Bead-rod-spring models in random flows

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Bead-rod-spring models are the foundation of the kinetic theory of polymer solutions. We derive the
diffusion equation for the probability density function of the configuration of a general bead-
rod-spring model in short-correlated Gaussian random flows. Under isotropic conditions, we solve
this equation analytically for the elastic rhombus model introduced by Curtiss, Bird, and Hassager
[Adv. Chem. Phys. 35, 31 (1976)].

The study of polymer solutions generally requires a
coarse-grained description of a polymer molecule. A suc-
cessful and well-established approach consists in using
bead-rod-spring models, where a polymer is described
as a sequence of beads connected by rigid or elastic
links [14]. By selecting the number of beads and the
nature of the links, it is possible to build flexible, semi-
flexible, or rigid molecules with various internal struc-
tures. bead-rod-spring models play a central role across
different fields, including rheology, non-Newtonian fluid
mechanics, chemical physics, soft matter [1 5]. Analy-
cetical solutions of these models represent an essential
step towards the derivation of constitutive equations and
hence the prediction of the non-Newtonian properties of
polymeric fluids [1 3 5]. However, in spite of their con-
tceptual simplicity, the internal dynamics of bead-rod-
spring models may be exceedingly complex. For this
reason bead-rod-spring models have been solved analyti-
cally only in simplified settings. In the case of laminar
flows, analytical results are restricted to linear velocity
fields with elementary time dependence, namely steady,
steady, or oscillatory extensional and shear flows [1 3 5].
In the case of randomly fluctuating flows, exact solu-
tions are only available for dumbbells, which are sim-
ply composed of two beads and a single elastic or rigid
link [7 14]. Nevertheless, in recent years there has been a
growing interest in the Lagrangian dynamics of complex-
shaped objects in turbulent flows, such as elastic poly-
mers [13 19], triaxial ellipsoids [20], flexible fibers [21],
crosses and jacks [22], isotropic helicoids and four-bead
particles [23], chiral dipoles [24]. It is therefore impor-
tant to advance the analytical tools needed for the study
of this problem. Here we first derive the diffusion equa-
tion for the probability distribution function of the config-
uration of a general bead-rod-spring polymer in a Gaussian
random flow with short correlation time. Short-correlated
stochastic fields have been widely employed in the theo-
retical study of turbulent flows and have yielded funda-
mental results on passive-scalar mixing and the turbu-

lent dynamo [25]; moreover, they have been used to pre-
dict the coil–stretch transition of polymers in turbulent
flows [9] and the associated critical slowing down [14].
By using the aforementioned diffusion equation, we then
analytically calculate the stationary configuration of the
elastic rhombus model in an isotropic random flow. The
rhombus model was introduced by Curtiss, Bird, and
Hassager [20] and is a prototype of a finitely extensible
multibead polymer that includes both elastic and rigid
internal links.

We start by briefly recalling the diffusion equation for
the probability density function (PDF) of the config-
uration of a bead-rod-spring polymer following Refs. [1 3].
Consider N spherical beads with mass \( m_\mu \), \( \mu = 1, \ldots, N \). Let \( \mathbf{x}_\mu \) denote the position vector of the \( \mu \)th bead with
respect to a space-fixed coordinate system. The posi-
tion of the center of mass of the polymer is
\[
\mathbf{r}_c = \frac{\sum_\mu m_\mu \mathbf{x}_\mu}{\sum_\mu m_\mu},
\]
and the position vector of the \( \mu \)th bead referred to the center of mass is
\[
\mathbf{r}_\mu = \mathbf{r}_c - \mathbf{x}_\mu.
\]
The polymer is immersed in a Newtonian fluid, whose
motion is described by the incompressible velocity field
\( \mathbf{u}(\mathbf{x}, t) \). The velocity gradient, \( \kappa = \nabla \mathbf{u}, \kappa_\mu = \partial u_\mu/\partial x_\mu \),
is assumed to be uniform over the length of the poly-
mer. If the flow is turbulent, this assumption means that
the size of the polymer is much smaller than the viscous-
dissipation scale. The force of the flow on bead \( \mu \) is given
by Stokes’s law with drag coefficient \( \zeta_\mu \); the inertia of the
beads is disregarded. Furthermore, the concentration of
the solution is sufficiently small for polymer–polymer hy-
drodynamic interactions to be negligible, and the flow
is unperturbed by the presence of polymers.

Assume that the beads are subject to \( D' \) rigidity con-
straints. Then, the number of degrees of freedom of the
polymer in the frame of reference of the center of mass is
\( D = d(N - 1) - D' \), where \( d \) is the dimension of the flow.
It is therefore convenient to specify the configuration of
the polymer in terms of \( D \) coordinates \( \mathbf{q} = (q^1, \ldots, q^D) \),
which describe its degrees of freedom. The statistics of the
coordinates \( \mathbf{q} \) is given by the PDF \( \psi(\mathbf{q}; t) \).

We define the tensors \( \zeta_{\mu\nu} \) implicitly from the equation:
\[
\sum_\mu \zeta_{\mu\nu} : (\delta_{\nu\rho} \delta_{\rho\lambda} - 1) \mathbf{I} + \Omega_{\mu\nu} \mathbf{I} = \delta_{\mu\nu} \mathbf{I},
\]
where \( \delta_{\mu\nu} \) is the Kro-

necker delta, \( \mathbf{I} \) is the identity matrix, and the tensors \( \Omega_{\mu\nu} \) describe the hydrodynamic interactions between the \( \mu \)th
and the \( \nu \)th bead (in the simplest approximation \( \Omega_{\mu\nu} = \mathbf{0} \) is the
Oseen tensor). Define also the tensors \( \Lambda_{\nu} = \mathbf{Z}^{-1} \sum_\mu \zeta_{\mu\nu}, \Lambda_{\mu} = \mathbf{Z}^{-1} \sum_\mu \zeta_{\mu\nu}, \) and \( \zeta_{\nu\mu} = \zeta_{\mu\nu} - \Lambda_{\mu}^T \cdot \mathbf{Z} \cdot \Lambda_{\nu} \).
Finally, \( f_{\mu\nu} \) is the force exerted by the \( \nu \)th bead over the \( \mu \)th one
through the springs and \( f_{\mu} \) is the external force on bead
\( \mu \) (which is assumed to be independent of \( \mathbf{r}_c \)). Then,
\( \psi(\mathbf{q}; t) \) satisfies the diffusion equation [1 3] (summation
over repeated indices is understood throughout):
\[
\frac{\partial \psi}{\partial t} = - \frac{\partial}{\partial q^j} \left\{ G^{ij} \left[ (M^{kij} K^{kl} - F^j + \tilde{\sigma}^j) \psi - KT \sqrt{h} \frac{\partial}{\partial q^j} \left( \frac{\psi}{\sqrt{h}} \right) \right] \right\}, \tag{1}
\]
where \( K \) is the Boltzmann constant, \( T \) is temperature, and \( h = \det(H) \), and \( \tilde{G} = \tilde{H}^{-1} \) with:
\[
H^{ij} = m_{ij} \frac{\partial \tilde{r}_i^k}{\partial q^j} \frac{\partial \tilde{r}_j^k}{\partial q^i}, \quad \tilde{H}^{ij} = \tilde{\zeta}_{ij} \frac{\partial \tilde{r}_i^k}{\partial q^j} \frac{\partial \tilde{r}_j^k}{\partial q^i}.
\]
The stationary solution of Eq. (1) can be calculated exactly when hydrodynamic bead-bead interactions are negligible (\( \Omega_{\mu\nu} = 0 \) for all \( \mu, \nu = 1, \ldots, N \)) or equilibrium averaged (\( \Omega_{\mu\nu} \) is replaced with its average value at equilibrium) and the velocity gradient is time-independent and symmetric (\( \kappa = \kappa^T \)) \[28\]. For other flows, Bird et al. \[1\] note that the analytical solution of Eq. (1) is in general a formidable problem.

Let us consider the case in which the velocity gradient fluctuates randomly in time, as in turbulent flows. Assume that \( \kappa(t) \) is a delta-correlated-in-time \((d \times d)\)-dimensional Gaussian stochastic process with zero mean and correlation: \( \langle \kappa^{ij}(t) \kappa^{mn}(t') \rangle = \delta^{jm} \delta^{in} \delta(t-t') \), where the specific form of the tensor \( \kappa \) depends on the statistical symmetries of the flow. Equation (1) is now stochastic and describes the evolution of \( \psi(q; t) \) for a given realization of the flow; \( \kappa(t) \) is a multiplicative noise and is interpreted in the Stratonovich sense. Under this assumption on the velocity gradient, the stochastic differential equation associated with Eq. (1) is (see Ref. \[28\]):
\[
dq^j = A^i dt + B^{ij} dq^i + C^{ijkl} dt^{kl}(t), \tag{4}
\]
where \( W(t) \) is \( D \)-dimensional Brownian motion and \( \Gamma(t) \) is such that \( \kappa(t) = \Gamma(t)/dt \), i.e. \( \Gamma(t) \) is a Gaussian process with \( \langle \Gamma^{kl}(t) \Gamma^{mn}(t') \rangle = K^{klmn} \delta(t-t') \) \[27\]. The symbol \( \circ \) indicates that the stochastic differential equation is interpreted in the Stratonovich sense. The coefficients are
\[
A^i = \tilde{G}^{ij}(F^j + \tilde{\sigma}^j) + KT \sqrt{h} \frac{\partial}{\partial q^j} \left( \frac{\tilde{\sigma}^{\mu} \beta^{\nu}}{\sqrt{h}} \right), \tag{5}
\]
\[
B^{ij} = \sqrt{2KT} \beta^{ij}, \quad C^{ijkl} = \tilde{G}^{ij} M^{kl}. \tag{6}
\]
In the above equations, \( \beta \) is such that \( \beta \beta^T = \tilde{G} \) (it is assumed that \( G \) is positive definite—this condition is easily verified when the masses and the drag coefficients are the same for all beads). The Itô form of Eq. (1) is (appendix A):
\[
dq^j = \left( A^i + \frac{1}{2} B^{il} \frac{\partial B^{ia}}{\partial q^j} + \frac{1}{2} K^{klmn} C^{ijmn} \frac{\partial C^{ikl}}{\partial q^j} \right) dt + B^{ij} dW^j(t) + C^{ijkl} dt^{kl}(t). \tag{7}
\]
We denote by \( p(q; t) \) the PDF of the configuration of the polymer with respect to the realizations both of the velocity gradient and of thermal noise. The diffusion equation corresponding to Eq. (7) is (appendix A):
\[
\frac{\partial p}{\partial t} = - \frac{\partial}{\partial q^j} \left[ \left( A^i + \frac{1}{2} B^{il} \frac{\partial B^{ia}}{\partial q^j} + \frac{1}{2} K^{klmn} C^{ijmn} \frac{\partial C^{ikl}}{\partial q^j} \right) p \right] + KT \frac{\partial^2}{\partial q^j \partial q^k} \tilde{G}^{ij} p + \frac{K^{klmn}}{2} \frac{\partial^2}{\partial q^j \partial q^k \partial q^l \partial q^m} \left( C^{ijkl} \right) p. \tag{8}
\]
Rearranging the terms in Eq. (8), we obtain:
\[
\frac{\partial p}{\partial t} = \frac{\partial}{\partial q^j} \left\{ 1 \frac{K^{klmn} \tilde{G}^{ia} M^{ikl}}{2} \frac{\partial}{\partial q^j} \left( \sqrt{h} \right) \right\} + \tilde{G}^{ij} \left[ - (F^j + \tilde{\sigma}^j) p + KT \sqrt{h} \frac{\partial}{\partial q^j} \left( \frac{p}{\sqrt{h}} \right) \right]. \tag{9}
\]
Equation (9) determines the evolution of the PDF of the configuration of a general bead-rod-spring model in a short-correlated Gaussian flow. Note that Eq. (9) can also be derived by applying Gaussian integration by parts \[29\] to Eq. (1).

We now consider a bead-rod-spring model for which the stationary solution of Eq. (9) can be calculated exactly. The elastic plane rhombus model was introduced by Curtiss, Bird, and Hassager \[26\]. It describes a finitely extensible polymer and consists of four coplanar identical beads connected by four rods and of an elastic spring between two opposing beads (Fig. 1). The angle \( 0 \leq \sigma \leq \pi/2 \) between the spring and one of the rods describes the deformation of the rhombus. The spring is at rest if the rods are perpendicular to each other. If \( \sigma \neq \pi/4 \), the spring stretches or compresses the rhombus back to its equilibrium; the force that it exerts on the beads is given by the harmonic potential \( \phi(q) = A(\sqrt{2} \cos \sigma - 1)^2/2 \). Let \( m_\mu = m, \mu = \zeta \) for all \( \mu = 1, \ldots, 4 \) and \( \ell \) be the length of the rods. In addition, hydrodynamical bead-bead interactions are disregarded (\( \Omega_{\mu\nu} = 0 \)), and no external forces act on the polymer (\( f_\mu = 0 \)). Under these assumptions, we have \( \zeta_{\mu\nu} = \zeta_{\delta \mu \ell}, \tilde{\sigma} = 0 \), and
\[
M^{ikl} = \zeta_{\mu\nu} \frac{\partial \tilde{r}_i^k}{\partial q^j} \frac{\partial \tilde{r}_j^l}{\partial q^k}, \quad F^j = - \frac{\partial \phi}{\partial q^j}, \quad \tilde{H}^{ij} = \zeta_{\mu\nu} \frac{\partial \tilde{r}_i^k}{\partial q^j} \frac{\partial \tilde{r}_j^l}{\partial q^k}. \tag{10}
\]

The contribution of the rhombic particles to the viscoelastic properties of a solution, such as the normal stress coefficient and the viscosity, have been calculated exactly \[26\]. In particular, the addition of \( n \) rhombuses increases the viscosity by \( 3nC^2 r^2 \). This result also holds for other variants of the rhombus model, namely the freely-jointed and the rigid models. The normal stress coefficient of the polymer solution, by contrast, varies according to the flexibility of the rhombus. A fully elastic
rhombus model has been used to investigate the motion of deformable active particles [30]. The rhombus model could also be used to examine how deformability influences the alignment and orientation statistics of microscopic particles in turbulent flows [31].

If the random flow is incompressible and statistically invariant under rotations and reflections, the components of $K$ take the form: $K_{ijkl} = 2\lambda[d(1)d_{ijkl} - \delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk}]/[d(d - 1)]$, where $\lambda$ is the maximum Lyapunov exponent of the flow [25]. Denoting $G = \zeta G$, we write Eq. (8) as a Fokker–Planck equation [28]:

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial q^i}(V^i p) + \frac{1}{2} \frac{\partial^2}{\partial q^i \partial q^j}(D^{ij} p),$$

(11)

where the drift and diffusion coefficients are

$$V^i = \frac{1}{2} K^{mn} G^{a^i b^i \mu} \frac{\partial r^a_{\mu}}{\partial q^m} \frac{\partial q^a}{\partial q^m} \left( G^{a^i b^i \mu} \frac{\partial r^a_{\mu}}{\partial q^m} \right) - \frac{G^{ij}}{\zeta} \frac{\partial \phi}{\partial q^j} + KT \frac{1}{\sqrt{\zeta \sqrt{h}}} \frac{\partial^2}{\partial q^i \partial q^j} \left( G^{ij} \sqrt{h} \right),$$

(12)

and

$$D^{ij} = K^{mn} G^{a^i b^i \mu} \frac{\partial r^a_{\mu}}{\partial q^m} G^{b^i c^i \nu} \frac{\partial r^c_{\nu}}{\partial q^m} + 2G^{ij} KT \frac{1}{\zeta}.$$

(13)

In the case of a two-dimensional flow ($d = 2$), the rhombus may be described by $q = (\theta, \sigma)$, where $\theta$ gives the orientation of $x_3 - x_1$ with respect to the horizontal axis. The vectors $r_\mu$ can be expressed as:

$$r_1 = \ell (-\cos \theta \cos \sigma, -\sin \theta \cos \sigma) = -r_3,$$

(14)

$$r_2 = \ell (-\sin \theta \sin \sigma, \cos \theta \sin \sigma) = -r_4.$$

(15)

We also have $G^{ij} = \delta_{ij}/2\ell^2$ and $h = 4\ell^2$. After time is rescaled by the characteristic time scale of the restoring potential $\tau_p = \zeta \ell^2/A$ and Eqs. (14), (15) are replaced into Eqs. (12), (13), the drift and diffusion coefficients in Eq. (11) become:

$$V^\sigma = -\left( \sqrt{2} - 2 \cos \sigma \right) \sin \sigma / 2,$$

(16)

$$D^{\phi \theta} = Z^{-1} + Wi (\cos 4\sigma)/2,$$

(17)

$$D^{\sigma \sigma} = Z^{-1} + Wi (1 - \cos 4\sigma)/2,$$

(18)

$$V^\theta = D^{\sigma \sigma} = D^{\phi \phi} = 0,$$

(19)

where $Z = A/KT$ is the stiffness parameter and the Weissenberg number $Wi = \lambda \tau_p$ measures the relative strength of the flow to that of the restoring potential $\phi(\sigma)$. The fact that all the coefficients are independent of $\theta$ reflects the isotropy of the flow and implies that the long-time PDF of the configuration is a function of $\sigma$ alone. Given reflecting boundary conditions at $\sigma = 0$ and $\sigma = \pi/2$, the stationary PDF $p_{st}(\sigma)$ can be analytically calculated to be [28]

$$p_{st}(\sigma) \propto \frac{1}{D^{\sigma \sigma}} \exp \left( 2 \int_0^\sigma \frac{V^\sigma(\omega)}{D^{\sigma \sigma}(\omega)} d\omega \right).$$

(20)

We can evaluate the integral in Eq. (20) by using Eqs. (3.3.23) and (4.6.22) of Ref. [32], whence the explicit form of the PDF of $\sigma$:

$$p_{st}(\sigma) \propto \frac{1}{D^{\sigma \sigma}} \left[ \frac{C_2^2 - C_1^2}{C_2^2 + C_1^2} \right]^{Z/AC_1} \exp \left\{ \frac{Z \sqrt{W_i Z}}{2C_1} \left[ \arctanh \left( C_2/C_+ \right) + \arctan \left( C_2/C_- \right) \right] \right\},$$

(21)

with $C_+ = \sqrt{2W_i Z \cos \sigma}$, $C_1 = \sqrt{W_i Z (W_i Z + 1)}$, and $C_\pm = \sqrt{C_1 \pm W_i Z}$. Figure 2 illustrates the graph of $p_{st}(\sigma)$ for $Z = 1$ and different values of $Wi$. The probability of the rhombus being fully stretched ($\sigma = 0$) or fully compressed ($\sigma = \pi/2$) increases with $Wi$, i.e. the rhombus exhibits an almost rod-like configuration when a very strong flow dominates the dynamics. However, the stretched configuration is favored compared to the compressed one, because the restoring force is weaker for $\sigma = 0$ than for $\sigma = \pi/2$.

In a three-dimensional flow, the number of degrees of freedom of the elastic planar rhombus is $D = 4$. We consider $q = (\alpha, \beta, \gamma, \sigma)$, where the first three coordinates are the Euler angles used to define the configuration of the rhombus in a fixed frame of reference. The details on the definition of the Euler angles, as well as the explicit expressions of $G$ and $h$ can be found in Refs. [11], [20]. Note that our $G$ differs from that of Ref. [20] by a factor.
of $m$. The PDF $p(q)$ of the configuration again satisfies Eq. (11), where $V^i$ and $D^ij$ are given in appendix B. In view of the isotropy of the flow, we assume that the stationary PDF of the configuration takes the form $p_{st}(q) = \tilde{p}(\sigma) \sin \beta \sin 2\sigma$, where the factor $\sin \beta \sin 2\sigma$ is proportional to the Jacobian of the coordinate transformation from $r_p$ to $q$. Substituting $p_{st}(q)$ into Eq. (11) results into a Fokker–Planck equation in the variable $\sigma$ alone:

$$0 = \frac{\partial p_{st}(q)}{\partial \sigma} = -\frac{\partial}{\partial \sigma} (V^\sigma p_{st}) + \frac{1}{2} \frac{\partial^2}{\partial \sigma^2} (D^{\sigma \sigma} p_{st}),$$

where $s = t/\tau_p$, $V^\sigma = \cot 2\sigma/Z - (\sqrt{2} - 2 \cos \sigma) \sin \sigma/2$ and $D^{\sigma \sigma} = Z^{-1} + Wi (1 - \cos 4\sigma)/4$. The partial derivatives with respect to the Euler angles indeed cancel each other. Under reflecting boundary conditions at $\sigma = 0$ and $\sigma = \pi/2$, the solution of Eq. (22) takes the form given in Eq. (20) with modified expressions for $V^\sigma$ and $D^{\sigma \sigma}$. Invoking again Eqs. (3.3.23) and (4.6.22) of Ref. [32], we derive the exact form of the stationary PDF of $\sigma$ in three dimensions:

$$\tilde{p}(\sigma) \propto \frac{1}{D^{\sigma \sigma} \sqrt{Wi Z \sin^2 2\sigma + 2}} \left[ \frac{C^2_\sigma - C^2_+}{C^2_\sigma + C^2_-} \right]^{Z/4C_1} \times \exp \left\{ \frac{Z \sqrt{Wi Z/2}}{2C_1} \left[ \arctanh \left( \frac{C_\sigma}{C_+} \right) + \arctan \left( \frac{C_\sigma}{C_-} \right) \right] \right\}$$

with $C_\sigma = \sqrt{Wi Z \cos \sigma}$, $C_1 = \sqrt{Wi Z (Wi Z + 2)/2}$, and $C_\pm = \sqrt{C_1 \pm Wi Z/2}$. The graph of $\tilde{p}(\sigma)$ is shown in Fig. 3. The statistics of the internal angle $\sigma$ is qualitatively the same for $d = 2$ and $d = 3$ (the curves in Figs. 2 and 3 indeed differ only slightly for the same Wi). This behavior is attributed to the fact that the rhombus can only deform in the plane to which it belongs and cannot undergo three-dimensional deformations, which makes its dynamics weakly sensitive to the dimension of the flow.

Bead-rod-spring models are the foundation of the kinetic theory of polymer solutions. There is a broad literature on the analytic solutions of these models for laminar flows. In the case of fluctuating flows, such as turbulent flows, analytical results are restricted to dumbbells. We have given a general description of bead-rod-spring models in short-correlated random flows. In addition, we have exactly solved the elastic rhombus model under isotropic conditions. To the best of our knowledge, this is the first instance of an exact solution of a multibead model that include both elastic and rigid links and is transported by a randomly fluctuating flow. We hope that the tools developed here will stimulate new studies on the dynamics of complex-shaped particles in turbulent flows. The stretching dynamics of bead-spring chains has also received attention in the context of nonequilibrium statistical mechanics [33]; the probability of work and entropy production have been studied for laminar gradient flows [41, 57]. It would be interesting to generalize those studies to the case considered here, where the velocity gradient is a tensorial noise (see, e.g., Ref. [38]).

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Appendix A: Derivation of Eqs. (7) and (8)

The Itô version of Eq. (4) can be derived formally by generalizing the standard transformation rules for stochastic differential equations (see, e.g., Refs. 28, 30) to tensorial Brownian motion. Let us assume that the Itô version is:

$$dq^i(t) = \mathcal{A}^i dt + \mathcal{B}^{ij} dW^j(t) + \mathcal{C}^{ikl} d\Gamma^{kl}(t),$$

(A1)

where the coefficients $\mathcal{A}, \mathcal{B}, \mathcal{C}$ are to be determined. We first write Eq. (4) in integral form:

$$q^i(t) = q^i(t_0) + \int_{t_0}^t \mathcal{A}^i dt' + \int_{t_0}^t \mathcal{B}^{ia} \circ dW^a(t')$$

$$+ \int_{t_0}^t \mathcal{C}^{ikl} \circ d\Gamma^{kl}(t').$$

(A2)

Consider a partition of $[t_0, t]$ into $N$ subintervals $[t_{\tau - 1}, t_{\tau}], \tau = 1, \ldots, N$. The Stratonovich integrals in Eq. (A2) are, by definition:

$$\int_{t_0}^t \mathcal{B}^{ia} \circ dW^a(t') = \lim_{N \to \infty} \sum_{\tau = 1}^N \mathcal{B}^{ia} (q^i_{\tau}, t_{\tau - 1}) \Delta W^a_{\tau},$$

(A3)

$$\int_{t_0}^t \mathcal{C}^{ikl} \circ d\Gamma^{kl}(t') = \lim_{N \to \infty} \sum_{\tau = 1}^N \mathcal{C}^{ikl} (q^i_{\tau}, t_{\tau - 1}) \Delta \Gamma^{kl}_{\tau},$$

(A4)
where the limits are understood in the mean-square, $q^2 = (q_t + q_{t-1})^2/2, q_t = q(t, \tau), \Delta W^a = W^a(t, \tau) - W^a(t, \tau-1)$, and $\Delta \Gamma^a = \Gamma^a(t, \tau) - \Gamma^a(t, \tau-1)$. We also introduce the notations $\Delta t^a = t - t', \Delta q^a = q(t, \tau)$ for the tensor $X$ and set of indices I. Define $\Delta q_{t-1}^a = q_t^a - q_{t-1}^a$, whence $q^2 = q_{t-1}^2 + \Delta q_{t-1}^2/2$. Expanding the coefficients in (A3) and (A4) at $q_{t-1}^a$ yields:

$$B^{ia}(q_{t-1}^a, t-1) = B_{t-1}^{ia} + \frac{\Delta q_{t-1}^a}{2} \frac{\partial B_{t-1}^{ia}}{\partial q^a} + \text{h.o.t.}, \quad (A5)$$

$$C^{ikl}(q_{t-1}^a, t-1) = C_{t-1}^{ikl} + \frac{\Delta q_{t-1}^a}{2} \frac{\partial C_{t-1}^{ikl}}{\partial q^a} + \text{h.o.t.}, \quad (A6)$$

where h.o.t. refers to higher order terms. We now write $\Delta q^j_{t-1}$ according to its Itô discretization:

$$\Delta q^j_{t-1} = \mathbb{X}^j_{t-1} \Delta t + \mathbb{B}^{ja}_{t-1} \Delta W^a + \mathbb{C}^{jmn}_{t-1} \Delta \Gamma^m_{t-1} + \text{h.o.t.} \quad (A7)$$

After substituting Eqs. (A5), (A6), (A7) into Eqs. (A3), (A4) and using the formal rules $\Delta \Gamma^a = \Gamma^a(t, \tau) - \Gamma^a(t, \tau-1)$, we can write Eqs. (A3) and (A4) as:

$$\int_{t_0}^t B^{ia} \circ dW^a(t') = \lim_{N \to \infty} \sum_{\tau=1}^N \left( B^{ia}_{t-1} \Delta W^a_{\tau} + \frac{1}{2} \frac{\partial B^{ia}_{t-1}}{\partial q^a} \Delta t^a \right),$$

$$\int_{t_0}^t C^{ikl} \circ d\Gamma^k(t') = \lim_{N \to \infty} \sum_{\tau=1}^N \left( C^{ikl}_{t-1} \Delta \Gamma^k_{\tau} + \frac{1}{2} \frac{\partial C^{ikl}_{t-1}}{\partial q^a} \Delta \Gamma^k_{\tau} \right).$$

The first terms in the sums yield Itô stochastic integrals, whereas the second terms give ordinary integrals, hence:

$$\int_{t_0}^t B^{ia} \circ dW^a(t') = \int_{t_0}^t B^{ia} \circ dW^a(t') + \int_{t_0}^t \frac{\partial B^{ia}}{\partial q^a} \circ dB_{t-1}^a \circ dW^a, \quad \int_{t_0}^t C^{ikl} \circ d\Gamma^k(t') = \int_{t_0}^t C^{ikl} \circ d\Gamma^k(t') + \int_{t_0}^t \frac{\partial C^{ikl}}{\partial q^a} \circ dB_{t-1}^a \circ d\Gamma^k \circ d\Gamma^k.$$

Therefore, for Eq. (A1) to be equivalent to Eq. (4), the coefficients must satisfy $\mathbb{B} = \mathbb{B}, \mathbb{C} = \mathbb{C}$, and

$$\mathbb{A}^i = A^i + \frac{1}{2} B^{ja} \frac{\partial B^{ia}}{\partial q^a} + \frac{1}{2} K^{iklm} \frac{\partial C^{ikl}}{\partial q^a} \circ dB_{t-1}^a \circ d\Gamma^k \circ d\Gamma^k.$$

We now derive the diffusion equation (5). Let $f(q)$ be a function of $q$. We first generalize Itô’s lemma for a tensorial Brownian motion. By expansion, we have:

$$f(q + \Delta q) - f(q) = \Delta q^i \frac{\partial f}{\partial q^i} + \frac{\Delta q^i \Delta q^j}{2} \frac{\partial^2 f}{\partial q^i \partial q^j} + \text{h.o.t.}$$

By substituting $\Delta q^i$ and $\Delta q^j$ from Eq. (A1) and using the formal rules as above, we obtain:

$$\frac{df}{dt} = \left[ A^i + \mathbb{B}^{ia} \frac{dW^a(t)}{dt} + \mathbb{C}^{ikl} \frac{d\Gamma^k(t)}{dt} + \frac{1}{2} \frac{\partial f}{\partial q^j} \frac{\partial^2 f}{\partial q^i \partial q^j} \right] \partial q^i + \frac{1}{2} \frac{\partial f}{\partial q^j} \frac{\partial^2 f}{\partial q^i \partial q^j}.$$

By taking the average over the noises and by using the properties of the Itô integral, we have:

$$\frac{1}{\sqrt{5}} \left[ f_{t}(\frac{df}{dt}) = \int f \left( \frac{\partial p}{\partial t} \right) dq, \right.$$\n
$$\left. = \int f \left( \frac{\partial f}{\partial q^j} \frac{\partial^2 f}{\partial q^i \partial q^j} + \frac{1}{2} \frac{\partial f}{\partial q^j} \frac{\partial^2 f}{\partial q^i \partial q^j} \right) dq. \right]$$

Integrating the right-hand side by parts gives:

$$\int f \left( \frac{\partial f}{\partial q^j} \right) dq = \int f \left( \frac{\partial f}{\partial q^j} \right) dq + \frac{1}{2} \frac{\partial f}{\partial q^j} \frac{\partial^2 f}{\partial q^i \partial q^j} \left( \mathbb{B}^{ia} \mathbb{B}^{ja} + \mathbb{C}^{ikl} \mathbb{C}^{imn} \right) \frac{\partial^2 f}{\partial q^i \partial q^j}.$$
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[26] Equation (4) may also be written as: $dq_i = A_i dt + Q_{ij} \circ d\eta_j(t)$, where $\eta$ is $D$-dimensional Brownian motion and $(QQ^\top)_{ij} = B_{ia}B_{ja} + K_{klmn}C_{ikl}C_{jmn}$. The thermal and velocity fluctuations would thus be merged into a single noise and the prefactor $Q_{ij}$ would contain the information on the correlations of the random medium.
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