normal diffusion to one of subdiffusion [3, 22–24]. However we see from equation (68) that when $\kappa_y\neq 0$ then the vanishing of $\kappa_e^{(q)}$ does not cause the diffusion constant to vanish as the result has an additive property. Indeed if $\kappa_e^{(q)}=0$ then we find

$$\kappa_{\rm e} = \frac{\kappa_x \kappa_y}{\kappa_x + \kappa_y} \tag{69}$$

throughout the parameter region where the quenched problem shows subdiffusion.

The quenched diffusion constant $\kappa_{\rm e}^{(q)}$ can be computed exactly in a limited number of cases [3], notably in one dimension where it is given by

$$\frac{\kappa_{\rm e}^{(q)}}{\kappa_{\rm x}} = \frac{1}{\langle \exp(-\beta V) \rangle \langle \exp(\beta V) \rangle} \tag{70}$$

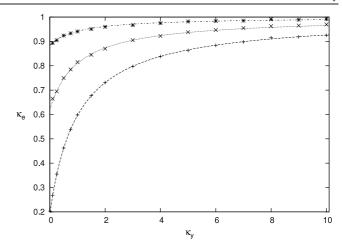


Figure 1. Effective diffusion coefficient versus field evolution velocity for the model of equations (58) and (59) in one dimension for $V(x) = \cos(x)$ and temperatures T = 0.5(+), $1(\times)$ and 2(*). The continuous lines correspond to the analytical result.

where

$$\langle \exp(\pm \beta V) \rangle = \lim_{L \to \infty} \frac{1}{L} \int_0^L \exp(\pm \beta V(x)) dx$$
 (71)

which exists for translationally invariant potentials.

An exact result also exists in two dimensions in the case where the field V is statistically equivalent to -V (either functionally or statistically) [3]; it has the simple form

$$\frac{\kappa_{\rm e}^{(q)}}{\kappa_{\rm r}} = \frac{1}{\langle \exp(\beta V) \rangle}.$$
 (72)

As a test of this result in one dimension we took the potential $V(x) = \cos(x)$ and equations (68) and (70) then give

$$\frac{\kappa_{\rm e}}{\kappa_{\rm x}} = \frac{I_0(\beta)^{-2}\kappa_{\rm x} + \kappa_{\rm y}}{\kappa_{\rm x} + \kappa_{\rm y}},\tag{73}$$

where $I_0(z)$ denotes the modified Bessel function. Numerical simulations were carried out for $\kappa_x = 1$ and κ_y varying between 0.1 and 10 and at temperatures T = 0.5, 1 and 2. The results given figures (1) show an excellent agreement with the analytical result equation (73).

6. Discussion

We have examined the diffusion of an active tracer particle coupled to a fluctuating field. Most previous studies have been carried out on passive tracers in time dependent or quenched fields. The action of the tracer on the field means that diffusion is always slowed down with respect to the non-interacting case; this fact is explicit in equation (46). This result may seem odd from a physical point of view as one would naively expect that the fluctuating field would help the particle to diffuse. Indeed we have seen that in the adiabatic approximation a passive diffuser diffuses more quickly when driven by the field. However when the effect of the tracer on the field is taken into account the effect of the extra noise from the

fluctuating field is eliminated by a additional drag due to the action of the tracer on the field. Although it is in a limiting case, the adiabatic calculation carried out here shows how these two effects compete and lead to slowing down of the diffusion with respect to the free case. As an example we analyzed the diffusion constant of magnetic fields diffusing in Gaussian ferromagnets; here we found that the diffusion rate decreases as the correlation length of the field increases. This result is presumably linked to the fact that the field is trapped in domains where the field has the same sign and also its presence leads to the formation of these domains about it. As the correlation length increases the size of the domains containing the field increases and the diffusion constant of the field effectively becomes that of it surrounding domain. It seems physically reasonable that the diffusion constant of the surrounding domain becomes smaller as its size increases.

We have also analyzed the active diffusion problem in the weak coupling limit where the existence of an underlying Gibbs measure allows us to write down a Kubo-type formula for the diffusion constant. As well as rigorously establishing that diffusion is slowed down with respect to the free case, this formula can be used to give a first order expression for the modified diffusion constant.

Finally we have analyzed a toy model for a particle interacting with a scalar field in the simple case where this scalar field is another diffusing particle. In this case the effective diffusion constant can be formally computed in terms of the effective diffusion constant for a particle diffusing in a quenched random potential. The effect of the dynamics of the second diffuser can be thoroughly understood, and as its bare diffusion constant is increased so is that of the tracer.

Clearly there are still a large number of questions about diffusion of active scalars in fluctuating fields, for the precise problem examined here the whole regime beyond the perturbative and adiabatic regimes studied here remains open. It would also be interesting to understand in more detail the cross over from the active to passive cases and understand under what circumstances field fluctuations increase/decrease the tracer diffusion constant.

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