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Advective-diffusive motion on large scales from small-scale dynamics with an internal symmetry

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We consider coupled diffusions in n-dimensional space and on a compact manifold and the resulting effective advective-diffusive motion on large scales in space. The effective drift (advection) and effective diffusion are determined as a solvability conditions in a multiscale analysis. As an example, we consider coupled diffusions in three-dimensional space and on the group manifold SO(3) of proper rotations, generalizing results obtained by H. Brenner [J. Colloid Interface Sci. **80**, 548 (1981)]. We show in detail how the analysis can be conveniently carried out using local charts and invariance arguments. As a further example, we consider coupled diffusions in two-dimensional complex space and on the group manifold SU(2). We show that although the local operators may be the same as for SO(3), due to the global nature of the solvability conditions the resulting diffusion will differ and generally be more isotropic.

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I. INTRODUCTION

The transition from the microscopic to the macroscopic is the central problem in statistical physics [1]. Posed as early as the 19th century, it can be understood as the emergence of qualitatively different phenomena on larger scales from averaging of (typically simpler) phenomena on smaller scales, cf. Refs. [2–4]. Analogous considerations were later extended to hydrodynamics [5] and more general systems of ordinary or partial differential equations and are today usually referred to as homogenization [6] or as multiscale methods [7].

In this paper we consider effective diffusion on large scales from averaging motion involving additional degrees of freedom on small scales. Our setting is mesoscopic physics where the small scale motion is understood as an overdamped dynamics with given transport coefficients and where the large-scale motion is described by other, effective, transport coefficients. As will be described in detail below we thus apply the multiscale method to the analysis of overdamped Fokker-Planck equations (FPE) where we start with an FPE on configuration space and an internal symmetry and end up with an FPE on configuration space only. The effective transport coefficients on large scales are computed as averages over the small scales.

In a recent joint work with Bo, Dias, and Eichhorn, we considered the instance of the problem where the configuration space is ordinary three-dimensional space and the internal symmetry the group of rotations SO(3) [8]. We were thus able to recover results obtained by H. Brenner in the early 1980s [9]. The most striking of these results is a contribution to the effective diffusivity which is inversely proportional to $k_B T$ and which depends quadratically on the applied force field. As stressed already by Brenner this effect should completely dominate the diffusion of, e.g., nonspherical micron-sized particles settling in a gravitational field and is thus quite important for the understanding of sedimentation and aggregation during sedimentation. Further physical consequences of this theory will be discussed in a forthcoming separate contribution [10].

The objectives of the present paper are threefold. First, we will separate the different strands of the analysis with the aim to more clearly distinguish the technical and conceptual points. We will thus show that advection-diffusion on large scales is quite general and holds if the internal symmetry is described by a compact manifold of otherwise arbitrary internal geometry. The steps in the multiscale analysis can be posed as solving elliptic partial differential equations on the manifold and then computing weighted averages of these solutions. These are both well defined, though generally nontrivial, tasks, and, consequently, it is only determining the effective transport coefficients in closed form which necessitates additional assumptions. Second, we will give further details on the analysis in Ref. [8] focusing on a local representation of rotations [elements of SO(3)] as charts and on the computation of the effective transport coefficients by the use of SO(3) invariant theory. We will also present results going beyond a diagonalizability assumption made in Ref. [8], predictions which we compare to numerical simulations. Third, we will show that the first step of the multiscale analysis can be carried out also for a process that satisfies a detailed balance condition. In this case, however, the transport coefficients cannot be analytically computed as averages of known terms over the manifold using simply invariant theory.

As an illustration we also include a discussion of the example where the configuration space is $\mathbb{C}^2$, two-dimensional complex space, and the internal symmetry is the Lie group SU(2) of 2×2 unitary matrices of unit determinant. The small-scale motion is thus coupled advection-diffusion on $\mathbb{C}^2$ and on the group manifold of SU(2) while the large-scale motion is advection-diffusion on $\mathbb{C}^2$ only. As a consequence of the Lie algebras su(2) and so(3) being isomorphic the equations to solve on the consecutive levels of the multiscale analysis are

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equivalent to those for SO(3), but the solvability conditions, being global, differ.

The paper is organized as follows. In Sec. II we introduce our basic model of coupled diffusions in space and on a manifold and the basic notions of differential geometry which we need in the following. In Sec. III we carry out a multiscale analysis on the basic model and show that it leads to large-scale drift and diffusion. In Sec. IV we apply the basic model to motion in space and a symmetry group acting on that space, and in Sec. V we discuss the example where space is three dimensional and the symmetry is rotation group SO(3). In Sec. VI we similarly discuss the case of SU(2), in Sec. VII we present numerical results, and in Sec. VIII we sum up and discuss what has been done. Some standard material is for completeness included as appendices.

II. DIFFUSION WITH INTERNAL STATES

In this section we introduce our basic model, coupled diffusion on n-dimensional space and on a manifold $\mathcal{M}$ with dimension m. The general theory of Brownian motion on manifolds was developed by Kolmogorov, Itô, and Yosida and others in the middle of the 20th century and is described in many monographs, cf. Refs. [11–14]. The case of Brownian motion on SO(3), which will be one of our main examples, was explicitly constructed by McKean in an early but still very instructive paper [15].

A. Brownian motion on manifolds

Our purpose in this section is to introduce the notation and set the stage for the general multiscale analysis in Sec. III. We therefore start from the dictionary definition that an m-dimensional manifold is a topological space, each point of which has a neighborhood that is homeomorphic to the Euclidean space of dimension m. This means that the manifold can be covered by a collection of open sets U_i which are one to one and smoothly related to open sets $V_i \in \mathbb{R}^m$. One set V_i is called a local coordinate patch for the set U_i, and the map $\psi_i : U_i \to V_i$ is called a local coordinate. Suppose a point p on the manifold belongs to two sets U_i and U_j and U' is an open set in $U_i \cap U_j$ containing p. Then we can define two sets $V'_i = \psi_i(U')$ and $V'_j = \psi_j(U')$ and two maps $\psi_{ij} = \psi_j \circ \psi_i^{-1} : V'_i \to V'_j$ and $\psi_{ji} = \psi_i \circ \psi_j^{-1} : V'_j \to V'_i$ which have the meaning of a change of coordinate, locally around point p. Obviously, $\psi_{ji} = \psi_{ij}^{-1}$.

On the manifold is defined a metric g which can be expressed as a matrix g_{ij} in local coordinates. This means that if two points p and q are close and have coordinates $\alpha_p = \psi_i(p)$ and $\alpha_q = \psi_i(q)$ in the same patch such that $\alpha_q = \alpha_p + \Delta\alpha$, then the squared distance $d^2(p,q)$ equals $\sum_{ab} g_{ab}(\alpha)\Delta\alpha^a\Delta\alpha^b$. Under a change of coordinate $\alpha \to \alpha'$ with Jacobian $J^a_b = \frac{\partial\alpha'^a}{\partial\alpha^b}$ the metric g therefore transforms as a second-order contravariant tensor

$$g'_{ab}(\alpha') = \sum_{cd}(J^{-1})^c_a(J^{-1})^d_b g_{cd}[\psi_{ji}(\alpha')],$$

The manifold also has a volume element $\sqrt{\det g}$, which we will write $\sqrt{g}$, and which under a coordinate change transforms as $\sqrt{g'} = \sqrt{g}/|\det J|$. We will from now on use the Einstein convention where repeated indices, one upper and one lower, are summed.

Let now $\mathbb{R}^n \otimes V_i$ be parametrized as $(x^1,\dots,x^n,\alpha^1,\dots,\alpha^m)$. The building blocks of our basic model are systems of coupled stochastic differential equations

$$\begin{aligned} dx^i &= A_1(\vec{x},\vec{\alpha},t)^i dt + B_{11}(\vec{x},\vec{\alpha},t)^i_j \bullet dW^j \\ &\quad + B_{12}(\vec{x},\vec{\alpha},t)^i_b \bullet dW'^b, \\ d\alpha^a &= A_2(\vec{x},\vec{\alpha},t)^a dt + B_{21}(\vec{x},\vec{\alpha},t)^a_j \bullet dW^j \\ &\quad + B_{22}(\vec{x},\vec{\alpha},t)^a_b \bullet dW'^b, \end{aligned} \tag{1}$$

where dW^j and dW'^b are independent standard n-dimensional and m-dimensional Wiener noises, $\vec{A}_1$ and $\vec{A}_2$ n- and m-dimensional vector fields, and B_{11}, B_{12}, B_{21}, and B_{22} are, respectively, $n \times n$, $n \times m$, $m \times n$, and $m \times m$-dimensional matrix fields. All functions are assumed to depend smoothly on their arguments. The symbol $\bullet$ denotes a product evaluated in the Itô sense. The generator of the diffusion is the operator

$$\begin{aligned} \mathcal{L} &= A_1(\vec{x},\vec{\alpha},t)^i \frac{\partial}{\partial x^i} + A_2(\vec{x},\vec{\alpha},t)^a \frac{\partial}{\partial\alpha^a} \\ &\quad + \frac{1}{2} b_{11}(\vec{x},\vec{\alpha},t)^{ij} \frac{\partial^2}{\partial x^i \partial x^j} + \frac{1}{2} b_{22}(\vec{x},\vec{\alpha},t)^{ab} \frac{\partial^2}{\partial\alpha^a\partial\alpha^b} \\ &\quad + b_{12}(\vec{x},\vec{\alpha},t)^{ia} \frac{\partial^2}{\partial x^i \partial\alpha^a}, \end{aligned} \tag{2}$$

with

$$\begin{aligned} b_{11}^{ij} &= \left(B_{11}B_{11}^T + B_{12}B_{12}^T\right)^{ij}; \\ b_{22}^{ab} &= \left(B_{22}B_{22}^T + B_{21}B_{21}^T\right)^{ab}; \\ b_{12}^{ia} &= \left(B_{11}B_{21}^T + B_{12}B_{22}^T\right)^{ia}. \end{aligned}$$

The generator determines the time change of expectation values of future events through $\partial_t E + \mathcal{L}E = 0$. The evolution of a probability density is given by the Fokker-Planck equation $\partial_t P = \mathcal{F}P$, where

$$\begin{aligned} \mathcal{F}P &= -\frac{\partial}{\partial x^i}(A_1(\vec{x},\vec{\alpha},t)^i P) - \frac{\partial}{\partial\alpha^a}(A_2(\vec{x},\vec{\alpha},t)^a P) \\ &\quad + \frac{1}{2}\frac{\partial^2}{\partial x^i\partial x^j}(b_{11}(\vec{x},\vec{\alpha},t)^{ij} P) \\ &\quad + \frac{1}{2}\frac{\partial^2}{\partial\alpha^a\partial\alpha^b}(b_{22}(\vec{x},\vec{\alpha},t)^{ab} P) \\ &\quad + \frac{\partial^2}{\partial x^i\partial\alpha^a}(b_{12}(\vec{x},\vec{\alpha},t)^{ia} P). \end{aligned} \tag{3}$$

Note that being a density, P transforms as $P' = P/|\det J|$.

During a sufficiently short time interval the solutions of (1) will, with high probability, not leave $\mathbb{R}^n \otimes V_i$ and then specify a trajectory in $\mathbb{R}^n \otimes \mathcal{M}$. Assume that the trajectory is contained in a set $\mathbb{R}^n \otimes U'$ centered around point p parametrized by two coordinate systems $(\alpha^1,\dots,\alpha^m) \in V_i$ and $(\alpha'^1,\dots,\alpha'^m) \in V_j$ with Jacobian J. The Itô lemma specifies the motion in the second coordinate system to be

$$\begin{aligned} dx^i &= A_1'(\vec{x},\vec{\alpha}',t)^i dt + B_{11}'(\vec{x},\vec{\alpha}',t)^i_j \bullet dW^j \\ &\quad + B_{12}'(\vec{x},\vec{\alpha}',t)^i_b \bullet dW'^b, \\ d\alpha'^a &= A_2'(\vec{x},\vec{\alpha}',t)^a dt + B_{12}'(\vec{x},\vec{\alpha}',t)^a_j \bullet dW^j \\ &\quad + B_{22}'(\vec{x},\vec{\alpha}',t)^a_b \bullet dW'^b, \end{aligned} \tag{4}$$

where

$$\begin{aligned} A_1'^i &= A_1(\vec{x},\alpha(\vec{\alpha}'),t)^i; \\ A_2'^a &= J^a_b A_2(\vec{x},\alpha(\vec{\alpha}'),t)^b + \frac{1}{2}\left(\frac{\partial^2\alpha'^a}{\partial\alpha^c\partial\alpha^d}\right) b_{22}^{cd}; \\ B_{11}'{}^i_j &= B_{11}(\vec{x},\alpha(\vec{\alpha}'),t)^i_j; \\ B_{12}'{}^i_b &= B_{12}(\vec{x},\alpha(\vec{\alpha}'),t)^i_b; \\ B_{21}'{}^a_i &= J^a_c B_{21}(\vec{x},\alpha(\vec{\alpha}'),t)^c_i; \\ B_{22}'{}^a_b &= J^a_c B_{22}(\vec{x},\alpha(\vec{\alpha}'),t)^c_b. \end{aligned} \tag{5}$$

from which follows

$$\begin{aligned} b_{11}'{}^{ij} &= b_{11}^{ij}; \\ b_{12}'{}^{ia} &= J^a_c b_{12}^{ic}; \\ b_{22}'{}^{ab} &= J^a_c J^b_d b_{22}^{cd}. \end{aligned} \tag{6}$$

It is readily checked that the solutions of the Fokker-Planck equation (3) change by the transformations (5) and (6).

Diffusion on $\mathbb{R}^n \otimes \mathcal{M}$ is specified as a family of systems of stochastic differential equations (1) in local coordinates which transform as (4), (5), and (6) under any well-defined change of variables whatsoever.

B. Integration, adjoint, and Fokker-Planck

Integration on $\mathcal{M}$ is defined by first dividing it up in sets B_i, each contained in an open set U_i with local coordinates $(\alpha_i^1,\dots,\alpha_i^m)$ in local patch V_i. Let the metric g expressed in the coordinates of local patch V_i be the matrix-valued function $g^{(i)}_{ab}(\alpha_i)$ and let f be a function $f:\mathcal{M}\to\mathbb{R}$. Then

$$\int \sqrt{g} f = \sum_i \int_{\psi_i(B_i)} \sqrt{g^{(i)}} d\alpha_i^1 \cdots d\alpha_i^m f\left[\psi_i^{-1}(\alpha_i)\right]. \tag{7}$$

Integrating two functions specifies a scalar product

$$(f,h) = \int \sqrt{g} f h, \tag{8}$$

and the adjoint of an operator $\mathcal{L}$ is thus given by

$$(f,\mathcal{L}^\dagger[h]) = (\mathcal{L}[f],h) = \int \sqrt{g} h \mathcal{L}[f]. \tag{9}$$

These considerations are immediately extended to square integrable functions on the product manifold $\mathbb{R}^n \otimes \mathcal{M}$ which has the flat Euclidean metric on $\mathbb{R}^n$ and the metric g on $\mathcal{M}$. Let $\mathbb{R}^n$ be divided in sets $B_j^{(n)}$ and let $\mathbb{R}^n \otimes \mathcal{M}$ be divided in the sets $B_{ji}^{(n\times m)} = B_j^{(n)} \otimes B_i$. For the generator of diffusions in (2) the adjoint can be computed by integration by parts in each set $B_{ji}^{(n\times m)}$. It is a fundamental fact that the boundary conditions then cancel between neighboring sets and

$$\begin{aligned} \mathcal{L}^\dagger = \frac{1}{\sqrt{g}}\bigg[&-\partial_i \sqrt{g} A_1^i - \frac{\partial}{\partial\alpha^a}\sqrt{g}A_2^a + \frac{1}{2}\partial^2_{ij}\sqrt{g} b_{11}^{ij} \\ &+ \frac{1}{2}\frac{\partial^2}{\partial\alpha^a\partial\alpha^b}\sqrt{g} b_{22}^{ab} + \partial_i \frac{\partial}{\partial\alpha^a}\sqrt{g} b_{12}^{ai}\bigg]. \end{aligned} \tag{10}$$

By comparing (10) and (3) we can write the Fokker-Planck operator as

$$\mathcal{F}[P] = \sqrt{g}\mathcal{L}^\dagger\left[\frac{P}{\sqrt{g}}\right]. \tag{11}$$

For the following it is convenient to write

$$P = \hat{P}\sqrt{g}, \tag{12}$$

where $\hat{P}$ is a scalar function.

C. Closed solutions for the stationary state

The stationary state of the Fokker-Planck equation in ordinary space can be found in closed form if either the diffusion process satisfies detailed balance or when the drift field is incompressible. In this subsection we state the generalization of these results to diffusions on a compact manifold. To streamline the notation we use here only one d-dimensional drift vector A with components A^μ and one $d\times d$-dimensional diffusion matrix b with components $b^{\mu\nu}$. Taking the manifold to be $T^n \otimes \mathcal{M}$ where T^n is the n-dimensional torus ($d = m + n$), these stationary states can then be used as zeroth-order probabilities in the multiscale analysis in Sec. III and in the following.

The starting point is the observation that the Hänggi-Klimontovich drift

$$D^\mu = A^\mu - \frac{1}{2\sqrt{g}}\partial_\nu(\sqrt{g} b^{\mu\nu}) \tag{13}$$

transforms as a covariant vector. For completeness, a demonstration is given in the Appendix A. If for some scalar function V and in some coordinate system we have

$$D^\mu = -\tfrac{1}{2} b^{\mu\nu}\partial_\nu V, \tag{14}$$

then this must therefore be true in every coordinate system. The fluxless stationary states of (3) are determined by

$$\tfrac{1}{2} b^{\mu\nu}(\partial_\nu P) = \left[A^\mu - \tfrac{1}{2}\partial_\nu(b^{\mu\nu})\right] P. \tag{15}$$

Using the scalar $\hat{P} = P/\sqrt{g}$ we have instead

$$\frac{1}{2} b^{\mu\nu}(\partial_\nu \log\hat{P}) = \left(A^\mu - \frac{1}{2}\partial_\nu(b^{\mu\nu}) - \frac{1}{2} b^{\mu\nu}\frac{\partial_\nu\sqrt{g}}{\sqrt{g}}\right) = D^\mu. \tag{16}$$

Therefore, if (14) is true, then the stationary state is given by

$$P^* = \frac{1}{\mathcal{N}}\sqrt{g} e^{-V}, \tag{17}$$

where $\mathcal{N}$ is a normalization constant. The mean drift with respect to this measure must vanish:

$$\begin{aligned} V^\mu &= \frac{1}{\mathcal{N}}\int \sqrt{g} e^{-V} A^\mu \\ &= \frac{1}{\mathcal{N}}\int \sqrt{g} e^{-V} D^\mu - \frac{1}{\mathcal{N}}\int \sqrt{g} e^{-V} D^\mu = 0. \end{aligned} \tag{18}$$

Therefore we can only use (or hope to use) this solution method when the average drift in the internal states vanishes, which for a rotating Brownian particles means that it cannot have a mean rotation around an axis. On the other hand, for motion in space we can go to a comoving frame where the average drift is zero and then compute the effective diffusion in that frame.

The other class of closed-form solutions is obtained by noting that

$$c = \partial_a(D^a) + D^a \frac{\partial_a \sqrt{g}}{\sqrt{g}} \tag{19}$$

is a scalar. The condition $c = 0$ is thus the natural generalization of incompressibility, $\partial_\mu A^\mu = 0$ in local flat coordinates. Consider, then,

$$S = \frac{1}{2}\int \sqrt{g}\left(\hat{P} - \frac{1}{\mathcal{N}}\right)^2, \tag{20}$$

where $\int \sqrt{g}\hat{P} = \int \sqrt{g}\frac{1}{\mathcal{N}} = 1$. Using (10) we have

$$\begin{aligned}\partial_t S &= \int \sqrt{g}\left(\hat{P} - \frac{1}{\mathcal{N}}\right)\partial_t \hat{P} \\ &= 2\int \sqrt{g} c \hat{P}^2 - \frac{1}{2}\int \sqrt{g} b^{ab}\partial_a \hat{P}\partial_b \hat{P}.\end{aligned} \tag{21}$$

If $c = 0$, then the solutions must therefore relax to $\hat{P} = \frac{1}{\mathcal{N}}$.

III. MULTISCALE WITH INTERNAL STATES

In a pioneering contribution published in the mid-1990s, Vergassola and Avellaneda showed that scalar transport in a velocity field that varies on a small scale leads to advection and diffusion on large scales with transport coefficients that can be computed in a hierarchy of solvability conditions and solutions [16]; further results in the same direction were later obtained in Refs. [17] and [18]. We will here apply the same method to the analysis of the Fokker-Planck equation on a product manifold $\mathbb{R}^n \otimes \mathcal{M}$ written

$$\partial_t \hat{P} = \mathcal{L}^\dagger \hat{P}, \tag{22}$$

where $\mathcal{L}^\dagger$ is defined in (10) and where the auxiliary scalar function $\hat{P}$ is defined in (12). From a technical point of view, the material in this section is not very new, except that we keep track of the manifold $\mathcal{M}$ of internal states which adds to the notational complications; readers familiar with the multiscale formalism may want to skip to Sec. IV.

The first step is to identify a characteristic time $t_\mathcal{M}$ in which diffusion spreads out probability mass on the manifold $\mathcal{M}$. By order of magnitude $t_\mathcal{M} \sim D^2_\mathcal{M}/b$, where $D_\mathcal{M}$ is the diameter of $\mathcal{M}$ and b is a characteristic size of the diffusion coefficients b_{22} in (10). The second step is to identify a characteristic spatial scale $L_\mathcal{M}$ which the diffusion process will reach during time $t_\mathcal{M}$. For the case of diffusion of the position and orientation of a three-dimensional body in space and on SO(3), and for physically reasonable diffusion coefficients, $L_\mathcal{M}$ is on the order of the radius of the body [8]. We will from now on assume that scales of time and space and distances on the manifold have been chosen such that $t_\mathcal{M}$, $L_\mathcal{M}$, and $D_\mathcal{M}$ are all of order one, meaning that all the diffusion coefficients b_{11}, b_{22}, and b_{12} in (10) are also of order one. We will further assume that in the same coordinates the drift coefficients A_1^i and A_2^a are also of order one. If in fact A_1^i and A_2^a would be smaller, then this would mean that the drift is relatively small (a special case of what will be considered below) while if A_1^i and A_2^a would be larger, then diffusion would not be the fastest process on the scale of the internal states, and the starting point of the analysis should differ. The third step is to identify a larger spatial scale L and a small dimension-less ratio $\epsilon = \frac{L_\mathcal{M}}{L}$. We seek an effective description of the motion in space on scale L. To do so, we assume that there are processes on time scale $t_\mathcal{M}$ which act to spread out probability mass over $\mathcal{M}$ and distances $L_\mathcal{M}$ in space, processes on time scale $\epsilon^{-1}t_\mathcal{M}$ where the probability mass is advected over length scale L, and processes on time scale $\epsilon^{-2}t_\mathcal{M}$ where the probability mass diffuses relative distance L.

The multiscale step proper is to let physical space be represented by two variables $\tilde{x}$ on scale $L_\mathcal{M}$ and X on scale L and similarly time by $\tilde{t}$ on scale $t_\mathcal{M}$, τ on scale $\epsilon^{-1}t_\mathcal{M}$ and θ on scale $\epsilon^{-2}t_\mathcal{M}$. Derivatives with respect to physical time and space are then represented as

$$\begin{aligned}\frac{\partial}{\partial t} &\to \partial_{\tilde{t}} + \epsilon\partial_\tau + \epsilon^2\partial_\theta, \\ \frac{\partial}{\partial x^i} &\to \partial_i + \epsilon\nabla_i,\end{aligned} \tag{23}$$

where ∂_i stands for $\frac{\partial}{\partial \tilde{x}^i}$ and ∇_i for $\frac{\partial}{\partial X^i}$ and ϵ is the small parameter. The probability density function is expressed in local coordinates and expanded as

$$\begin{aligned}P &= P^{(0)}(\tilde{x},X,\alpha,\tilde{t},\tau,\theta) + \epsilon P^{(1)}(\tilde{x},X,\alpha,\tilde{t},\tau,\theta) \\ &\quad + \epsilon^2 P^{(2)}(\tilde{x},X,\alpha,\tilde{t},\tau,\theta) + \dots \\ &= \sqrt{g}(\hat{P}^{(0)}(\tilde{x},X,\alpha,\tilde{t},\tau,\theta) + \epsilon\hat{P}^{(1)}(\tilde{x},X,\alpha,\tilde{t},\tau,\theta) \\ &\quad + \epsilon^2\hat{P}^{(2)}(\tilde{x},X,\alpha,\tilde{t},\tau,\theta) + \dots)\end{aligned} \tag{24}$$

and (22) is solved order by order in ϵ. All functions $P^{(0)}, P^{(1)}, P^{(2)}, \dots$ are assumed periodic in the small-scale variable $\tilde{x}$ with period $L_\mathcal{M}$.

An important role is now played by the part of the operator $\mathcal{L}^\dagger$ in (10) which is of leading order in ϵ. In local coordinates $(\tilde{x},\alpha)$ it is written in the same way as (10), i.e.,

$$\begin{aligned}\mathcal{L}_0^\dagger = \frac{1}{\sqrt{g}}\bigg[&-\partial_i\sqrt{g}A_1^i - \frac{\partial}{\partial\alpha^a}\sqrt{g}A_2^a + \frac{1}{2}\partial_{ij}^2\sqrt{g}b_{11}^{ij} \\ &+ \frac{1}{2}\frac{\partial^2}{\partial\alpha^a\partial\alpha^b}\sqrt{g}b_{22}^{ab} + \partial_i\frac{\partial}{\partial\alpha^a}\sqrt{g}b_{12}^{ia}\bigg],\end{aligned} \tag{25}$$

but is an elliptic partial differential operator not on $\mathbb{R}^n \otimes \mathcal{M}$, but on the compact manifold $T^n \otimes \mathcal{M}$, where T^n is the n-dimensional torus with radii $L_\mathcal{M}$. The coefficients of $\mathcal{L}_0^\dagger$ depend in principle on $\tilde{x}$, X, and α. We now appeal to standard results on spectra of elliptic operators on compact spaces; $\mathcal{L}_0^\dagger$ should have a discrete spectrum

$$\mathrm{Spec}(\mathcal{L}_0) = \{\lambda_0, \lambda_1, \dots\}, \tag{26}$$

and $\lambda_0 = 0$ is a unique zero mode. Physically, this corresponds the solutions of (22) relaxing for long time to a unique stationary state; as total probability mass is conserved the corresponding eigenvalue must then be zero. The operator $\mathcal{L}_0^\dagger$ and its adjoint $\mathcal{L}_0$ have the same eigenvalues but not necessarily the same eigenfunctions. Let these be given as

$$\begin{aligned}\mathcal{L}_0 n_l &= \lambda_l n_l;\\ \mathcal{L}_0^\dagger m_l &= \lambda_l m_l,\end{aligned} \tag{27}$$

where $(n_l,m_k) = \mathbf{1}_{lk}$. Since in $\mathcal{L}_0$ all derivatives stand to the right of all variable-dependent coefficients, n_0 must be a constant. We can choose that to be 1; the orthogonality condition for m_0 and n_0 then gives a normalization of m_0:

$$\int_{T^n\otimes\mathcal{M}} \sqrt{g} m_0 = 1. \tag{28}$$

The scalar density $\sqrt{g}m_0$ is then a normalized probability density on $T^n \otimes \mathcal{M}$.

The multiscale is now posed by the following hierarchy:

$$\begin{aligned}
\mathcal{L}_0^\dagger \hat{P}^{(0)} &= 0;\\
\mathcal{L}_0^\dagger \hat{P}^{(1)} &= \partial_\tau \hat{P}^{(0)} + \frac{1}{\sqrt{g}}\nabla_i\big[\sqrt{g}A_1^i\hat{P}^{(0)}\big]\\
&\quad - \frac{1}{\sqrt{g}}\partial_i\nabla_j\big[\sqrt{g}b_{11}^{ij}\hat{P}^{(0)}\big] - \frac{1}{\sqrt{g}}\frac{\partial}{\partial\alpha^a}\nabla_i\big[\sqrt{g}b_{12}^{ia}\hat{P}^{(0)}\big];\\
\mathcal{L}_0^\dagger \hat{P}^{(2)} &= \partial_\tau \hat{P}^{(1)} + \frac{1}{\sqrt{g}}\nabla_i\big[\sqrt{g}A_1^i\hat{P}^{(1)}\big]\\
&\quad - \frac{1}{\sqrt{g}}\partial_i\nabla_j\big[\sqrt{g}b_{11}^{ij}\hat{P}^{(1)}\big] - \frac{1}{\sqrt{g}}\frac{\partial}{\partial\alpha^a}\nabla_i\big[\sqrt{g}b_{12}^{ia}\hat{P}^{(1)}\big]\\
&\quad + \partial_\theta\hat{P}^{(0)} - \frac{1}{2}\frac{1}{\sqrt{g}}\nabla_i\nabla_j\big[\sqrt{g}b_{11}^{ij}\hat{P}^{(0)}\big].
\end{aligned} \tag{29}$$

All equations are solved in the relaxation limit for the fast time $\tilde{t}$. We note that, by assumption, $\sqrt{g}$ only depends on the internal coordinates, hence it commutes with ∇_i, the derivative on the large scale.

A. Dependence of $P^{(0)}$ on $\tilde{x}$ and internal states

The solution to zeroth order is

$$\hat{P}^{(0)}(\vec{\tilde{x}},\vec{\alpha},\vec{X},\tau,\theta) = m_0(\vec{\tilde{x}},\vec{\alpha};\tau,\theta,X)C^{(0)}(\vec{X},\tau,\theta), \tag{30}$$

where $m_0(\vec{\tilde{x}},\vec{\alpha};\tau,\theta,X)$ is the zero mode of $\mathcal{L}_0^\dagger$ with normalization (28). Note that m_0 depends parametrically on τ, θ, and X because the coefficients of $\mathcal{L}_0^\dagger$ may depend on all these variables. $C^{(0)}$ is, on the other hand, a (so far undetermined) proportionality coefficient. The zeroth other probability $P^{(0)}$ is then $\sqrt{g}m_0C^{(0)}$. Except for the special cases discussed above in Sec. II C, solving for m_0 is in general not straightforward and requires numerical methods. For the general discussion in this section it is, however, enough to assume that it exists and that it depends smoothly on $\tilde{x}$, α, and (τ,θ,X).

B. Solvability conditions and solution to order ϵ

Generally, we must have

$$\mathcal{L}_0^\dagger\hat{P}^{(1)} \in \mathrm{Im}(\mathcal{L}_0^\dagger) = \mathrm{Span}\{m_1,m_2,\ldots\}, \tag{31}$$

where the zero mode m_0 does not appear on the right-hand side. By Fredholm alternative we then have $(\mathcal{L}_0^\dagger\hat{P}^{(1)},n_0) = 0$ and, using the second line of (29) and the solution $P^{(0)}$ obtained above, we have a *solvability condition* (two terms vanish because the are gradients with respect to the small scales that are integrated over):

$$\left(n_0,\frac{\partial}{\partial\tau}(m_0C^{(0)})\right) + \nabla_i\big(n_0,A_1^i m_0C^{(0)}\big). \tag{32}$$

Since $C^{(0)}$ does not depend on the small scales, the first term in (32), $(n_0,\frac{\partial}{\partial\tau}(m_0C^{(0)}))$, is equal to $C^{(0)}(n_0,\frac{\partial}{\partial\tau}(m_0)) + \frac{\partial}{\partial\tau}(C^{(0)})(n_0,m_0)$. On the other hand, by orthogonality $(n_0,m_0) = 1$ for any values of (τ,θ,X) and n_0 has been chosen independent of τ. Therefore $(n_0,\frac{\partial}{\partial\tau}(m_0)) = 0$ and (32) simplifies to

$$\partial_\tau C^{(0)}(\vec{X},\tau,\theta) + \nabla_i[C^{(0)}(\vec{X},\tau,\theta)(n_0,A_1^i m_0)] = 0. \tag{33}$$

Equation (33) describes advective motion with effective drift velocity

$$V^i(\tau,\theta,X) = \big(n_0,A_1^i m_0\big) = \int_{T^n\otimes\mathcal{M}} \sqrt{g}\,A_1^i m_0. \tag{34}$$

The above is a straightforward generalization of the result given in Eqs. (17) and (18) in Ref. [16].

To *solve* for $P^{(1)}$ we first write

$$\begin{aligned}\mathcal{L}_0^\dagger\hat{P}^{(1)} &= m_0\frac{\partial C^{(0)}(\vec{X},\tau,\theta)}{\partial\tau} + C^{(0)}(\vec{X},\tau,\theta)\frac{\partial m_0}{\partial\tau}\\ &\quad + \nabla_i\big[A_1^iC^{(0)}(\vec{X},\tau,\theta)m_0\big] + \tilde{P}^{(1)},\end{aligned} \tag{35}$$

where the remainder term is

$$\tilde{P}^{(1)} = -\frac{1}{\sqrt{g}}\partial_i\nabla_j\big[b_{11}^{ij}P^{(0)}\big] - \frac{1}{\sqrt{g}}\frac{\partial}{\partial\alpha^a}\nabla_i\big[b_{12}^{ia}P^{(0)}\big] \in \mathrm{Im}(\mathcal{L}_0^\dagger). \tag{36}$$

Using the solvability condition, the first term in (35) can be rewritten $-m_0\nabla_i[C^{(0)}V^i]$, and we have

$$\begin{aligned}\mathcal{L}_0^\dagger\hat{P}^{(1)} &= C^{(0)}\left(\frac{\partial m_0}{\partial\tau} + V^i\nabla_i m_0\right)\\ &\quad + \nabla_i\big[C^{(0)}\big(A_1^i - V^i\big)m_0\big] + \tilde{P}^{(1)}.\end{aligned} \tag{37}$$

By the same argument as given above, $(n_0,\nabla_i m_0) = 0$, and all terms on the right-hand side of (37) are therefore in $\mathrm{Im}(\mathcal{L}_0^\dagger)$. The inverse $(\mathcal{L}_0^\dagger)^{-1}$ is an integral operator on functions on $T^n\otimes\mathcal{M}$ defined on all functions orthogonal to n_0, and

$$\begin{aligned}\hat{P}^{(1)} &= C^{(0)}\left((\mathcal{L}_0^\dagger)^{-1}\frac{\partial m_0}{\partial\tau} + V^i(\mathcal{L}_0^\dagger)^{-1}\nabla_i m_0\right)\\ &\quad + [\nabla_iC^{(0)}](\mathcal{L}_0^\dagger)^{-1}\big[\big(A_1^i - V^i\big)m_0\big]\\ &\quad + C^{(0)}(\mathcal{L}_0^\dagger)^{-1}\nabla_i\big[\big(A_1^i - V^i\big)m_0\big]\\ &\quad + (\mathcal{L}_0^\dagger)^{-1}\tilde{P}^{(1)} + \hat{P}^{(1),\mathrm{hom}},\end{aligned} \tag{38}$$

where $\hat{P}^{(1),\mathrm{hom}}$ is the homogenous solution which can be written $C^{(1)}m_0$, where $C^{(1)}$ is another proportionality. The way in which $(\mathcal{L}_0^\dagger)^{-1}$ does not commute with ∇_i is illustrated by second and third terms in (38). Even though $(\mathcal{L}_0^\dagger)^{-1}$ acts on functions on $T^n\otimes\mathcal{M}$ its coefficients depend (by assumption) on the slow variables. To bring $(\mathcal{L}_0^\dagger)^{-1}$ completely inside the action of ∇_i we would have to write these two terms as

$$\nabla_i\big[C^{(0)}(\mathcal{L}_0^\dagger)^{-1}\big[\big(A_1^i - V^i\big)m_0\big]\big] + C^{(0)}(\mathcal{L}_0^\dagger)^{-1}[\nabla_i\mathcal{L}_0^\dagger](\mathcal{L}_0^\dagger)^{-1}\big[\big(A_1^i - V^i\big)m_0\big],$$

where $(\mathcal{L}_0^\dagger)^{-1}(\nabla_i\mathcal{L}_0^\dagger)(\mathcal{L}_0^\dagger)^{-1}$ is another operator.

C. Solvability conditions to order ϵ^2

The effective diffusion on large scales if determined by the solvability condition on second order, i.e.,

$$\mathcal{L}_0^\dagger \hat{P}^{(2)} \in \mathrm{Im}(\mathcal{L}_0^\dagger). \tag{39}$$

Considering the right-hand side of the third line of (29), this means

$$\partial_\tau[(n_0,\hat{P}^{(1)})] + \nabla_i\big[\big(n_0,A_1^i\hat{P}^{(1)}\big)\big] + \partial_\theta C^{(0)} - \tfrac{1}{2}\nabla_i\nabla_j\big[\big(n_0,b_{11}^{ij}m_0\big)C^{(0)}\big] = 0, \tag{40}$$

where $\hat{P}^{(1)}$ is given by (38). The last term gives a first effective diffusion term with effective diffusion coefficient matrix

$$\kappa_{(1)}^{ij} = \tfrac{1}{2}\big(n_0,b_{11}^{ij}m_0\big). \tag{41}$$

The homogeneous part $\hat{P}^{(1),\mathrm{hom}}$ enters in the first two terms in (40) as a continuity equation for the proportionality $C^{(1)}$ with the same effective drift velocity as in (34), while the other terms in $P^{(1)}$ can be written

$$\hat{P}^{(1)} - \hat{P}^{(1),\mathrm{hom}} = [\nabla_k C^{(0)}]\chi^k + C^{(0)}\xi, \tag{42}$$

with two auxiliary functions χ^k (given below) and ξ. Overall, the second term in (40) therefore contributes

$$\nabla_i\big[\big(n_0,A_1^i\hat{P}^{(1)}\big)\big] = \nabla_i\nabla_k\big[C^{(0)}\big(n_0,A_1^i\chi^k\big)\big] + \nabla_i\big[C^{(0)}\big(n_0,A_1^i\xi\big) - \nabla_k\big[\big(n_0,A_1^i\chi^k\big)\big]\big], \tag{43}$$

of which the first is a diffusion and the second is a higher-order advection with effective drift velocity $V_1^i = [(n_0,A_1^i\xi) - \nabla_k[(n_0,A_1^i\chi^k)]]$. The second effective diffusion term therefore depends only on

$$\chi^k = (\mathcal{L}_0^\dagger)^{-1}\Big[\big(A_1^k - V^k\big)m_0 - \partial_j\big(b_{11}^{kj}m_0\big) - \frac{1}{\sqrt{g}}\frac{\partial}{\partial\alpha^a}\big(\sqrt{g}b_{12}^{ka}m_0\big)\Big], \tag{44}$$

and we can also write

$$\kappa_{(2)}^{ik} = \Big((\mathcal{L}_0)^{-1}\big[\big(V^i - A_1^i\big)n_0\big],\big(A_1^k - V^k\big)m_0 - \partial_j\big(b_{11}^{kj}m_0\big) - \frac{1}{\sqrt{g}}\frac{\partial}{\partial\alpha^a}\big(\sqrt{g}b_{12}^{ka}m_0\big)\Big). \tag{45}$$

Naturally, only the components symmetric in interchanging indices i and k matter in the above; (45) is hence the generalization of Eq. (64) in Ref. [16].

D. Semianalytic solutions for χ^k

For generalized potential motion discussed above, where $m_0 = \frac{1}{\mathcal{N}_{(V)}}e^{-V}$ and where $\partial_a V = -2(b^{-1})_{ab}D^b$, where D^b is the Hänggi-Klimontovich drift, the calculation of the transport coefficient can be simplified. First recall that for consistency we must then be in a comoving frame where the drift velocity V^k is zero. Equation (44) determining χ^k is then

$$\mathcal{L}_V^\dagger\chi_{(V)}^k = -A_1^k\frac{1}{\mathcal{N}_{(V)}}e^{-V}, \tag{46}$$

where $\mathcal{L}_V^\dagger[\cdot] = \frac{1}{2\sqrt{g}}\partial_\mu(e^{-V}\sqrt{g}b^{\mu\nu}\partial_\nu(e^V[\cdot]))$. Suppose now that for some drift field A_2 in the internal states, e.g., $A_2 = 0$ in local flat coordinates, we have found as a solution the uniform measure $m_0 = \frac{1}{\mathcal{N}_{(0)}}$. For that drift field there is an auxiliary field $\chi_{(0)}^k$ which satisfies

$$\mathcal{L}_0^\dagger\chi_{(0)}^k = -A_1^k\frac{1}{\mathcal{N}_{(0)}}, \tag{47}$$

and the contribution to the effective diffusion coefficient (45) is

$$\kappa_{(2)}^{ik}(V=0) = -\frac{1}{\mathcal{N}_{(0)}}\int\sqrt{g}\chi_{(0)}^k A_1^i. \tag{48}$$

A solution of (46) can be found by:

$$\chi_{(V)}^k = -(\mathcal{L}_V^\dagger)^{-1}\Big[A_1^k\frac{1}{\mathcal{N}_{(V)}}e^{-V}\Big], \tag{49}$$

and for general potential motion we thus have

$$\kappa_{(2)}^{ik}(V) = -\frac{1}{\mathcal{N}_{(V)}}\int\sqrt{g}\chi_{(V)}^k A_1^i. \tag{50}$$

We, therefore, must solve equation (46) for every potential and average on the manifold.

E. Collapsing equation on orders ϵ and ϵ^2

To bring out one final equation we introduce the adjusted advective velocity $\tilde{V}^i = V^i + \epsilon V_1^i$ and the adjusted zero-order proportionality,

$$\tilde{C} = C^{(0)} + \epsilon C^{(1)}, \tag{51}$$

and bring back the original variables in time and space. By the above we then have

$$\partial_t\tilde{C} = -\partial_i[\tilde{V}^i\tilde{C}] + \partial_i\partial_k\big[\big(\kappa_{(1)}^{ik} + \kappa_{(2)}^{ik}\big)\tilde{C}\big], \tag{52}$$

where all terms are of order $(\epsilon)^2$ (diffusive time scale) and where the first correction is of order $(\epsilon)^3$.

IV. MULTISCALE WITH INTERNAL SYMMETRY

In this section we apply the general results of the previous section to the physical setting where the system of stochastic differential equations (1) are overdamped equations of motion and where the manifold describes a symmetry of the motion in space. We then assume a drift field $\vec{F}$ in the spatial directions which we call force and a drift field $\vec{M}$ in the tangent space of the manifold which we call torque.

A. Overdamped motion

We assume that $\vec{F}$ only depends on the large-scale $\vec{X}$ but not on the internal state or on the small scale $\vec{\tilde{x}}$, while $\vec{M}$ may depend on both the internal state and the large-scale $\vec{X}$. Further assume a friction matrix

$$\Gamma = \begin{pmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{pmatrix},$$

which has to have only real positive eigenvalues such that the underdamped motion on a faster time scale is purely relaxational. In the examples discussed below of motion on $\mathbb{R}^3$ or $\mathbb{C}^2$ Γ will be real symmetric or Hermitian. Γ therefore has a square root in the sense that $\Gamma = \sigma\sigma^T$

$$\sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$$

such that Eq. (1) can be written

$$\begin{aligned} &\gamma_{11}{}^i_j dx^j + \gamma_{12}{}^i_b d\alpha^b \\ &\quad = F^i dt + \sqrt{2k_BT}\big[(\sigma_{11})^i_j dW^j + (\sigma_{12})^i_b dW'^b\big], \\ &\gamma_{21}{}^a_j dx^j + \gamma_{22}{}^a_b d\alpha^b \\ &\quad = M^a dt + \sqrt{2k_BT}\big[(\sigma_{21})^a_j dW^j + (\sigma_{22})^a_b dW'^b\big], \end{aligned} \tag{53}$$

where T is the temperature. The inverse of the friction matrix is a symmetric mobility matrix

$$\Gamma^{-1} = \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix},$$

and the drift fields in (1) are given by

$$A_1^i = \mu_{11}{}^i_j F^j + \mu_{12}{}^i_a M^a, \tag{54}$$

$$A_2^i = \mu_{21}{}^a_j F^j + \mu_{22}{}^a_b M^a, \tag{55}$$

while the diffusion amplitudes in (1) are

$$B = \sqrt{2k_BT}\,\Gamma^{-1}\sigma. \tag{56}$$

We will, for the rest of this section, assume that all Itô terms and other correction terms from spatial variation of temperature and friction matrix have been included in the physical force and torque as the need may be. The diffusion terms in the Fokker-Planck operator (10) follow from (56) and the expressions listed below Eq. (2). We will assume that the program of the previous section can be carried out, i.e., that we can compute m_0, $P^{(1)}$, etc., as needed.

Before introducing symmetry, let us remark that the advection velocity (57) can now be written as

$$V^i(\tau,\theta,X) = \left(n_0, A_1^i m_0\right) = \overline{\mu}^i_j F^j + \overline{V}^i \tag{57}$$

with an effective mobility

$$\overline{\mu}^i_j = \int \sqrt{g}\,\mu_{11}{}^i_j m_0, \tag{58}$$

and a drift generated by torsion and cross-mobility

$$\overline{V}^i = \int \sqrt{g}\,\mu_{12}{}^i_a M^a m_0. \tag{59}$$

If two bodies experience opposite torques but are otherwise equivalent, then they would hence typically migrate at different speeds when the cross-mobility μ_{12} is nonzero.

B. Overdamped motion with a symmetry

Let us now assume that the internal states are a symmetry group of the motion in n-dimensional space. Abstractly defined, a *group* G is a collection of elements g with the following properties:

(i) There is a rule for multiplying any two elements, and their product g_1g_2 is also an element of G; this rule for multiplication is *associative*, so for any three element of $(g_1g_2)g_3 = g_1(g_2g_3)$;

(ii) There is an identity element of G, say, e, such that $eg = ge = g$ for any element g;

(iii) For every element g, there is a unique inverse element g^{-1} such that $gg^{-1} = g^{-1}g = e$.

That the manifold $\mathcal{M}$ is a symmetry group of $\mathbb{R}^n$ means that there is a map from points g on $\mathcal{M}$ to operators $R(g)$ acting on $\mathbb{R}^n$ which are a faithful representation of the group, i.e.,

(i) $R(g_1g_2) = R(g_1)R(g_2)$;

(ii) $R(e) = \mathbf{1}$, such that $R(eg) = R(ge) = R(g)$ for any element g;

(iii) $R(g^{-1}) = (R(g))^{-1}$.

All the products in the above are ordinary matrix products. Let now U_e be a patch of the manifold around the identity element e and let $V_e = \psi_e(U_e) \in \mathbb{R}^m$ be local coordinates for that patch. By the group action we can construct patches $U_g = g(U_e)$ around each point g, and we can therefore construct local coordinates for patch U_g as $V_g = \psi_e[g^{-1}(U_g)]$. From now on we will consider motions (1) expressed in these local coordinates. Furthermore, we will in this section only consider patches that are very small so the drift terms in (54) and (55) and the diffusion terms in (56) are practically constant in each patch. The values of the various quantities around e will be indexed B for "body."

That $\mathcal{M}$ is a symmetry group of the motion means that for any g the overdamped motion described by (53) should look the same if described in the equivalent local coordinates V_g and in the transformed spatial coordinates

$$x'^i = R^i_j(g)x^j. \tag{60}$$

The deterministic and random forces in (53) are also be transformed in the same way, while the transformation properties of the Wiener noises is a matter of convention; here we will take them to be unchanged. Clearly invariance of the motion in space only holds if the friction matrices transform as

$$\gamma_{11}(g) = R(g)\gamma^B{}_{11}R^{-1}(g); \tag{61}$$

$$\gamma_{12}(g) = R(g)\gamma^B{}_{12}; \tag{62}$$

and the spatial noise terms as

$$\sigma_{11}(g) = R(g)\sigma^B{}_{11}; \tag{63}$$

$$\sigma_{12}(g) = R(g)\sigma^B{}_{12}. \tag{64}$$

We have to assume that γ_{21} and γ_{22} transform as needed to preserve positivity; for a real symmetric friction matrix this means $\gamma_{21}(g) = \gamma_{21}R^T(g)$ and $\sigma_{21}(g) = \sigma^B{}_{21}R^T(g)$.

Although somewhat more general cases could be considered we will assume that the friction and noise in the manifold directions are the same at every point, i.e., $\gamma_{22}(g) = \gamma_{22}^B$ and

$\sigma_{22}(g) = \sigma_{22}^B$. The mobilities in (54) then transform as

$$\mu_{11}(g) = R(g)\mu^B{}_{11}R^{-1}(g),$$
$$\mu_{12}(g) = R(g)\mu^B{}_{12},$$

and the effective mobility in (58) is

$$\overline{\mu}^i_j = \int \sqrt{g}R^i_l\left(\mu^B{}_{11}\right)^l_k R^{-1}{}^k_j m_0. \tag{65}$$

As we will see below for the examples of SO(3) and SU(2), when m_0 is constant this simplifies considerably and $\overline{\mu}^i_j$ then becomes proportional to the identity matrix. The same result holds for the first (simple) component of the effective diffusivity in (41).

For invariance to be complete we would finally have to assume that the torque M^a be the same at each point of $\mathcal{M}$ (expressed in the local coordinates). Since, physically, the torque is (or could be) externally determined we will, however, relax this requirement, and the drift generated by cross-diffusion and torque is then

$$\overline{V}^i = \int \sqrt{g}R^i_l(g)\left(\mu^B_{12}\right)^l_a M^a m_0. \tag{66}$$

This can be nonzero if the variations of $R^i_l(g)$ and $M^a m_0$ combine constructively but would be zero if, for instance, M^a is constant and m_0 is uniform.

V. MOTION ON $\mathbb{R}^3$ AND ROTATIONS IN THE LIE GROUP SO(3)

We will now make the previous section more concrete by considering translation and rotations in ordinary three-dimensional space. The Lie group SO(3) is the set of rotations about the origin of the three-dimensional Euclidean space $\mathbb{R}^3$ where the group product is composition of rotations. Physically, the situation is described by two frames: the laboratory frame and the body frame, where everything that depends on the external world (force $\vec{F}$ and perhaps partly torque $\vec{M}$) are simply expressed in the laboratory frame, and everything else is simply expressed in the body frame. A rotation is a transformation that changes the body frame to the laboratory frame (active interpretation, left action of the group). Rotations, being linear transformations, can be represented as matrices once a basis of $\mathbb{R}^3$ has been chosen. Specifically, if we choose an orthonormal basis of $\mathbb{R}^3$, every proper rotation is described by an orthogonal 3×3 matrix with determinant one, which is the set SO(3). The following facts about SO(3) are well known, cf. Ref. [19]:

(i) SO(3) preserves the scalar product $(x,y) = \sum_i x^i y^i$. SO(3) therefore preserves the Euclidean metric tensor diag(1,1,1), which is the Kronecker symbol δ_{ij}. As a consequence, all spatial tensor indices can be lowered and raised at will. SO(3) additionally preserves the three-dimensional volume element and the Levi-Civita tensor ϵ_{ijk}.

(ii) SO(3) is compact manifold of dimension 3.

(iii) The tangent space of SO(3) at the identity element e is the Lie algebra so(3). An element of the Lie algebra can be written $v = \sum_i \alpha_i L_i$ where $(\alpha_1,\alpha_2,\alpha_3)$ are three real parameters and (L_1,L_2,L_3) are three basis elements. so(3) is hence isomorphic to $\mathbb{R}^3$.

(iv) The exponential map of the Lie algebra covers the group.

The last point means that every element $g \in$ SO(3) can be written $\exp(v)$ for some v. This representation is, of course, not unique. However, if the real parameters α lie sufficiently close to the origin, then they determine a set $V_e \subset \mathbb{R}^3$ such that the map $\alpha \to \exp(\sum_i \alpha_i L_i)$ is one to one. The α's can therefore be used to construct a very convenient system of local coordinates used in Ref. [20] and earlier in Ref. [15]. In Appendix B we summarize useful facts about this system of charts.

A. No cross-diffusion and m_0 constant

In this section and in the next we will make successive assumptions to make the problem of computing large-scale advective-diffusive motion analytically solvable. The first of these assumptions is to assume that the cross-frictions in (53) are absent. Our starting point is therefore the simpler set of overdamped equations,

$$\begin{aligned} dx^i &= \gamma^{-1}{}^i_j F^j dt + \sqrt{2k_BT}(\gamma^{-\frac{1}{2}})^i_j dW^j, \\ d\alpha^b &= \eta^{-1}{}^a_b M^b dt + \sqrt{2k_BT}(\eta^{-\frac{1}{2}})^a_b dW'^b, \end{aligned} \tag{67}$$

where we have introduced γ (spatial friction matrix) for γ_{11} and η (rotation friction matrix) for γ_{22}. Note that for space (indices i and j) we do not need to distinguish upper and lower indices, but for motion on the group manifold (indices a and b) we do. We restate the assumptions already made on the dependence of the various quantities in (67):

$$\begin{aligned} T &= T(\vec{X},\tau,\theta); \\ \gamma^i_j &= \gamma^i_j(\vec{X},\vec{\alpha},\tau,\theta); \\ \eta^a_b &= \eta^a_b(\vec{X},\tau,\theta); \\ F^i &= F^i(\vec{X},\tau,\theta); \\ M^a &= M^a(\vec{X},\vec{\alpha},\tau,\theta). \end{aligned} \tag{68}$$

where γ, η, and $\vec{F}$ transform as discussed above in Sec. IV B.

A consequence of these assumptions is that the zero-order probability $P^{(0)} = \sqrt{g}C^{(0)}m_0$ does not depend on the small length scale $\tilde{x}$. From now on we will additionally ignore the dependency of T, γ, and η on τ and θ as they are not our concern here; similarly as in Sec. IV above, we have in (67) also assumed that all Itô terms and other correction terms from spatial variation of temperature and friction matrix have been included in the physical force $\vec{F}$.

Second, we assume that the dynamics is such that m_0 is constant. As discussed above in Sec. II C, this is so when the drift $(\eta^{-1})^a_b M^b$ is zero and when the generalized incompressibility condition in (20) is satisfied. One example of when the latter holds is when M^a is constant (a particle that tends to rotate around an axis fixed in the body), and another is when the torque is constant in the laboratory frame.

We now discuss the effective mobility (65), which we write as

$$\overline{\mu}_{ij} = \sum_{lk}\int \sqrt{g}R_{il}\left(\gamma_B^{-1}\right)_{lk}R^{-1}_{kj}m_0, \tag{69}$$

where $R^{-1}_{kj} = R_{jk}$. Consider the quadratic form $s(x,y) = \sum_{ij} \overline{\mu}_{ij} x_i y_j$ where x and y are two vectors. From the above, this is

$$s(x,y) = \sum_{lk} \int \sqrt{g}\left(\sum_i x_i R_{il}\right)(\gamma_B^{-1})_{lk}\left(\sum_j y_i R_{jk}\right) m_0.$$

As m_0 is constant, the value of the integral is the same for every joint rotation of the two vectors; $s(Rx,Ry) = s(x,y)$. Since the quadratic form invariant by SO(3) is the Kronecker δ and since $\mathrm{Tr} R(\gamma_B^{-1})R^{-1} = \mathrm{Tr}(\gamma_B^{-1})$, we therefore have

$$\overline{\mu}_{ij} = \frac{\mathrm{Tr}(\gamma^{-1})}{3}\delta_{ij}, \tag{70}$$

and the advective velocity is

$$V_i = \frac{\mathrm{Tr}(\gamma^{-1})}{3}F_i. \tag{71}$$

The same reasoning gives the first component of the effective diffusion tensor obtained in (41) as

$$\kappa^{ij}_{(1)} = k_B T \frac{\mathrm{Tr}(\gamma^{-1})}{3}\delta^{ij}. \tag{72}$$

The invariant method used here is described in more detail in Appendix C.

B. No torque and η diagonal

To proceed further, we need to solve for the first-order probability $P^{(1)}$, and to do so in closed form we assume that there is no torque. We will also assume that the angular friction matrix η is diagonal, which amounts to a choice of basis for the body frame. Note that we will not assume that γ is diagonalizable in the same basis, a simplifying assumption made in Refs. [8] and [9].

Let us first recall that the goal is to compute the second component of the effective diffusion tensor obtained in (45), which is

$$\kappa^{ij}_{(2)} = -\big(n_0,(\tilde{\gamma}^{-1})^i_l F^l \chi^j\big), \tag{73}$$

where χ^j is given in (44).

Under the assumptions made, the second term on the right-hand side of this equation $[\partial_j(B^{kj}_{11} m_0)]$ vanishes, and, as discussed in Appendix B, the third term is proportional to α in the local coordinates. By making the local patches sufficiently small (evaluating the right-hand side sufficiently close to the reference point in the center of patch), this term can therefore also be neglected, and the auxiliary equation to solve is more simply

$$\mathcal{L}_0^\dagger \chi^i = m_0\big[(\gamma^{-1})^i_l F^l - V^i\big]. \tag{74}$$

As $\vec{F}$ does not depend on the small scales we can look for solutions through a secondary auxiliary equation,

$$\mathcal{L}_0^\dagger \lambda^{ij} = (\tilde{\gamma}^{-1})^{ij}, \tag{75}$$

where λ is a tensor and $\tilde{\gamma}^{-1}$ is the traceless part of the mobility matrix. We note that this quantity is an element of the irreducible representation $\underline{\mathbf{5}}$ of SO(3) which transforms as

$$\tilde{\gamma}^{-1} = R^* r(\alpha)\tilde{\gamma}_B^{-1} r^{-1}(\alpha)(R^*)^{-1}, \tag{76}$$

where $\tilde{\gamma}_B^{-1}$ is the traceless part of the mobility tensor in the body frame.

We now consider the operator $\mathcal{L}_0^\dagger$ in (10) acting on λ. As we have assumed no dependence on the small spatial scales, no cross-diffusion, and no torque, the only term that matters are the partial derivatives with respect to the rotations. For a small patch the terms $\frac{1}{2}\sqrt{g} b^{ab}_{22}$ will be close to $k_B T(\eta^{-1})^{ab}$ and, as discussed in Appendix B, we can interchange the order of the derivative and $\frac{1}{2}\sqrt{g} b^{ab}_{22}$ such that

$$\mathcal{L}_0^\dagger = k_B T(\eta^{-1})^{ab}\frac{\partial^2}{\partial\alpha^a \partial\alpha^b}. \tag{77}$$

We then make the ansatz that λ also lies in $\underline{\mathbf{5}}$:

$$\lambda = R^* r(\alpha) Q_B r^{-1}(\alpha)(R^*)^{-1}, \tag{78}$$

where Q_B is an auxiliary traceless symmetric tensor in the body frame. Note that if Q_B^s would have a component $q\mathbf{1}$ where q is a scalar, then $\mathcal{L}_0^\dagger Q_B^s$ would be zero, and, furthermore, it would not contribute to (73). We therefore prefer to solve (75) for a general symmetric matrix Q_B and then show that these solutions are only determined up to an arbitrary term proportional to the identity matrix, after which by adding or subtracting such a term we can always adjust the trace of Q_B to be zero.

The equation to solve is thus

$$\left[k_B T(\eta^{-1})^{mn}\frac{\partial}{\partial\alpha^m}\frac{\partial}{\partial\alpha^n}(R^* r(\alpha) Q_B r^{-1}(\alpha)(R^*)^{-1})^{ij}\right]_{\alpha=0} = (\tilde{\gamma}^{-1})^{ij}. \tag{79}$$

The pertinent terms inside the differentials are the quadratic, and using (B3), one obtains:

$$\begin{aligned}(\tilde{\gamma}^{-1})^{ij} = k_B T[&(3R^* Q_B \eta^{-1}(R^*)^{-1} + 3R^*\eta^{-1} Q_B (R^*)^{-1}\\ &- 4\mathrm{Tr}(\eta^{-1})R^* Q_B (R^*)^{-1} - 2\mathrm{Tr}(Q_B)R^*\eta^{-1}(R^*)^{-1})^{ij}\\ &+ 2(\mathrm{Tr}(\eta^{-1})\mathrm{Tr}(Q_B) - \mathrm{Tr}(\eta^{-1}Q_B))\delta^{ij}].\end{aligned} \tag{80}$$

It is seen that the factors R^* and $(R^*)^{-1}$ can be removed on both sides.

The *diagonal* elements obey coupled equations

$$\begin{pmatrix}\frac{\tilde{\gamma}^{-1}_{B_{11}}}{2k_B T}\\ \frac{\tilde{\gamma}^{-1}_{B_{22}}}{2k_B T}\\ \frac{\tilde{\gamma}^{-1}_{B_{33}}}{2k_B T}\end{pmatrix} = \begin{pmatrix}2(\eta^{-1}_{11} - a) & -\eta^{-1}_{22} & -\eta^{-1}_{33}\\ -\eta^{-1}_{11} & 2(\eta^{-1}_{22} - a) & -\eta^{-1}_{33}\\ -\eta^{-1}_{11} & -\eta^{-1}_{22} & 2(\eta^{-1}_{33} - a)\end{pmatrix} \times \begin{pmatrix}Q_{B_{11}}\\ Q_{B_{22}}\\ Q_{B_{33}}\end{pmatrix}. \tag{81}$$

The general solution of (81) can be written as

$$Q_{B_{ii}} = -\frac{1}{6bk_B T}\left(3\eta^{-1}_{ii}\tilde{\gamma}^{-1}_{B_{ii}} - \sum_j \eta^{-1}_{jj}\tilde{\gamma}^{-1}_{B_{jj}}\right) + q, \tag{82}$$

where $b = (\eta^{-1}_{11}\eta^{-1}_{22} + \eta^{-1}_{22}\eta^{-1}_{33} + \eta^{-1}_{11}\eta^{-1}_{33})$ and q is arbitrary. By choosing $q = 0$ we adjust the trace of Q_B to be zero.

When $\tilde{\gamma}_B^{-1}$ commutes with η^{-1} (82) is the full result, but in the more general case $\tilde{\gamma}_B^{-1}$ is not diagonal in the chosen basis and the off-diagonal elements of Q_B are

$$Q_{B_{ij}} = -\frac{\tilde{\gamma}_{B_{ij}}^{-1}}{(k_B T)\big(4\mathrm{Tr}(\eta^{-1}) - 3\eta_{ii}^{-1} - 3\eta_{jj}^{-1}\big)} \quad i \neq j \tag{83}$$

Using the invariant method, we obtain the general formula for the effective diffusion tensor:

$$\begin{aligned}(K^{\mathrm{eff}})^{ik} &= \kappa_{(1)}^{ik} + \kappa_{(2)}^{ik} \\ &= \delta^{ik}\frac{k_B T\,\mathrm{Tr}(\gamma^{-1})}{3} + \mathrm{Tr}\big(\tilde{\gamma}_B^{-1}Q_B\big) \\ &\quad \times \sum_{l,j}\left[\frac{1}{30}\big(\delta^{ij}\delta^{kl}F_l F_j\big) + \frac{1}{10}\big(\delta^{ik}\delta^{lj}F_l F_j\big)\right],\end{aligned} \tag{84}$$

where

$$\begin{aligned}\mathrm{Tr}(\tilde{\gamma}_B^{-1}Q_B) &= \frac{\sum_i (\tilde{\gamma}_B^{-1})^{ii}(\tilde{\gamma}_B^{-1})^{ii}(\eta^{-1})^{ii}}{2bk_B T} \\ &\quad + \frac{2}{k_B T}\left\{\frac{\big[(\tilde{\gamma}_B^{-1})_{21}\big]^2}{\mathrm{Tr}(\eta^{-1}) + 3\eta_{33}^{-1}} + \frac{\big[(\tilde{\gamma}_B^{-1})_{23}\big]^2}{\mathrm{Tr}(\eta^{-1}) + 3\eta_{11}^{-1}}\right. \\ &\quad \left. + \frac{\big[(\tilde{\gamma}_B^{-1})_{13}\big]^2}{\mathrm{Tr}(\eta^{-1}) + 3\eta_{22}^{-1}}\right\}.\end{aligned} \tag{85}$$

In the special case where $\tilde{\gamma}_B^{-1}$ commutes with η^{-1} only the first term in (85) is nonzero, which can be seen to be the result derived in Refs. [21] and [8].

C. General potential motion on SO(3)

We now return to the setting of Sec. III D and assume that there is another set of torques which satisfy a detailed balance condition but with a nontrivial zeroth probability $P^{(0)} = \sqrt{g}e^{-V}/\mathcal{N}_{(V)}$. Using (50) the contribution to the effective diffusivity is

$$\kappa_{(2)}^{ik}(V) = T^{ik}{}_{jl}F^j F^l, \tag{86}$$

where the fourth-order tensor is given by

$$T_{jl}^{ik} = -\int \sqrt{g}(\tilde{\gamma}^{-1})_j^i(\mathcal{L}_V^\dagger)^{-1}\left[(\tilde{\gamma}^{-1})_l^k \frac{1}{\mathcal{N}_{(V)}}e^{-V}\right] \tag{87}$$

with a tensor differing from Eqs. (78), (82), and (83) above.

VI. MOTION ON $\mathbb{C}^2$ AND TRANSFORMATIONS IN THE LIE GROUP $SU(2)$

As a further example we consider motion in four real dimensions with an internal symmetry differing from the four-dimensional rotation group SO(4). Let four real coordinates (x_1,y_1,x_2,y_2) be grouped into two complex coordinates (z_1,z_2). An overdamped dynamics in (x_1,y_1,x_2,y_2), analogous to the first line of (67), can then be taken to be

$$\begin{pmatrix} dz_1 \\ dz_2\end{pmatrix} = \mathbf{S}\begin{pmatrix} f_1 \\ f_2\end{pmatrix}dt + \sqrt{2k_B T}\,\mathbf{S}^{\frac{1}{2}} \bullet \begin{pmatrix} d\omega_1 \\ d\omega_2\end{pmatrix}, \tag{88}$$

where $\mathbf{S}$ is a Hermitian mobility matrix, f_1 and f_2 are two complex forces, and $d\omega_1$ and $d\omega_2$ are two complex Wiener process such that

$$\begin{aligned}\langle d\omega_\mu(t)d\omega_\nu(s)\rangle &= 0; \\ \langle d\omega_\mu(t)\overline{d\omega_\nu}(s)\rangle &= 2dt\delta_{\mu\nu}\delta(t-s).\end{aligned} \tag{89}$$

Two-dimensional complex space has the symmetry of the *special unitary group* [SU(2)] of 2×2 unitary matrices with determinant 1. To have diffusion on $\mathbb{C}^2$ with the internal symmetry of SU(2) we should therefore add to (88)

$$d\vec{\alpha} = \eta^{-1}\vec{M}dt + \sqrt{2k_B T}\,\eta^{-\frac{1}{2}} \bullet d\vec{\xi}, \tag{90}$$

where α is the coordinate in some local chart of SU(2) and the mobility tensor transforms as

$$\mathbf{S}(g) = U(g)\mathbf{S}(e)U^{-1}(g). \tag{91}$$

Equations (88)–(91) define the model we will study in this section.

The following facts about SU(2) are well known:

(i) If $z = (z_1,z_2)$ and $w = (w_1,w_2)$ are two pairs of complex numbers, then SU(2) preserves the scalar product $(z,w) = \overline{z_1}w_1 + \overline{z_2}w_2$. Introducing the covariant vector ("ket") z^i and the contravariant vector ("bra") $z_i = \overline{z^i}$ SU(2) hence preserves the identity operator $\mathbf{1}_j^i$. In particular, SU(2) preserves the norm $|z|^2 = (z,z) = \sum_i z_i z^i$.

(ii) SU(2) is a compact manifold of dimension 3, and is the twofold covering group of SO(3).

(iii) The tangent space of SU(2) at the identity element e is the Lie algebra su(2), isomorphic to $\mathbb{R}^3$ [and to so(3)]. An element of the Lie algebra can be written $v = i\sum_i \alpha_i\sigma_i$ where $(\alpha_1,\alpha_2,\alpha_3)$ are three real parameters and $(\sigma_1,\sigma_2,\sigma_3)$ are three Hermitian traceless matrices, commonly chosen to be the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}.$$

(iv) The exponential map of the Lie algebra covers the group. If H is a Hermitian 2×2 matrix with zero trace, then $U = e^{iH}$ is in SU(2).

In this setting the analysis proceeds much as above for SO(3). Qualitatively speaking, one main difference is that SU(2) only preserves the identity matrix $\mathbf{1}_j^i$ and not, as SO(3), both an identity matrix and a three-dimensional Euclidean metric. A simplifying feature is, on the other hand, that the friction operator $\mathbf{S}$ can be expressed in the same basis as the Lie algebra. Let us therefore write

$$\mathbf{S} = \mu_0\mathbf{1} + \sum_l \mu_l\sigma_l \quad \mathrm{Tr}(\mathbf{S}) = 2\mu_0. \tag{92}$$

The advection velocity is then

$$V^\mu = \mu_0 f^\mu. \tag{93}$$

We also introduce the traceless mobility tensor,

$$\tilde{\mathbf{S}}_\nu^\mu = \sum_l \mu_l(\sigma_l)^\mu{}_\nu. \tag{94}$$

The analog of the auxiliary tensor field λ for SO(3) above is now a Hermitian 2×2 matrix, and the analog of the ansatz (78) is

$$\lambda^\mu{}_\nu = U^\mu{}_\lambda(Q_B)_\kappa^\lambda(U^{-1})^\kappa{}_\nu. \tag{95}$$

As Q_B is Hermitian, it can be written

$$Q_B = q_0\mathbf{1} + \sum_l q_l\sigma_l \tag{96}$$

and the analog of (79) is

$$k_BT\sum_i(\eta^{-1})^{ii}\frac{\partial^2}{\partial\alpha_i^2}\left\{U(\vec{\alpha})\left(q_0\mathbf{1}+\sum_k q_k\sigma_k\right)U^{-1}(\vec{\alpha})\right\}$$
$$= -U(\vec{\alpha})\sum_k \mu_k\sigma_k U^{-1}(\vec{\alpha}), \tag{97}$$

with solution

$$q_p = \frac{1}{4k_BT}\frac{\mu_p}{\mathrm{Tr}(\eta^{-1})-\eta^{-1}_{pp}} \tag{98}$$

and q_0 arbitrary.

The effective diffusion on C^2 is determined by the fourth-order tensor

$$T^{\mu\nu}{}_{\kappa\lambda} = \langle \tilde{\mathbf{S}}^{\mu}_{\kappa}\lambda^{\nu}{}_{\lambda}\rangle, \tag{99}$$

which by SU(2) invariance can be written $A\mathbf{1}^{\mu}_{\kappa}\mathbf{1}^{\nu}_{\lambda}+B\mathbf{1}^{\mu}_{\lambda}\mathbf{1}^{\nu}_{\kappa}$. The coefficients are determined by the two equations

$$0 = 4A + 2B, \tag{100}$$

$$\mathrm{Tr}[\tilde{\mathbf{S}}\lambda] = 2A + 4B, \tag{101}$$

and it therefore suffices to compute

$$\mathcal{B} = 4k_BT\,\mathrm{Tr}[\tilde{\mathbf{S}}\lambda] = \sum_p \frac{\mu_p^2}{\mathrm{Tr}(\eta^{-1})-(\eta^{-1})^{pp}}. \tag{102}$$

The effective diffusion has two components of which the first is

$$2\left(\mathrm{Re}\left(\nabla^2_{z_\mu\bar{z}_\mu}\right)\right)\left(\kappa^{\mu\mu}_{(2)}C^{(0)}\right)$$
$$= \left(\nabla_{x_\mu}\nabla_{x_\mu}+\nabla_{y_\mu}\nabla_{y_\mu}\right)\left(C^{(0)}\frac{\mathcal{B}}{3k_BT}f^\mu f^\mu\right) \tag{103}$$

and the second is

$$\mathrm{Re}\left(\nabla^2_{z_\mu z_\nu}\kappa^{\mu\nu}_{(2)}C^{(0)} - \nabla^2_{\bar{z}_\mu\bar{z}_\nu}\kappa^{\mu\bar{\nu}}_{(2)}C^{(0)}\right)$$
$$= \mathrm{Re}\left(\nabla^2_{z_\mu z_\nu}\frac{\mathcal{B}}{6k_BT}f^\mu f^\nu C^{(0)} - \nabla^2_{\bar{z}_\mu\bar{z}_\nu}\frac{\mathcal{B}}{6k_BT}f^\mu\overline{f}^\nu C^{(0)}\right). \tag{104}$$

VII. NUMERICAL SIMULATIONS

In this section we compare our result (84) to numerical simulations of a Brownian particle, which can translate and rotate in three dimensions and subjected to an external constant force field. During the simulation we solve numerically the equations in (67), where the evolution of translational Brownian motion is computed in the laboratory frame, while the rotational Brownian motion is computed in the body frame. We also assume that:

(i) The translational friction tensor is only dependent by orientation in the laboratory frame.

(ii) The rotational friction tensor and the translational friction tensor are not diagonal in the same base in the body frame.

(iii) The force is constant in the laboratory frame and is applied only in one direction.

(iv) The torque is set to zero.

For the simulations, we choose a quaternion as a concrete parametrization of rotation, i.e., the model is supplemented by the equation of motion for the quaternion q,

$$\dot{q} = \tfrac{1}{2}q\circ\Omega, \tag{105}$$

where the symbol $\circ$ denotes a *quaternion* product [22] evaluated in the Stratonovich sense and Ω is the angular velocity in the body frame (from the equation describing the rotational motion), represented as a pure quaternion [22].

We solve translational and rotational equations describing the motion of Brownian body with the Euler algorithm with time step 10^{-4} s and temperature $T = 300$ K. The result of the simulations averaged over 10^4 realizations of the noise sources (with identical initial conditions) are shown in the following figures.

In Fig. 1 a trajectory in the laboratory frame of a Brownian body is shown. The shape of the particle is identified by translational friction tensor and rotational friction tensor in the body frame:

$$\gamma_B = \begin{pmatrix}25 & 0 & 0.2\\ 0 & 16 & 0\\ 0.2 & 0 & 13\end{pmatrix}\left(\frac{\mathrm{fN\,s}}{\mu\mathrm{m}}\right),$$
$$\eta = \begin{pmatrix}17 & 0 & 0\\ 0 & 16 & 0\\ 0 & 0 & 8\end{pmatrix}\quad(\mathrm{fN}\,\mu\mathrm{m\,s}). \tag{106}$$

As expected, the motion of the body is enhanced along the direction where the force is applied, while diffusion governs the motion along the other two directions. In this specific case, the force is applied along the x direction with magnitude equal to $\|\vec{F}\| = 10$ fN.

Figure 2, instead, shows the probability distribution functions of the final position of all trajectories for the same body described before. Here the asymmetry given by the application

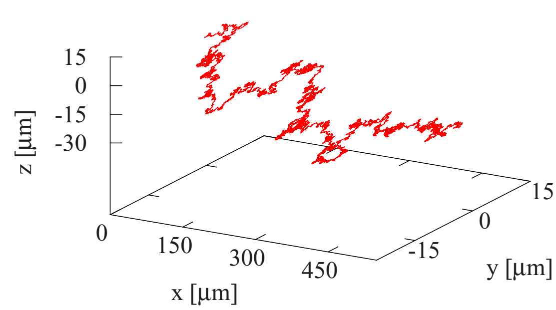

FIG. 1. The figure describes a trajectory in laboratory frame of a Brownian body in three dimensions. Body: $(\gamma_B)^{11} = 25\ \frac{\mathrm{fN\,s}}{\mu\mathrm{m}}, (\gamma_B)^{22} = 16\ \frac{\mathrm{fN\,s}}{\mu\mathrm{m}}, (\gamma_B)^{33} = 13\ \frac{\mathrm{fN\,s}}{\mu\mathrm{m}}$, $(\gamma_B)^{13} = 0.2\ \frac{\mathrm{fN\,s}}{\mu\mathrm{m}}\ (\gamma_B)^{12} = (\gamma_B)^{23} = 0\ \frac{\mathrm{fN\,s}}{\mu\mathrm{m}}$, $(\eta)^{11} = 17$ fN μm s, $(\eta)^{22} = 16$ fN μm s, $(\eta)^{33} = 8$ fN μm s. The external force is $\vec{F} = (10\,\mathrm{fN}, 0\,\mathrm{fN}, 0\,\mathrm{fN})$.

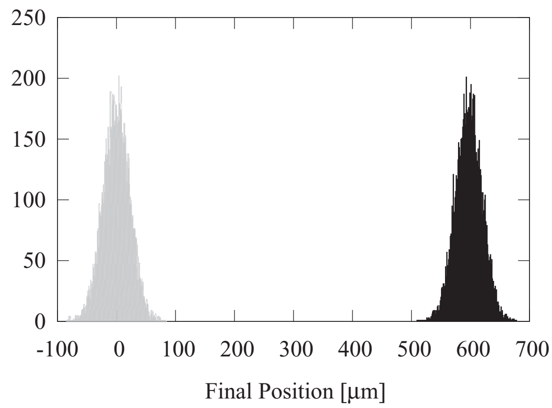

FIG. 2. The figure describes the final position distribution probability functions for the x and z components in the laboratory frame of all trajectories for a Brownian body, respectively (black) right and (gray) left probability distributions (the y-component probability distribution function is not shown. It overlaps with the z-component probability distribution function, as expected). The asymmetry is given by the application of an external force field on the body. Body: $(\gamma_B)^{11} = 25\ \frac{\text{fN s}}{\mu\text{m}}$,$(\gamma_B)^{22} = 16\ \frac{\text{fN s}}{\mu\text{m}}$,$(\gamma_B)^{33} = 13\ \frac{\text{fN s}}{\mu\text{m}}$, $(\gamma_B)^{13} = 0.2\ \frac{\text{fN s}}{\mu\text{m}}\ (\gamma_B)^{12} = (\gamma_B)^{23} = 0\ \frac{\text{fN s}}{\mu\text{m}}$, $(\eta)^{11} = 17\ \text{fN}\,\mu\text{m s}$,$(\eta)^{22} = 16\ \text{fN}\,\mu\text{m s}$,$(\eta)^{33} = 8.\ \text{fN}\,\mu\text{m s}$. The external force is $\vec{F} = (10\,\text{fN},0\,\text{fN},0\,\text{fN})$.

of an external force is well displayed. Indeed, the final position mean of Brownian particle, along the coordinate where the force is applied, can be computed as:

$$\langle \vec{x}_{\text{final}} \rangle = \vec{V}_b t_{\text{final}}, \tag{107}$$

where $\vec{V}_b$ is given by Eq. (71) and t_{final} is set to 1000 s. In this case, the ballistic velocity of the Brownian body is $V_b^x = 0.60\ \frac{\mu\text{m}}{\text{s}}$. The final position mean is therefore $\langle x_{\text{final}} \rangle = 600\ \mu\text{m}$.

In Fig. 3 we show the temporal evolution of the translational diffusion tensor along the three different axes and, in the inset, the ballistic velocity, component x, for a Brownian body. The components of the effective diffusion tensor computed in Eq. (84) are in very good agreement with the long-term coefficients obtained by the simulation. The external force applied to the system is $\vec{F} = (200\,\text{fN},0\,\text{fN},0\,\text{fN})$, while the translational friction tensor and rotational friction tensor in the body frame have the following form:

$$\gamma_B = \begin{pmatrix} 12 & 2.0 & 0 \\ 2.0 & 10 & 0 \\ 0 & 0 & 10 \end{pmatrix} \left(\frac{\text{fN s}}{\mu\text{m}}\right),$$

$$\eta = \begin{pmatrix} 7.12 & 0 & 0 \\ 0 & 6.84 & 0 \\ 0 & 0 & 4.12 \end{pmatrix} (\text{fN}\,\mu\text{m s}). \tag{108}$$

The two full horizontal lines represent the theoretical long-term prediction given by Eq. (84):

$$\mathbf{K}^{eff} = \begin{pmatrix} 1.18 & 0 & 0 \\ 0 & 0.99 & 0 \\ 0 & 0 & 0.99 \end{pmatrix} \left(\frac{\mu\text{m}^2}{\text{s}}\right). \tag{109}$$

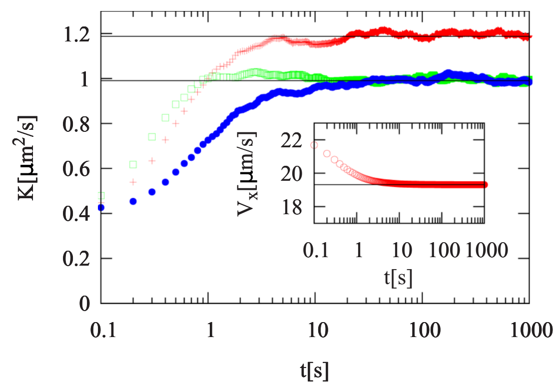

FIG. 3. The figure describes the diffusion coefficient along the x axis, y axis, and z axis in the laboratory frame, respectively (red) cross, (green) empty square, and (blue) full circle points, as function of the time for a body at room temperature $T = 300$ K, averaged over 10^4 realization of the Gaussian noise source, but for identical initial position and orientation of the body. The two full horizontal lines represent the theoretical long-term prediction from (84), $(K^{\text{eff}})^{xx} = 1.18\ \mu\text{m}^2/\text{s}$, $(K^{\text{eff}})^{yy} = (K^{\text{eff}})^{zz} = 0.99\ \mu\text{m}^2/\text{s}$. Body: $(\gamma_B)^{11} = 12.\ \frac{\text{fN s}}{\mu\text{m}}$,$(\gamma_B)^{22} = (\gamma_B)^{33} = 10\ \frac{\text{fN s}}{\mu\text{m}}$, $(\gamma_B)^{12} = 2\ \frac{\text{fN s}}{\mu\text{m}}\ (\gamma_B)^{13} = (\gamma_B)^{23} = 0\ \frac{\text{fN s}}{\mu\text{m}}$, $(\eta)^{11} = 7.12\ \text{fN}\,\mu\text{m s}$, $(\eta)^{22} = 6.84\ \text{fN}\,\mu\text{m s}$,$(\eta)^{33} = 4.12\ \text{fN}\,\mu\text{m s}$. The external force is $\vec{F} = (200\,\text{fN},0\,\text{fN},0\,\text{fN})$. In the inset is plotted the x component of the ballistic velocity of the particle (red) empty circle points, the full horizontal line is equal to $V^x = 19.31\ \ \mu\text{m/s}$ (the other net velocity components are zero, not shown).

The inset shows the evolution of the x component of the ballistic velocity of the body. The full horizontal line is the long-term prediction computed by Eq. (71) and it is equal to $V^x = 19.31\ \frac{\mu m}{s}$.

Figure 4 shows the temporal evolution of the translational diffusion tensor along the three different axes and, in the inset, the component x of the ballistic velocity of a Brownian body. The components of the effective diffusion tensor computed in Eq. (84) are in very agreement with the long-term coefficients obtained by the simulation. The external force applied to the system is $\vec{F} = (200\,\text{fN},0\,\text{fN},0\,\text{fN})$ and the translational friction tensor in the body frame has the following form:

$$\gamma_B = \begin{pmatrix} 12 & 2.0 & 0 \\ 2.0 & 11 & 0 \\ 0 & 0 & 10 \end{pmatrix} \left(\frac{\text{fN s}}{\mu\text{m}}\right). \tag{110}$$

The rotational friction tensor is the same as that of Eq. (108). The two full horizontal lines represent the theoretical long-term prediction given by Eq. (84):

$$\mathbf{K}^{\text{eff}} = \begin{pmatrix} 1.41 & 0 & 0 \\ 0 & 1.15 & 0 \\ 0 & 0 & 1.15 \end{pmatrix} \left(\frac{\mu\text{m}^2}{\text{s}}\right). \tag{111}$$

The inset shows the evolution of the x component of the ballistic velocity of the body. The full horizontal line is the long-term prediction computed by Eq. (71) and it is equal to $V^x = 18.70\ \frac{\mu m}{s}$.

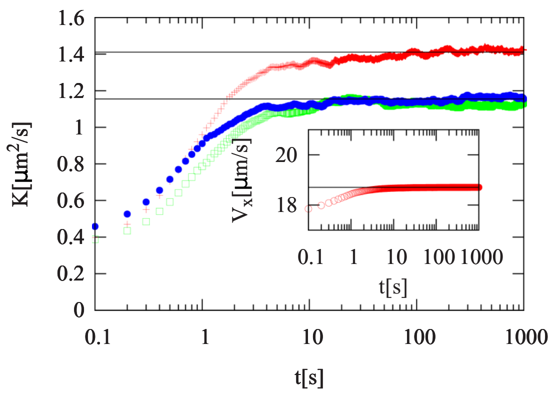

FIG. 4. The figure describes the diffusion coefficient along the x axis, y axis, and z axis in the laboratory frame, respectively (red) cross, (green) empty square, and (blue) full circle points, as function of the time for a body at room temperature $T = 300$ K, averaged over 10^4 realization of the Gaussian noise source but for identical initial position and orientation of the body. The two full horizontal lines represent the theoretical long-term prediction from (84), $(K^{\text{eff}})^{xx} = 1.41\ \mu\text{m}^2/\text{s}$, $(K^{\text{eff}})^{yy} = (K^{\text{eff}})^{zz} = 1.15\ \ \mu\text{m}^2/\text{s}$. Body: $(\gamma_B)^{11} = 12\ \frac{\text{fN s}}{\mu\text{m}}, (\gamma_B)^{22} = 11\ \frac{\text{fN s}}{\mu\text{m}}, (\gamma_B)^{33} = 10\ \frac{\text{fN s}}{\mu\text{m}}$, $(\gamma_B)^{12} = 2\ \frac{\text{fN s}}{\mu\text{m}}\ (\gamma_B)^{13} = (\gamma_B)^{23} = 0\ \frac{\text{fN s}}{\mu\text{m}}$, $(\eta)^{11} = 7.12\ \text{fN}\,\mu\text{m s}, (\eta)^{22} = 6.84\ \text{fN}\,\mu\text{m s}, (\eta)^{33} = 4.12\ \text{fN}\,\mu\text{m s}$. The external force is $\vec{F} = (200\,\text{fN}, 0\,\text{fN}, 0\,\text{fN})$. In the inset is plotted the x component of the ballistic velocity of the particle (red) empty circle points; the full horizontal line is equal to $V^x = 18.7\ \ \mu\text{m/s}$ (the other net velocity components are zero, not shown).

VIII. DISCUSSION

In this paper we have analyzed the coupled overdamped motion in space and on a manifold of internal states. We have shown that on large scales in space and time the probability distribution over the internal states and on small scales in space is slaved to the large-scale spatial probability distribution, which is that of an advection-diffusion process. This process is described by an effective drift field and an effective diffusion matrix, as is to be expected on physical grounds. The method to arrive at these results is the multiscale formalism, which here amounts to solving auxiliary elliptic partial differential equations on the manifold, and computing weighted averages of these solutions, over the manifold. In general, the solutions of the auxiliary equations and the averages can only be found numerically. For the drift field we identified settings including cross-mobility between space and internal states where particles that are acted on by different internal drifts (torques), but are otherwise equivalent, may migrate at different speeds in space.

We then showed that when the drift field obeys a detailed balance condition with respect to the diffusion operator the auxiliary equations must be solved to compute the effective diffusion.

A condition for such a solution to exist is that the average drift velocity vanishes, and the analysis therefore has to be carried out in a comoving frame in space. We have assumed that this comoving frame moves with constant speed; effects of the speed of co-moving frames varying on large scales of space and time have not been considered in this work.

We then applied our general approach to the Brownian translations and rotations, which is advection-diffusion on $\mathbb{R}^3$ and on Lie group SO(3) of rotations in three dimensions. We considered the special case of constant angular friction and no torque and showed that the auxiliary equations then can be solved in closed form. The solution can be described as follows: the traceless mobility tensor $\tilde{\gamma}^{-1}$ is a traceless symmetric 3×3 matrix and, hence, an element of SO(3) irrep $\underline{\mathbf{5}}$. Its value at a given group element g is determined by its value at the group identity $\tilde{\gamma}_B^{-1}$, which is the traceless part of the mobility tensor in the body frame, and a rotation matrix $R(g)$, through the formula $\tilde{\gamma}^{-1} = R(g)\tilde{\gamma}_B^{-1}R^T(g)$. We then find another element of irrep $\underline{\mathbf{5}}$, $\lambda = R(g)Q_B R^T(g)$, where Q_B is a linear transform of $\tilde{\gamma}_B^{-1}$. The effective diffusion matrix is then computed as an average of the product $\tilde{\gamma}^{-1}\lambda$ over a uniform measure on rotations (Haar measure). As discussed in the main text, these averages can be computed in closed form using invariant theory. We compare our predictions to numerical simulations with excellent results.

Compared to results reported recently [8] we have not assumed that the spatial mobility matrix γ_B commutes with the angular diffusion matrix in the body frame. Hence, we have here enlarged the set of cases where the effective diffusion can be computed analytically in closed form. We have also shown that the effective diffusion of Brownian translations and rotations, which has the same angular diffusion and which is in detailed balance, can be computed when an analytic expression of the solution of Eq. (46) can be found. When the measure over rotations is not uniform, these averages cannot be computed using invariant theory and would require further study. We hope to be able to return to this issue and other applications of the methods developed here in future contributions.

ACKNOWLEDGMENTS

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APPENDIX A: TRANSFORMATION PROPERTIES OF THE HÄNGGI-KLIMONTOVICH DRIFT

We want to show that

$$D^a = A^a - \frac{1}{2\sqrt{g}}\partial_{\alpha^b}(\sqrt{g}b^{ab}), \tag{A1}$$

defined in Eq. (13) above, transforms as a vector. Consider therefore in a transformed coordinate system

$$D'^a = A'^a - \frac{1}{2\sqrt{g'}}\partial_{\alpha'^b}(\sqrt{g'}b'^{ab}). \tag{A2}$$

Using the transformation properties of A, b, $\sqrt{g}$, and derivatives, this is

$$D'^a = J^a_b A^b + \frac{1}{2}\frac{\partial^2 \alpha'^a}{\partial\alpha^a\partial\alpha^b} b^{pq} - \frac{d}{2\sqrt{g}}(J^{-1})^q_b \frac{\partial}{\partial\alpha^q}\left(\sqrt{g}\frac{1}{d}J^a_p J^b_r b^{pr}\right), \quad \text{(A3)}$$

where $J^a_b = \partial\alpha'^a/\partial\alpha^b$ and $d = \det J$. Identifying terms, this is

$$D'^a = J^a_b D^b + \frac{1}{2}\frac{\partial^2\alpha'^a}{\partial\alpha^a\partial\alpha^b} b^{pq} - \frac{d}{2}(J^{-1})^q_b b^{pr}\frac{\partial}{\partial\alpha^q}\left(\frac{1}{d}J^a_p J^b_r\right). \quad \text{(A4)}$$

The second line in above gives three terms,

$$2^{\rm nd}\text{line} = \frac{d}{2}(J^{-1})^q_b b^{pr}\frac{\partial d}{\partial\alpha^q}\frac{1}{d^2}J^a_p J^b_r - \frac{d}{2}(J^{-1})^q_b b^{pr} \times \frac{\partial^2\alpha'^a}{\partial\alpha^q\partial\alpha^p}\frac{1}{d}J^b_r - \frac{d}{2}(J^{-1})^q_b b^{pr}\frac{\partial^2\alpha'^b}{\partial\alpha^q\partial\alpha^r}\frac{1}{d}J^a_p. \quad \text{(A5)}$$

Since $(J^{-1})^q{}_b J^b_r = \mathbf{1}^q{}_r$ the second line in the above cancels with the second term in the first line of (A4). The first line in the above can similarly be be rewritten $\frac{1}{2}J^a_p b^{pq}\partial_{\alpha^q}\log d$. Since $\partial_{\alpha^q}\log d = \mathrm{Tr}[J^{-1}\frac{\partial J}{\partial\alpha^q}]$ this cancels with the third line and we have hence simply

$$D'^a = J^a_b D^b + \text{all other terms cancel}. \quad \text{(A6)}$$

APPENDIX B: LOCAL CHARTS OF THE SO(3) GROUP MANIFOLD

Let e be the unit element of SO(3) and let $\mathbf{1}$ be its representation as a unit rotation matrix. The matrices

$$\mathbf{M}(\alpha) = \begin{pmatrix} 0 & -\alpha_3 & \alpha_2 \\ \alpha_3 & 0 & -\alpha_1 \\ -\alpha_2 & \alpha_1 & 0 \end{pmatrix}, \quad \text{(B1)}$$

can be identified with elements in the Lie algebra so(3). Let V_e be a neighborhood of the origin in $\mathbb{R}^3$ with $|\alpha| \leqslant C$, a neighborhood of e in SO(3) is then given by

$$U_e : r(\alpha) = \exp[\mathbf{M}(\alpha)] \quad \alpha \in V_e. \quad \text{(B2)}$$

Let g^* be another element of SO(3) and let $R^* = r(\alpha)$ be its representation as a rotation matrix. The local patch around g^* is then given by

$$U_{g*} : R(\beta) = R^* r(\beta) \quad \beta \in V_e. \quad \text{(B3)}$$

As the exponential is smooth, (B5) provides a one-to-one mapping between vectors in the open ball $\sqrt{\vec\beta^T\vec\beta} < C$ and sets U_{g*} if the maximal radii C are small enough. In fact, the elements along a line in α correspond to rotations around a given axis which give distinct outcomes as long as the angle of rotation is less than half a turn; the constant C therefore has to be less than π. Note that $r^{-1}(\alpha) = r(-\alpha)$.

Using the Levi-Civita tensor and the Einstein convention, we can write

$$r(\alpha)_{ij} = e^{-\epsilon_{ijs}\alpha_s}, \quad \text{(B4)}$$

which is convenient for calculation. However, it has to be remembered that when doing so we connect the basis of the Lie algebra with the body frame (they have to rotate together to keep ϵ invariant). In the main text and below we use a basis such that the angular diffusion matrix $b_{22} = k_B T\eta^{-1}$ entering the elliptic operator $\mathcal{L}_0$ is diagonal at the group identity element e. This together with (B4) means that we have chosen a frame of reference for the body system, the one for which the angular friction matrix η is diagonal, $\eta = \mathrm{diag}(\eta_{11},\eta_{22},\eta_{33})$.

Let now g be another group element close to g^*. As described above it can be represented by a rotation matrix which can be written either as $r(\alpha)r(\Delta\beta)$ with some small $\Delta\beta$ or as $r(\alpha+\Delta\alpha)$, with some small $\Delta\alpha$. This means

$$r(\Delta\beta) = r(-\alpha)r(\alpha+\Delta\alpha), \quad \text{(B5)}$$

which, when the increments are infinitesimal, gives the inverse Jacobian (upper and lower indices do not need to be distinguished since both β and α are elements of $\mathbb{R}^3$)

$$(J^{-1})_{ab} = \frac{\partial\beta_a}{\partial\alpha_b} = \left[\delta_{ab} + \frac{1}{2}\epsilon_{abt}\alpha_t + \frac{1}{6}(\alpha_a\alpha_b - \alpha^2\delta_{ab})\right] + \mathcal{O}(\alpha^3). \quad \text{(B6)}$$

The Jacobian is, similarly,

$$(J)_{ab} = \frac{\partial\alpha_a}{\partial\beta_b} = \left[\delta_{ab} - \frac{1}{2}\epsilon_{abt}\alpha_t + \frac{1}{12}(\alpha_a\alpha_b - \alpha^2\delta_{ab})\right] + \mathcal{O}(\alpha^3). \quad \text{(B7)}$$

The volume element close to unit element is given by

$$d\mathrm{Vol} = d\beta_1 d\beta_2 d\beta_3. \quad \text{(B8)}$$

By above, the volume element in the local coordinate is therefore up to terms quadratic in α given by

$$\sqrt{g}d\alpha_1 d\alpha_2 d\alpha_3 = \left(1 - \tfrac{1}{12}\alpha^2\right)d\alpha_1 d\alpha_2 d\alpha_3. \quad \text{(B9)}$$

In the main text we are interested in the partial differential operator $\mathcal{L}_0^\dagger$. Suppose that at the group element g and in system of local coordinates β around g it is given by a torque (drift field) $T = 0$ and a constant diffusion matrix $\overline{b}$. In coordinates α' centered on g^* $\mathcal{L}_0^\dagger$ is then given by $\frac{1}{\sqrt{g'}}\partial_{\alpha'^a}(-\sqrt{g'}T'^a + \frac{1}{2}\partial_{\alpha'^b}(\sqrt{g'}b'^{ab}))$ where T' and b' follow from the transformations (5). In the case at hand this means

$$T'^a = \frac{1}{2}\frac{\partial^2\alpha'^a}{\partial_{\beta^p}\partial_{\beta^q}}\overline{b}^{pq}, \quad \text{(B10)}$$

$$b'^{ab} = \frac{\partial\alpha'^a}{\partial_{\beta^p}}\frac{\partial\alpha'^b}{\partial_{\beta^q}}\overline{b}^{pq}, \quad \text{(B11)}$$

$$\sqrt{g'} = \det\left(\frac{\partial\alpha'^a}{\partial_{\beta^p}}\right)^{-1}. \quad \text{(B12)}$$

We recognize that the combination $T'^a - \frac{1}{2\sqrt{g'}}\partial_{\alpha'^b}(\sqrt{g'}b'^{ab})$ is the Hänggi-Klimontovich drift which transforms as a vector and which therefore here is zero. The operator (acting on a function h) is hence

$$\mathcal{L}_0^{\dagger}[h] = \frac{1}{2} b'^{ab} \frac{\partial^2 h}{\partial_{\alpha'^a} \partial_{\alpha'^b}} + \frac{1}{2\sqrt{g'}} \partial_{\alpha'^a} (\sqrt{g'} b'^{ab}) \frac{\partial h}{\partial_{\alpha'^b}}. \quad \text{(B13)}$$

The factor $\partial_{\alpha^a}(\sqrt{g} b^{ab})$ is of order $\mathcal{O}(\alpha)$, which means that for a small-enough patch it can be ignored.

APPENDIX C: INVARIANT METHOD

In this section we show how the method to average over the orientations can be used to compute the effective diffusion tensor. The averages over orientations are of the type

$$M_{ijkl} = \langle Q_{ij} \tilde{\gamma}_{kl}^{-1} \rangle \quad \text{(C1)}$$

for some indices (i,j,k,l) and $Q_{ij} = R_{ik}^* Q_{B_{kk}} (R^*)_{kj}^{-1}$, and where the average is taken with respect to the uniform measure (Haar measure). This can be written

$$M_{ijkl} = \frac{\partial^4}{\partial_{x_i} \partial_{y_j} \partial_{z_k} \partial_{w_l}} I(x,y,z,w), \quad \text{(C2)}$$

$$I(x,y,z,w) = \langle Q_{ij} \tilde{\gamma}_{k'l'}^{-1} x_{i'} y_{j'} z_{k'} w_{l'} \rangle, \quad \text{(C3)}$$

where x, y, z, and w are three-dimensional vectors and (i',j',k',l') are summed-over indices (Einstein convention). When the measure is uniform, $I(x,y,z,w)$ must be an invariant of SO(3) since any overall rotation of the vectors can be brought over on the matrices $\tilde{\gamma}$ and Q, and all rotations of the matrices are included in the average. By general invariant theory and by symmetry under $x \leftrightarrow y$ and $z \leftrightarrow w$,

$$I(x,y,z,w) = A(x,y)(z,w) + B(x,z)(y,w) + B(x,w)(y,z),$$

which leads to

$$M_{ijkl} = A \mathbf{1}_{ij} \mathbf{1}_{kl} + B \mathbf{1}_{ik} \mathbf{1}_{jl} + B \mathbf{1}_{il} \mathbf{1}_{jk}, \quad \text{(C4)}$$

where A and B are constants to be determined. We observe that

$$\begin{aligned} \langle Q_{ii} \tilde{\gamma}_{jj}^{-1} \rangle &= 0, \\ \langle Q_{ij} \tilde{\gamma}_{ji}^{-1} \rangle &= \mathrm{Tr}(Q \tilde{\gamma}^{-1}), \end{aligned} \quad \text{(C5)}$$

which gives the equations

$$\begin{aligned} 9A + 6B &= 0, \\ 3A + 12B &= \mathrm{Tr}(Q \tilde{\gamma}^{-1}). \end{aligned} \quad \text{(C6)}$$

The solution is

$$\begin{aligned} A &= -\frac{\mathrm{Tr}(Q \tilde{\gamma}^{-1})}{15}, \\ B &= \frac{\mathrm{Tr}(Q \tilde{\gamma}^{-1})}{10}. \end{aligned} \quad \text{(C7)}$$

In summary, by the invariant method, we only need to compute one trace. A similar calculation was sketched in the main body of the paper for SU(2).

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