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Dipole diffusion in a random electrical potential

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Abstract

We study the Langevin dynamics of a dipole diffusing in a random electrical field \mathbf{E} derived from a quenched Gaussian potential. We show that in a suitable adiabatic limit (where the dynamics of the dipole moment is much faster than the dynamics of its position), one can reduce the coupled stochastic equations to an effective Langevin equation for a particle diffusing in an effective potential with a spatially varying and anisotropic local diffusivity κ_{ij} . Analytic results, close to the adiabatic limit, for the diffusion constant κ_e are found in one dimension and a finite temperature dynamical transition is found. The system is also studied numerically. In particular, we study the anomalous diffusion exponent in the low-temperature regime. Our findings strongly support the conclusion that the location of the dynamical transition and the anomalous diffusion exponents are determined by purely static considerations, i.e. they are independent of the relative values of the diffusion constants of the particle position and its dipole moment.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Computing bulk transport properties in random media is an important physical problem [1–8] having many applications. Two important models of random media have widely been studied (i) where the randomness is due to a random potential and (ii) where the local diffusion constant is random. There are mathematical relations between the problems (i) and (ii) and problems of type (ii) are also related to a wide variety of physical problems such as the effective conductivity and dielectric constants of random conductors and dielectrics and the effective permeability of porous media [1]. An important quantity to understand those properties is the *late time diffusion constant* of a Brownian tracer particle in interaction with the medium. In the system we will study, the local transport properties are modified by the interaction of the dipole moment of the tracer particle with a random electric field drawn from an appropriate

statistical ensemble. If the electric field disorder is statistically invariant under translation and short range correlated in space, we expect that the diffusion constant and mobility due to an applied force are self-averaging in the regime where the diffusion is normal. If the transport is normal, then in the long time limit ($t \rightarrow \infty$), the mean-squared displacement of the particle position behaves as

$$\langle (\mathbf{x}(t) - \mathbf{x}(0))^2 \rangle \sim 2D\kappa_e t, \quad (1)$$

where D is the dimension of space and κ_e is the late time diffusion or the effective diffusion constant. In general there are subdominant corrections to the above, which depend strongly on the dimensionality of the problem [9, 10].

If the random field is frozen or evolves over very long timescales with respect to those of the tracer particle, then one is in the situation of *quenched disorder*, where the potential does not depend on time. The motivation for studying models of particles diffusing in a random potential comes from the fact that such systems arise very naturally in nature; for instance in zeolites where random electric fields are generated by the presence of frozen charged impurities [11]. If the particle has a net charge, then the particle interacts with the electric field and the case of diffusion in a quenched scalar field has been extensively studied in the literature [1–3, 10, 12]. However, if the particle is polarizable but without charge, it also interacts with the field. In this case, the problem is quite different and much less well studied [12, 13]. We also note that systems with quenched disorder, spin glasses for example, are often good paradigms for systems having structural glass transition (where no random field is present). It is often argued heuristically, that for sufficiently complex and frustrated systems, a single particle in the system sees an effectively random potential due to the other particles. At a mean field level, there exist models where this analogy has been used successfully to analyse the statistical mechanics of frustrated but non-disordered models. In practice one can have two models, one with quenched disorder and the other without but highly frustrated, which exhibit the same thermodynamics in the high temperature phase and the same glass transition at low temperatures [14–16]. Even if the frustrated non-random system possesses a crystalline ground state, not shared by the disordered system, this fact is practically irrelevant as this state is dynamically never attained. Therefore, these models are often adopted as toy models for structural glass transition. In the liquid phase, we expect the tracer particle to have a non-zero diffusion constant κ_l . Now consider the situation in which the same particle diffuses in a quenched background, where all the other particles have been frozen in a particular configuration. A realistic choice would be to select a configuration from a Gibbs–Boltzmann equilibrium ensemble. If κ_e is the diffusion constant, it has been shown [17, 18] that $\kappa_e < \kappa_l$ which makes physical sense, because if the background particles can move about, the cages, which trap the tracer, will break up on some timescale and free it to disperse more quickly than in the quenched case. Moreover, in some special cases, κ_e can vanish at a critical temperature or disorder strength [10, 12]. If the system has a finite correlation length l_0 (which will be the case, as our field will be short range correlated), the diffusion constant can be used to give an effective relaxation time τ

$$\tau \sim \frac{l_0^2}{\kappa_e}. \quad (2)$$

If $\kappa_e \rightarrow 0$, it means that we have a diverging timescale in the same way in which a structural glass has a diverging timescale which, experimentally, can be extracted from the divergence of the liquid's viscosity.

In this paper we study the physical case of dipoles diffusing in a random electric field $\mathbf{E}(\mathbf{x})$ which is spatially varying but time independent (or quenched). It is generated by a random potential $\phi(\mathbf{x})$ which gives $\mathbf{E}(\mathbf{x}) = -\nabla\phi(\mathbf{x})$, with the correlation function

$$\langle\phi(\mathbf{x})\phi(\mathbf{x}')\rangle = \Delta(|\mathbf{x} - \mathbf{x}'|). \quad (3)$$

The potential $\phi(\mathbf{x})$ is thus statistically isotropic and invariant by translation in space. The most convenient choice is to take ϕ to be Gaussian. If the dipole moment, denoted by \mathbf{p} , is modelled as two opposite charges connected to a Harmonic spring and \mathbf{x} denotes the position of the dipole centre, then the total energy of a particle at the point (\mathbf{p}, \mathbf{x}) is given by

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2\chi}\mathbf{p}^2 - \mathbf{p} \cdot \mathbf{E}(\mathbf{x}). \quad (4)$$

The first term is the Harmonic energy of the spring, and χ is simply the dipole polarizability. The second term is the energy of the dipole's interaction with the field \mathbf{E} . The partition function for the system, where \mathbf{x} is confined to a volume denoted by \mathcal{V} of a D dimensional space, is given, up to an overall factor, by

$$Z = \int_{\mathcal{V}} d\mathbf{x} \int_{\mathbb{R}^D} d\mathbf{p} \exp\left(-\beta\frac{\mathbf{p}^2}{2\chi} + \beta\mathbf{p} \cdot \mathbf{E}(\mathbf{x})\right), \quad (5)$$

where $\beta = 1/k_B T$ is the inverse temperature. If we trace over the dependence on \mathbf{p} , we find an effective partition function for the variable \mathbf{x} given, again up to a constant, by

$$Z_{eff} = \int_{\mathcal{V}} d\mathbf{x} \exp(-\beta V(\mathbf{x})), \quad (6)$$

where V is the effective potential for \mathbf{x} and is given by

$$V(\mathbf{x}) = -\frac{\chi\mathbf{E}^2(\mathbf{x})}{2}. \quad (7)$$

This represents the case where the dipole moment adapted instantaneously to the external field and motivated the study in [10, 12] of diffusion in non-Gaussian potentials. In [10] the diffusion constant for a particle diffusing in non-Gaussian potentials such as given by equation (7) was computed exactly in one dimension, and in [12] a self-renormalization group scheme was developed to study the problem in higher dimensions.

In [10, 12] a critical temperature at which the diffusion constant vanishes, signalling a dynamical transition from a normal diffusive regime to a subdiffusive regime, was identified. We thus expect that, in a suitable adiabatic limit where the dynamics of the dipole degree of freedom \mathbf{p} is much more rapid than that of the spatial variable \mathbf{x} , the effective potential seen by the variable \mathbf{x} is V as defined by equation (7).

If we take an overdamped Langevin dynamics for both the dipole and positional degrees of freedom, the equations of motion are given by

$$\frac{dx_i}{dt} = \beta\kappa_x p_j \frac{\partial E_j}{\partial x_i} + \sqrt{2\kappa_x}\eta_{x_i} \quad (8)$$

$$\frac{dp_i}{dt} = -\kappa_p \beta \left(\frac{p_i}{\chi} - E_i\right) + \sqrt{2\kappa_p}\eta_{p_i}. \quad (9)$$

In the above equations κ_x is the bare diffusion constant for the spatial variable and the other diffusion constant κ_p sets the timescale for the relaxation of the dipole and the adiabatic limit is where $\kappa_p \rightarrow \infty$. In principle both diffusion constants depend on the temperature but for notational simplicity this dependence is suppressed. In the dynamical equations (8) and (9), terms of the form A_i represent the component of the vector \mathbf{A} in the direction i ; we have also

used the Einstein summation convention and will stick with this convention throughout the paper. The noise terms are white noise and their correlation functions are given by

$$\langle \eta_{p_i}(t)\eta_{p_j}(s) \rangle = \langle \eta_{x_i}(t)\eta_{x_j}(s) \rangle = \delta_{ij}\delta(t-s) \quad \text{and} \quad \langle \eta_{p_i}(t)\eta_{x_j}(s) \rangle = 0. \quad (10)$$

If we rewrite (9) and substitute it into equation (8) we find

$$\frac{dx_i}{dt} = \sqrt{2\kappa_x}\eta_{x_i} + \kappa_x\beta \frac{\partial}{\partial x_i} \frac{\chi E_j^2}{2} - \frac{\kappa_x}{\kappa_p} \chi \frac{\partial E_j}{\partial x_i} \left(\frac{dp_j}{dt} - \sqrt{2\kappa_p}\eta_{p_j} \right). \quad (11)$$

If we now take the adiabatic limit ($\kappa_p \gg \kappa_x$), equation (11) reduces to the Langevin equation for a particle in the potential $V(\mathbf{x})$ defined by equation (7). In the appendix, we rederive this result in a more rigorous way and also see, at first order, the effect of a finite value of κ_p . We thus expect that for very large values of κ_p , we find the same dynamics for \mathbf{x} studied in [10, 12, 13]. Consequently there should also be a dynamical transition in this problem when the field ϕ is Gaussian. We can now ask the question, what happens if the timescale for the relaxation of the dipole moment is non-zero? Will the dynamical transition remain or is it a pathology of the limit $\kappa_p \rightarrow \infty$?

In the appendix we derive the effective dynamics for the marginal distribution of \mathbf{x} to order κ_x/κ_p . To this order the effective dynamics of \mathbf{x} can still be described by a Langevin equation, with the same potential as equation (7) but with a spatially varying non-isotropic diffusion constant. This is a rather remarkable fact and can be shown using operator projection techniques [19]. However we will present a derivation based on a direct manipulation of the Langevin equations similar to that of [20]. We chose this route as it gives a physical feeling for why the effective process for \mathbf{x} is to this order Markovian and also because the computation in spaces of dimension greater than 1 is more straightforward within this formalism. We also compute the first-order corrections to the effective diffusion constant in the high temperature limit via a Kubo formula for the effective diffusion constant.

In section 3 we present the exact result for the diffusion constant in one dimension. In section 4 we confront our results with numerical simulation (stochastic second-order Runge–Kutta) of the coupled Langevin equations (8) and (9) in the diffusive and sub-diffusive regimes. Finally in section 5 we will conclude and discuss our results.

2. Large κ_p and small β approximations

The timescale for the relaxation of the dipoles should be proportional to κ_p^{-1} and thus the adiabatic limit (where the dipoles adapt very quickly to the local field) will correspond to the limit where κ_p becomes large. Interestingly, in this limit, one can simplify the coupled equations (8) and (9) to an effective Langevin equation for \mathbf{x} up to the order $O(\kappa_x/\kappa_p)$ by direct manipulation of the Langevin equations [20]. The exact derivation is a little long and technical and for clarity's sake it is thus given in the appendix. As a result, we can write the following Fokker–Planck equation which describes the effective process for \mathbf{x} ,

$$\frac{\partial \rho}{\partial t} = H\rho = \frac{\partial}{\partial x_k} \left[\kappa_{ki} \left(\frac{\partial \rho}{\partial x_i} + \beta \rho \frac{\partial V}{\partial x_i} \right) \right] \quad (12)$$

where V is the effective potential given by equation (7) and κ_{ij} is a spatially varying and anisotropic diffusivity tensor given by

$$\kappa_{ij} = \kappa_x \left[\delta_{ij} - \frac{\kappa_x}{\kappa_p} \chi^2 \frac{\partial E_k}{\partial x_i} \frac{\partial E_k}{\partial x_j} \right]. \quad (13)$$

The Fokker–Planck equation (12) has the correct Gibbs–Boltzmann equilibrium distribution with the effective potential V and from this one can write a Langevin equation which corresponds to the process

$$\frac{dx_i}{dt} = -\beta\kappa_x \frac{\partial}{\partial x_i} \frac{\chi E_j^2}{2} + \frac{\partial}{\partial x_i} \kappa_{ij} + \sqrt{2\kappa_{ij}} \eta_i. \quad (14)$$

We note that if we take the limit where $\kappa_p \rightarrow \infty$ in (14), the diffusivity reduces to $\kappa_{ij} = \kappa_x \delta_{ij}$ and we recover the Langevin equation for a particle in the potential $V(\mathbf{x})$ rigorously. In equation (A.21) of the appendix we performed an expansion in α^{-1} (with $\alpha = \kappa_p \beta / \chi$) and assumed α to be large. However if κ_p is large but finite we see that as β becomes small (the high temperature limit) the expansion will fail. To predict the behaviour of κ_e at high temperature we will thus use a Kubo formula for the effective diffusion constant. Integrating the stochastic differential equation (8) between 0 and t we have

$$x_i(t) - x_i(0) = \sqrt{2\kappa_x} B_i(t) + \beta\kappa_x \int_0^t ds p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)), \quad (15)$$

where \mathbf{B}_t is a standard D -dimensional Brownian motion with $\langle \mathbf{B}_t^2 \rangle = 2Dt$ and $x_i(0)$ is the initial position in the direction i . Thus squaring the above equation and taking the average yields

$$\begin{aligned} 2\kappa_x t = \langle (x_i(t) - x_i(0))^2 \rangle + 2\kappa_x \beta \left\langle (x_i(t) - x_i(0)) \cdot \int_0^t ds p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) \right\rangle \\ + (\kappa_x \beta)^2 \int_0^t ds \int_0^s ds' \langle p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) p_k(s') \cdot \nabla_i E_k(\mathbf{x}(s')) \rangle. \end{aligned} \quad (16)$$

Using the property of detail balance, which ensures time translation invariance at equilibrium, we have for any two functions A and B that

$$\langle A(\mathbf{x}(t)) B(\mathbf{x}(s)) \rangle = \langle A(\mathbf{x}(t-s)) B(\mathbf{x}(0)) \rangle, \quad (17)$$

and the Onsager symmetry relation

$$\langle A(\mathbf{x}(t)) B(\mathbf{x}(s)) \rangle = \langle B(\mathbf{x}(t)) A(\mathbf{x}(s)) \rangle. \quad (18)$$

Assuming that the system starts in equilibrium¹ one can thus apply (17) and (18) to the second term of (16) and show that it should vanish

$$\begin{aligned} \left\langle (x_i(t) - x_i(0)) \cdot \int_0^t ds p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) \right\rangle \\ = \int_0^t ds [\langle x_i(t) p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) \rangle - \langle x_i(0) p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) \rangle] \\ = \int_0^t ds [\langle x_i(t-s) p_j(0) \cdot \nabla_i E_j(\mathbf{x}(0)) \rangle - \langle x_i(0) p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) \rangle] \\ = \int_0^t ds [\langle p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) x_i(0) \rangle - \langle x_i(0) p_j(s) \cdot \nabla_i E_j(\mathbf{x}(s)) \rangle] \\ = 0. \end{aligned} \quad (19)$$

Thus, (16) reduces to

$$\begin{aligned} \langle (x_i(t) - x_i(0))^2 \rangle = 2\kappa_x t \\ - (\kappa_x \beta)^2 \int_0^t ds \int_0^s ds' \langle p_j(s-s') p_k(0) \nabla_i E_j(\mathbf{x}(s-s')) \nabla_i E_k(\mathbf{x}(0)) \rangle. \end{aligned} \quad (20)$$

¹ We assume that the system is in equilibrium in a finite volume and the subsequent late time diffusion constant is computed at times such that the particle has diffused over a distance much larger than the system's correlation length but much smaller than the system's size.

This equation is however exact and can be evaluated to order \mathbf{E}^2 by calculating the integral on its right-hand side using the statistics for \mathbf{x} and \mathbf{p} in the absence of \mathbf{E} , i.e. in the weak disorder limit which should become exact at high temperatures. Here \mathbf{p} and \mathbf{x} are purely Gaussian with correlation functions

$$\langle p_j(s)p_k(0) \rangle = \frac{\chi}{\beta} \exp\left(-\frac{\kappa_p \beta}{\chi} s\right) \delta_{jk}, \quad (21)$$

and

$$\langle (x_i(t) - x_j(0))^2 \rangle = 2\delta_{ij}\kappa_x t. \quad (22)$$

This approximation yields

$$\begin{aligned} & \langle p_j(s - s')p_k(0)\nabla_i E_j(\mathbf{x}(s - s'))\nabla_i E_k(\mathbf{x}(0)) \rangle \\ &= \frac{\chi}{\beta} \exp\left(-\frac{\kappa_p \beta}{\chi}(s - s')\right) \langle \nabla_i E_j(\mathbf{x}(s - s'))\nabla_i E_k(\mathbf{x}(0)) \rangle \delta_{jk}. \end{aligned} \quad (23)$$

Summing over the spatial indices then gives

$$\kappa_e = \kappa_x - \frac{\kappa_x^2 \beta \chi}{Dt} \int_0^t ds \int_0^s ds' \exp\left(-\frac{\kappa_p \beta}{\chi}(s - s')\right) \langle \nabla_i E_j(\mathbf{x}(s - s'))\nabla_i E_j(\mathbf{x}(0)) \rangle. \quad (24)$$

The correlation function of the random field component in the above can be computed in terms of the correlation function $\Delta(\mathbf{x})$ of the random electrostatic field ϕ :

$$\begin{aligned} \langle (\nabla_i E_j \mathbf{x}(s - s'))\nabla_i E_j(\mathbf{x}(0)) \rangle &= \int \frac{d\mathbf{k}}{(2\pi)^D} \tilde{\Delta}(\mathbf{k}) \mathbf{k}^4 \langle \exp(i\mathbf{k} \cdot \mathbf{x}(s - s')) \rangle \\ &= \int \frac{d\mathbf{k}}{(2\pi)^D} \tilde{\Delta}(\mathbf{k}) \mathbf{k}^4 \exp(-\mathbf{k}^2 \kappa_x (s - s')), \end{aligned} \quad (25)$$

where $\tilde{\Delta}(\mathbf{k})$ is the Fourier transform of $\Delta(\mathbf{x})$. Finally, we are left with a simple double integration over s and s' , and from the large time behaviour we can extract κ_e as

$$\kappa_e = \kappa_x - \frac{\kappa_x^2 \beta \chi}{D} \int \frac{d\mathbf{k}}{(2\pi)^D} \frac{\tilde{\Delta}(\mathbf{k}) \mathbf{k}^4}{\mathbf{k}^2 \kappa_x + \frac{\kappa_p \beta}{\chi}}. \quad (26)$$

3. Analytic results in one dimension

In the previous section, all the results we derived were for an arbitrary dimension D . To analyse our results to first order beyond the adiabatic limit, we will restrict our study to the one-dimensional case where one can compute exactly the diffusion constant κ_e for the effective Fokker–Planck equation (12). We apply the general results of [1] to compute the effective diffusivity via a static problem:

$$\kappa(x) \left(\frac{d\rho}{dx} + \beta\rho \frac{dV}{dx} \right) = j, \quad (27)$$

where j is the current and $\kappa(x)$ is the spatially varying diffusivity in one dimension

$$\kappa(x) = \kappa_x \left[1 - \frac{\kappa_x}{\kappa_p} \chi^2 \left(\frac{dE(x)}{dx} \right)^2 \right]. \quad (28)$$

We can solve (27) and find

$$\rho(x) = j e^{-\beta V(x)} \int_0^x \frac{e^{\beta V(y)}}{\kappa(y)} dy. \quad (29)$$

The diffusion constant κ_e is then given as $\kappa_e \langle \frac{d\rho}{dx} \rangle = j$ where $\langle \cdot \rangle$ is the average over the disorder in the random electrical field. This gives

$$\kappa_e \left\langle \frac{d\rho}{dx} \right\rangle = \lim_{L \rightarrow \infty} \frac{\kappa_e j}{L} \left\langle e^{-\beta V(L)} \int_0^L \frac{e^{\beta V(y)}}{\kappa(y)} dy \right\rangle = j, \quad (30)$$

and finally

$$\kappa_e = \frac{1}{\langle e^{-\beta V} \rangle \left\langle \frac{e^{\beta V}}{\kappa} \right\rangle}. \quad (31)$$

This result can also be obtained via a first passage time argument [21, 22]. The electrical potential $\phi(x)$ is Gaussian and if we choose a correlator of the form $\Delta(x) = f(x^2)$, where f is analytic at $x = 0$, then we find that $\langle E^2(0) \rangle = -2f'(0)$, and $\langle E'(0)E(0) \rangle = 0$. Therefore, E' and E are uncorrelated and we can write

$$\kappa_e = \frac{\langle \kappa^{-1} \rangle^{-1}}{\langle e^{-\beta V} \rangle \langle e^{\beta V} \rangle}. \quad (32)$$

In [10] (corresponding to the adiabatic case here) it was shown that the dynamical transition could be identified, via an Arrhenius-type argument, with the divergence of one or other of the first two terms on the denominator of the equation above. We thus see that to first order beyond the adiabatic approximation the location of the transition temperature should be the same in the adiabatic limit and close to this limit.

In the numerical simulations we will carry out we take the choice of correlation function $f(u) = \exp(-\frac{1}{2}u)$ for which we find

$$\kappa_e = \kappa_x (1 - \chi^2 \beta^2)^{1/2} \left(1 - \frac{\kappa_x \chi^2}{\kappa_p} \right). \quad (33)$$

4. Numerical simulations

In this section we test our analytical predictions against numerical simulations of the Langevin equations (8) and (9) in one dimension. In our simulation, we set the diffusion constant without disorder κ_x to 1 for convenience and we used rescaled variables $p_i = \tilde{p}_i \sqrt{\kappa_p}$ and $E_i = \tilde{E}_i \sqrt{\kappa_p}$, so that both equations have the same timescale,

$$\frac{dx_i}{dt} = \beta \kappa_p \tilde{p}_j \frac{\partial \tilde{E}_j}{\partial x_i} + \sqrt{2} \eta_{x_i} \quad (34)$$

$$\frac{d\tilde{p}_i}{dt} = -\kappa_p \beta \left(\frac{\tilde{p}_i}{\chi} - \tilde{E}_i \right) + \sqrt{2} \eta_{p_i}. \quad (35)$$

The coupled stochastic differential equations were integrated using second-order Runge–Kutta integration schemes developed in [23, 24] and reviewed in [1] with a time step $\Delta t = 0.001$. In all simulations the effective diffusion constant for a given realization of the disorder was obtained by fitting the mean-squared displacement averaged over 2000 particles at late times. The time of the simulation was chosen so that particles had typically diffused ten or so correlation lengths of the field. The fit of the average mean-squared displacement was done over the last half of the time of the simulation (to ensure that the mean-squared displacement is well within the linear regime) by a nonlinear form: $at + bt^\theta$, with $\theta < 1$. The correction to the linear term has to be taken into account as it becomes more and more relevant close to the transition due to the slowing down of the dynamics [10].

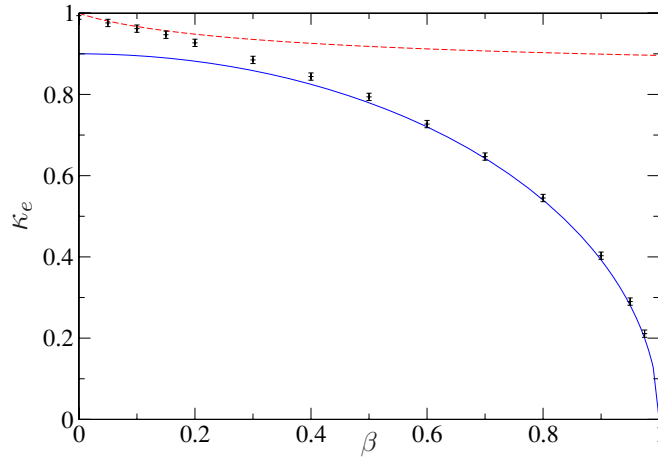


Figure 1. Numerical value of κ_e (stars) for $\kappa_p = 10$, compared with analytical results (26) (dashed line) and (33) (solid line).

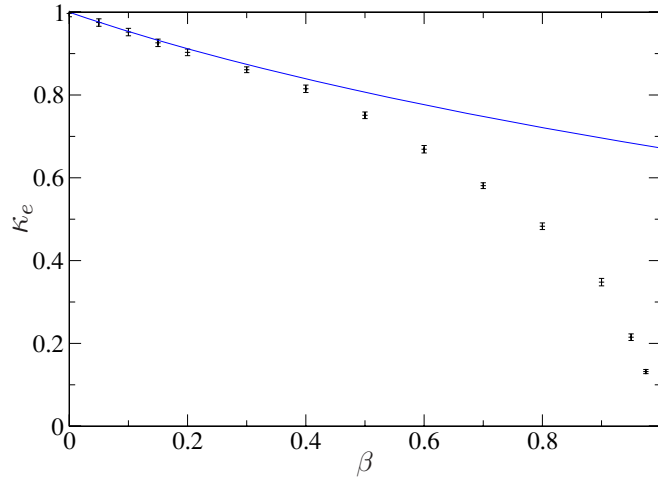


Figure 2. Numerical value of κ_e (plus) for $\kappa_p = 1$, compared with analytical results (26) (solid line).

To generate the Gaussian field characterized by a correlator (3), we used the technique presented in [25, 26]. The process can be written in a general form

$$\phi(x) = \int_{-\infty}^{+\infty} K(x - x')\eta(x') dx', \tag{36}$$

where K is a kernel function and $\eta(x)$ is a Gaussian white noise. The linear form of (36) ensures that $\phi(x)$ is a Gaussian process and the translational invariance of the kernel $K(x - x')$ ensures its stationarity. Now taking the Fourier transform defined by $\tilde{\phi}(\omega) = \int_{-\infty}^{+\infty} \phi(x) \exp(-i\omega x) dx$ of (36), we find

$$\tilde{\phi}(\omega) = \tilde{K}(\omega)\tilde{\eta}(\omega). \tag{37}$$

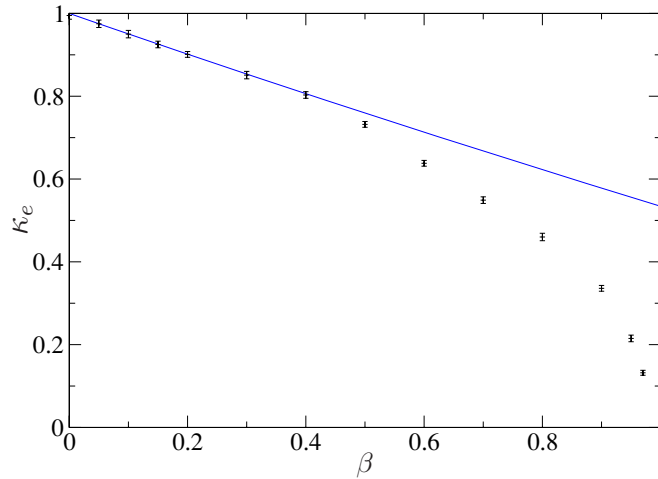


Figure 3. Numerical value of κ_e (plus) for $\kappa_p = 0.1$, compared with analytical results (26) (solid line).

If we now take the Fourier transform of the correlator (3) and the correlator $\langle \phi(\omega)\phi(\omega') \rangle$ from (37), then by identification we have $\tilde{\Delta}(\omega) = |\tilde{K}(\omega)|^2$ and thus from (37),

$$\tilde{\phi}(\omega) = \sqrt{\tilde{\Delta}(\omega)}\tilde{\eta}(\omega). \quad (38)$$

We can now create $\phi(x)$ by sampling $\tilde{\phi}(\omega)$ on a frequency mesh and taking the inverse fast Fourier transform (FFT). In [10, 12], the authors used a method due to Kraichnan [1, 27] which gives some finite size corrections for the diffusion constant close to the transition. However as we wish to precisely locate the transition and tests its dependence on κ_p (and as we do not have analytical results for all parameter ranges) we use this FFT-based method. Again we take a correlator of the form $\Delta(x) = \exp(-\frac{1}{2}x^2)$ and we average our sample over 2000 realizations of the field. In all our simulation we set $\chi = 1$. We measured the average value of κ_e over the field with an error bar estimated from the standard deviation from sample to sample. The result in one dimension is compared in figure 1 for $\kappa_p = 10$ with the analytical result (33) and the Kubo formula (26). As expected, we are well in the adiabatic regime and (33) is in very good agreement with the numerical simulations. Moreover, we find a dynamical transition at $\beta_c = 1$ where the diffusion constant becomes zero, and below the critical temperature T_c the diffusion turns out to be anomalous (see later). Finally, the agreement between (33) and the numerical results breaks down at high temperature, but fortunately in this regime the results agree with the weak disorder/high temperature analytical expression (26). We have thus a crossover between two analytical approximations which allows us to predict the behaviour of κ_e in the whole normal diffusion regime.

Beyond the adiabatic approximation, that is to say when κ_p is of the same order as κ_x or smaller, we lack analytical results (except for weak disorder), thus we must calculate κ_e numerically. The results are plotted in figure 2 for $\kappa_p = 1$ and figure 3 for $\kappa_p = 0.1$ and compared with the weak disorder result of equation (26). In both cases, the transition still appears to occur at, or very close to, the same critical temperature $T_c = 1$. Moreover, the diffusion constant clearly decreases monotonically with the value of κ_p at fixed temperature.

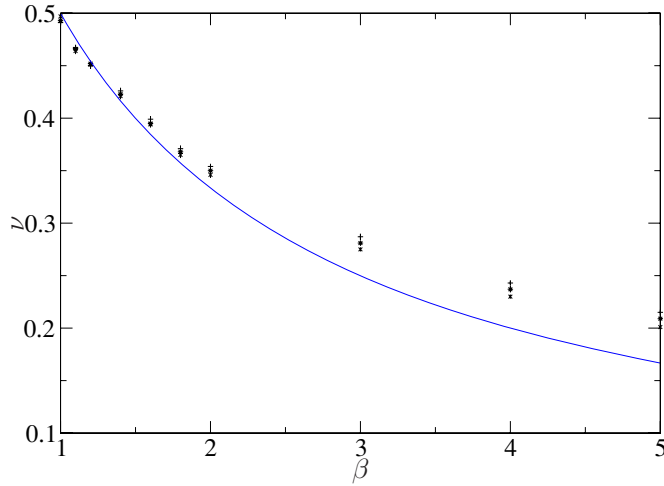


Figure 4. Numerical value of ν (cross) for $\kappa_p = 10$, (stars) for $\kappa_p = 1$ and (plus) for $\kappa_p = 0.1$ compared with analytical results (40) (solid line) in the low-temperature phase.

The low temperature phase, below T_c , is characterized by an anomalous sub-diffusive behaviour

$$\langle (\mathbf{x}(t) - \mathbf{x}(0))^2 \rangle \sim Ct^{2\nu}, \tag{39}$$

where the exponent associated with the anomalous diffusion $\nu < 1/2$. The subject of anomalous diffusion in disordered media has extensively been studied and a good review of it can be found in [9]. In the case of $\kappa_p \rightarrow \infty$ the authors in [10] were able to evaluate ν by means of first passage calculation and replica trick and they found

$$\nu = \frac{1}{1 + \beta}. \tag{40}$$

We plot in figure 4 the value of the exponent ν fitted from simulations with (39) for different values of κ_p . The results agree relatively well with equation (40) for temperatures below but close to the transition temperature. However for very low temperature, the exponent is significantly larger than that predicted by equation (40). However we have verified that as the time of the simulation is increased, the measured exponent appears to decrease (indeed this was the case in [10] where analytical results and an effective trap model were available to identify the correct exponent).

5. Conclusions and discussion

We have studied the dynamics of a dipole diffusing in a random electrical field \mathbf{E} derived from a quenched Gaussian potential. In the adiabatic limit (where the dipoles adapt very quickly to the local field), we showed that the coupled stochastic equation can be reduced, up to the order $O(\kappa_x/\kappa_p)$, to an effective Langevin equation for a particle diffusing in an effective potential with a spatially varying and anisotropic local diffusivity κ_{ij} . In one dimension, we could compute exactly the diffusion constant of this process and we found a dynamical transition at finite temperature $\beta_c = 1$ with a crossover between a diffusive and a sub-diffusive regime. The validity of the effective Langevin equation (14) breaks down for small β , but

a high-temperature treatment allowed us to compute a Kubo formula of κ_e for a given value of κ_p . We numerically checked our analytical predictions in one dimension, finding good agreement and confirming the presence of the transition. We also ran simulations far from the adiabatic regime and found strong indications that the transition remains at, or close to, the same β_c as for the adiabatic limit. Finally, we performed extensive numerical simulations in the low-temperature phase to compute the anomalous exponent ν . We found that it does not depend on the relative values of diffusion constants of the particle's position and dipole moment and agrees rather well with a calculation made for the adiabatic case [10].

In [12], the authors showed that in higher dimensions, for the adiabatic case $\kappa_p \rightarrow \infty$, the same type of dynamical transition is also present. It would be interesting to investigate the dipole problem in higher dimensions to see if the conclusions of our current study remain valid. It would also be interesting to see if renormalization group type treatments or other approximation schemes could be developed in order to obtain analytical results in higher dimensions.

Appendix. Derivation of the effective long-time Langevin equation for \mathbf{x}

This appendix gives the detail of the calculation of the effective long-time Langevin equation for \mathbf{x} . The first step is to formally integrate equation (9) for the variable \mathbf{p} to obtain

$$p_i(t) = p_i(0) \exp\left(-\frac{\beta\kappa_p}{\chi}t\right) + \int_0^t ds \exp\left(-\frac{\beta\kappa_p}{\chi}(t-s)\right) \kappa_p \beta E_i(\mathbf{x}(s)) + \sqrt{\frac{2}{\kappa_p}} \frac{\chi}{\beta} \zeta_i(t), \quad (\text{A.1})$$

where

$$\zeta_i(t) = \frac{\kappa_p \beta}{\chi} \int_0^t ds \exp\left(-\frac{\beta\kappa_p}{\chi}(t-s)\right) \eta_{p_i}(s) \quad (\text{A.2})$$

is a coloured noise. At late times the first term of equation (A.1) is exponentially suppressed and can thus be dropped giving

$$p_i(t) = \int_0^t ds \exp\left(-\frac{\beta\kappa_p}{\chi}(t-s)\right) \kappa_p \beta E_i(\mathbf{x}(s)) + \sqrt{\frac{2}{\kappa_p}} \frac{\chi}{\beta} \zeta_i(t). \quad (\text{A.3})$$

Substituting this into equation (8) yields

$$\frac{dx_i}{dt} = \beta\kappa_x \frac{\partial E_j}{\partial x_i} \left[\int_0^t ds \exp\left(-\frac{\beta\kappa_p}{\chi}(t-s)\right) \kappa_p \beta E_j(\mathbf{x}(s)) + \sqrt{\frac{2}{\kappa_p}} \frac{\chi}{\beta} \zeta_j(t) \right] + \sqrt{2\kappa_x} \eta_{x_i}. \quad (\text{A.4})$$

To proceed further we will find an effective Fokker–Planck equation corresponding to the stochastic equation (A.4). We follow the standard procedure of evaluating the change of an arbitrary function of $x(t)$:

$$\begin{aligned} \left\langle \frac{df(\mathbf{x}(t))}{dt} \right\rangle &= \int d\mathbf{x} \frac{\partial \rho(\mathbf{x}, t)}{\partial t} f(\mathbf{x}) \\ &= \int d\mathbf{x} H \rho(\mathbf{x}, t) f(\mathbf{x}) \\ &= \int d\mathbf{x} \rho(\mathbf{x}, t) H^\dagger f(\mathbf{x}) = \langle H^\dagger f(\mathbf{x}(t)) \rangle, \end{aligned} \quad (\text{A.5})$$

where $\rho(\mathbf{x}, t)$ is the probability density for the process \mathbf{x} at time t . The operator H is the forward Fokker–Planck operator and H^\dagger is its adjoint commonly called the backward Fokker–Planck

operator. We now write using the Stratonovich prescription for white noise in stochastic calculus (where normal differentiation applies) to give

$$\begin{aligned} \left\langle \frac{df(\mathbf{x}(t))}{dt} \right\rangle &= \left\langle \frac{\partial}{\partial x_i} f(\mathbf{x}(t)) \frac{d\mathbf{x}_i(t)}{dt} \right\rangle \\ &= T_1 + T_2 + T_3. \end{aligned} \tag{A.6}$$

The first term is

$$T_1 = \sqrt{2\kappa_x} \langle \nabla_i f(\mathbf{x}(t)) \eta_{x_i} \rangle, \tag{A.7}$$

which can be evaluated via Novikov's theorem as

$$T_1 = \sqrt{2\kappa_x} \left\langle \frac{\partial^2 f}{\partial x_i \partial x_j} \int_0^t ds \frac{\delta x_j(t)}{\delta \eta_{x_i}(s)} \langle \eta_{x_i}(s) \eta_{x_i}(t) \rangle \right\rangle, \tag{A.8}$$

which is true for any Gaussian noise. Now for a white noise correlation, if we work with a symmetrized Dirac delta function corresponding to the Stratonovich prescription, the above integral picks up half the weight of the delta function. And we obtain

$$T_1 = \sqrt{\frac{\kappa_x}{2}} \left\langle \frac{\partial^2 f}{\partial x_i \partial x_j} \frac{\delta x_j(t)}{\delta \eta_{x_i}(s)} \Big|_{s=t} \right\rangle. \tag{A.9}$$

The functional derivatives required in the above calculations can be evaluated using a path integral formalism as in [20]. However they can also be obtained directly from the stochastic equation as follows. Consider a general differential equation of the form

$$\frac{dx_i}{dt} = W_i + B_{ij} \xi_j. \tag{A.10}$$

In order to compute $\frac{\delta x_i(t)}{\delta \xi_j(s)}$ one can define the process

$$\frac{dx_i^\epsilon}{dt} = W_i + B_{ij} (\xi_j + \epsilon_j \delta(t - s)). \tag{A.11}$$

Now from one of the standard definitions of the functional integral we have

$$\frac{\delta x_i(t)}{\delta \xi_j(s)} = \frac{\partial x_i^\epsilon(t)}{\partial \epsilon_j} \Big|_{\epsilon=0}. \tag{A.12}$$

Integration of equation (A.11) in an infinitesimal interval about $t = s$ yields

$$x^\epsilon(t^+) = x(t^-) + B_{ij} \epsilon_j, \tag{A.13}$$

as long as the W_i do not depend on the derivative of x . We see that in the case considered here the W_i will be continuous at $s = t$ and thus give no contribution to the functional derivative. This thus yields

$$\frac{\delta x_i(t)}{\delta \xi_j(s)} \Big|_{s=t} = B_{ij}. \tag{A.14}$$

Using this result we obtain

$$\frac{\delta x_j(t)}{\delta \eta_{x_i}(s)} \Big|_{s=t} = \sqrt{2\kappa_x} \delta_{ij}, \tag{A.15}$$

which upon substitution into equation (A.9) gives

$$T_1 = \kappa_x \left\langle \frac{\partial^2}{\partial x_i \partial x_i} f(\mathbf{x}_t) \right\rangle. \tag{A.16}$$

This is the familiar Laplacian form arising for standard white noise. The second term T_2 is given by

$$T_2 = \sqrt{2\kappa_x\chi} \sqrt{\frac{\kappa_x}{\kappa_p}} \left\langle \frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \zeta_j(t) \right\rangle. \quad (\text{A.17})$$

Once again using Novikov's theorem we find

$$T_2 = \sqrt{2\kappa_x\chi} \sqrt{\frac{\kappa_x}{\kappa_p}} \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) \int_0^t ds \frac{\delta x_k(t)}{\delta \zeta_i(s)} \langle \zeta_j(t) \zeta_i(s) \rangle. \quad (\text{A.18})$$

The correlation function of the Gaussian field ζ is easily computed and is given for $t > s$ by

$$\langle \zeta_i(t) \zeta_j(s) \rangle = \alpha^2 \int_0^s du \exp(-\alpha(t + s - 2u)t), \quad (\text{A.19})$$

where $\alpha = \kappa_p \beta / \chi$. At large t and s this becomes

$$\langle \zeta_i(t) \zeta_j(s) \rangle = \frac{\alpha \delta_{ij}}{2} \exp(-\alpha(t - s)). \quad (\text{A.20})$$

We now consider the action of this correlation function as an operator on an arbitrary function $g(s)$ via the following operator expansion

$$\int_0^t ds \exp(-\alpha s) g(t - s) = \frac{1}{\alpha} \left[g(t) - \frac{1}{\alpha} \frac{d}{dt} g(t) + O\left(\frac{1}{\alpha^2}\right) \right] \quad (\text{A.21})$$

and to leading order in $1/\alpha$ we thus obtain

$$T_2 = \sqrt{2\kappa_x\chi} \sqrt{\frac{\kappa_x}{\kappa_p}} \left\langle \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) \frac{\delta x_k(t)}{\delta \zeta_j(s)} \Big|_{t=s} \right\rangle. \quad (\text{A.22})$$

Now repeating the argument leading to equation (A.15) we find that

$$\frac{\delta x_k(t)}{\delta \zeta_j(s)} \Big|_{t=s} = \sqrt{\frac{2}{\kappa_p}} \chi \kappa_x \frac{\partial E_j}{\partial x_k} \quad (\text{A.23})$$

and thus

$$T_2 = \kappa_x \chi^2 \left(\frac{\kappa_x}{\kappa_p} \right) \left\langle \frac{\partial E_j}{\partial x_k} \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) \right\rangle. \quad (\text{A.24})$$

One thus sees that the noise ζ is to leading order white noise interpreted via the Stratonovich prescription. The final term to evaluate is

$$T_3 = \beta^2 \kappa_x \kappa_p \left\langle \frac{\partial f(\mathbf{x}(t))}{\partial x_i} \frac{\partial E_j(\mathbf{x}(t))}{\partial x_i} \int_0^t ds \exp(-\alpha(t - s)) E_j(\mathbf{x}(s)) \right\rangle \quad (\text{A.25})$$

and so one needs to compute terms of the form

$$I = \left\langle A(\mathbf{x}(t)) \int_0^t ds \exp(-\alpha(t - s)) B(\mathbf{x}(s)) \right\rangle, \quad (\text{A.26})$$

bearing in mind that α is large. Now if $\rho(\mathbf{x}, t)$ is the probability density for the position \mathbf{x} and H the effective forward Fokker–Planck operator, we may write the above as

$$I = \int d\mathbf{x} B(\mathbf{x}) \rho(\mathbf{x}, s) \exp(-(t - s)(\alpha - H^\dagger)) A(\mathbf{x}). \quad (\text{A.27})$$

The density ρ obeys the Fokker–Planck equation

$$\frac{\partial \rho}{\partial t} = H\rho. \quad (\text{A.28})$$

The integration over s can be evaluated by integrating by parts, we have

$$\int_0^t ds \rho(\mathbf{x}, s) \exp(-(t-s)(\alpha - H^\dagger)) = \rho(\mathbf{x}, t) [1 - \exp(-t(\alpha - H^\dagger))] (\alpha - H^\dagger)^{-1} - \int_0^\infty ds \frac{\partial \rho(\mathbf{x}, s)}{\partial s} \exp(-(t-s)(\alpha - H^\dagger)) (\alpha - H^\dagger)^{-1}. \quad (\text{A.29})$$

Now because the eigenvalues of H must be negative or zero, we may neglect the second term in the square brackets on the right-hand side above. Another integration by parts yields

$$\int_0^t ds \rho(\mathbf{x}, s) \exp(-(t-s)(\alpha - H^\dagger)) = \rho(\mathbf{x}, t) (\alpha - H^\dagger)^{-1} - [H\rho(\mathbf{x}, t)] (\alpha - H^\dagger)^{-2}, \quad (\text{A.30})$$

where we have used equation (A.28) in the second term of the right-hand side and the operator H in this term only acts on ρ inside the square bracket. All other operators act on the right and we can now expand in powers of $1/\alpha$ to obtain

$$\int_0^t ds B(\mathbf{x}) \rho(\mathbf{x}, s) \exp(-(t-s)(\alpha - H^\dagger)) A(\mathbf{x}) = \rho(\mathbf{x}, t) \left[\frac{A(\mathbf{x})B(\mathbf{x})}{\alpha} + B(\mathbf{x}) \frac{H^\dagger}{\alpha^2} A(\mathbf{x}) - \frac{H^\dagger}{\alpha^2} A(\mathbf{x})B(\mathbf{x}) \right]. \quad (\text{A.31})$$

Now putting all these together yields

$$\begin{aligned} \langle H^\dagger f(\mathbf{x}) \rangle &= \kappa_x \left\langle \frac{\partial^2}{\partial x_i \partial x_i} f(\mathbf{x}_t) \right\rangle \\ &+ \kappa_x \left(\frac{\kappa_x}{\kappa_p} \right) \chi^2 \left\langle \frac{\partial E_j}{\partial x_k} \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) \right\rangle \\ &+ \kappa_x \beta \chi \left\langle \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} E_j + \frac{\chi}{\kappa_p \beta} E_j H^\dagger \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} - \frac{\chi}{\kappa_p \beta} H^\dagger \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} E_j \right\rangle. \end{aligned} \quad (\text{A.32})$$

This can be written in the form

$$\begin{aligned} \langle H^\dagger f(\mathbf{x}) \rangle &= \langle H_0^\dagger f(\mathbf{x}) \rangle + \chi^2 \frac{\kappa_x}{\kappa_p} \left[\left\langle \kappa_x \frac{\partial E_j}{\partial x_k} \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) \right. \right. \\ &\left. \left. + E_j H^\dagger \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} - H^\dagger \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} E_j \right\rangle \right] + O\left(\left(\frac{\kappa_x}{\kappa_p}\right)^2\right), \end{aligned} \quad (\text{A.33})$$

where

$$H_0^\dagger f = \kappa_x \left[\frac{\partial^2 f}{\partial x_i \partial x_i} + \beta \chi \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} E_j \right]. \quad (\text{A.34})$$

This is the only term remaining strictly in the limit $\kappa_p \rightarrow \infty$ and corresponds exactly to a Langevin particle in an effective potential V given by equation (11). Now keeping the first term of $O(\kappa_x/\kappa_p)$ we may write equation (A.33) as

$$\begin{aligned} \langle H^\dagger f(\mathbf{x}) \rangle &= \langle H_0^\dagger f(\mathbf{x}) \rangle \\ &+ \chi^2 \frac{\kappa_x}{\kappa_p} \left[\left\langle \kappa_x \frac{\partial E_j}{\partial x_k} \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) + E_j H_0^\dagger \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} - H_0^\dagger \frac{\partial f}{\partial x_i} \frac{\partial E_j}{\partial x_i} E_j \right\rangle \right] \\ &= \langle H_0^\dagger f(\mathbf{x}) \rangle - \kappa_x \frac{\kappa_x \chi^2}{\kappa_p} \left\langle \frac{\partial}{\partial x_k} \left(\frac{\partial E_j}{\partial x_k} \frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} \right) + \beta \chi \frac{\partial E_j}{\partial x_k} \frac{\partial E_j}{\partial x_i} \frac{\partial f}{\partial x_i} E_l \frac{\partial E_l}{\partial x_k} \right\rangle. \end{aligned} \quad (\text{A.35})$$

Finally the above may be written as

$$\langle H^\dagger f(\mathbf{x}) \rangle = \left\langle \frac{\partial}{\partial x_k} \left(\kappa_{ki} \frac{\partial f}{\partial x_i} \right) - \beta \kappa_{ki} \frac{\partial V}{\partial x_k} \frac{\partial f}{\partial x_i} \right\rangle, \quad (\text{A.36})$$

with κ_{ij} being the spatially varying and anisotropic diffusivity tensor given by (13) and V the potential defined by (7).

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