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STOCHASTIC MODE REDUCTION FOR THE IMMERSED BOUNDARY METHOD*

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Abstract. We apply the formulation of a stochastic mode reduction method developed in a recent paper of Majda, Timofeyev, and Vanden-Eijnden [*Comm. Pure Appl. Math.*, 54 (2001), pp. 891–974] (MTV) to obtain simplified equations for the dynamics of structures immersed in a thermally fluctuating fluid at low Reynolds (or Kubo) number, as simulated by a recent extension of the immersed boundary (IB) method by Kramer and Peskin [*Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics*, Elsevier Science, Oxford, UK, 2003, pp. 1755–1758]. The effective dynamics of the immersed structures are not obvious in the primitive equations, which involve both fluid and structure dynamics, but the procedure of MTV allows the rigorous derivation of a reduced stochastic system for the immersed structures alone. We find, in the limit of small Reynolds (or Kubo) number, that the Lagrangian particle constituents of the immersed structures undergo a drift-diffusive motion with several physically correct features, including the coupling between dynamics of different particles. The MTV procedure is also applied to the spatially discretized form of the IB equations with thermal fluctuations to assist in the design and assessment of numerical algorithms.

Key words. stochastic mode reduction, immersed boundary method, Brownian motion

AMS subject classifications. 60H10, 60H30, 60J60, 60J65, 60J70, 76R50, 82C31, 82C70, 82C80

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1. Introduction.

In several applications of modern interest, the governing equations can be written as a complex system of stochastic differential equations, with the variables (modes) evolving over a wide range of characteristic time scales. Sometimes, the variables can be grouped into a "fast" class of modes and a "slow" class of modes, with a wide separation between the time scales of the two classes. In such a situation, one can exploit singular perturbation techniques using the ratio of the fast to slow time scales as a small parameter to reduce the system by averaging the effects of the fast modes on the system. A rigorous procedure for averaging over fast fluctuations in a stochastic system was first provided by Khas'minskii [24, 23] and then later developed into more widely applicable theorems by Kurtz [30] (see also [9]), Ellis and Pinsky [7], and Papanicolaou [39]. (See the textbook [17] for an applied exposition.) Recently, Majda, Timofeyev, and Vanden-Eijnden [34, 35, 36] ([36] hereafter referred to as MTV) have developed these mathematical techniques into a methodological framework for climate modeling, where the governing equations are often essentially quadratically nonlinear and contain both slowly varying climate and "mean flow" modes and more rapidly fluctuating modes. In this work and the companion paper [26], we demonstrate how the MTV framework can be applied productively to a quite different class of applications, namely the simulation of microscale fluid systems with immersed structures and thermal fluctuations, such as microphysiological

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systems, colloid suspensions, and polymer suspensions. In the present paper, we focus on the immersed boundary (IB) method [42] for simulating biological systems, as extended recently by Kramer and Peskin [28] to include thermal fluctuations and thereby extend its applicability to small scales (microns).

The IB method emphasizes the dynamics of the fluid environment in which the biological structures, such as polymers, membranes, and particles, are immersed. The forces generated by the biological structures as they are deformed or interact with external fields are communicated locally as forces on the fluid. The fluid then responds dynamically to these forces in a way represented by the Navier–Stokes equations. The structures are then advected (and strained) by their local fluid velocity. Thermal fluctuations are introduced through forces on the fluid. The immersed structures are not directly thermally forced, but rather undergo thermal fluctuations through advection by the thermally fluctuating fluid [28].

The IB method, then, is described by a coupled system of differential equations with the fluid modes stochastically forced. The details of this dynamical system will be presented in section 2. In the microscopic systems for which the method is designed, viscosity plays a strong role. More precisely, one can define a thermal Reynolds number (product of particle size and thermal velocity divided by kinematic viscosity) which will often be small in typical systems of interest. In such instances, the MTV stochastic mode reduction framework can be applied based on this small parameter to deduce a simplified system governing the immersed particles and structures, with the fluid variables eliminated (see section 3). To unify the discussion with the other simulation methods in [26], it is useful to note that the thermal Reynolds number in the IB method can be identified with a "thermal Kubo number," defined as the ratio of the rate of decorrelation of a particle's (Lagrangian) thermal velocity due to its advection into different fluid regions relative to its rate of decorrelation due to viscous damping.

The main motivation for this work is to obtain a rigorous characterization of the effective dynamics of immersed structures in the IB method at low thermal Reynolds (or Kubo) number. These results can then be used to assess the physical fidelity of the simulation method, to point out possible areas for improvement in the simulation scheme, and to calibrate the numerical parameters in applications. As discussed in [27] and section 2 below, thermal fluctuations are incorporated into the IB simulation equations in a rational manner based on statistical mechanics, but because of a basic approximation in the IB method, it is not a priori clear that the simulated Brownian motion of particles displays physically appropriate behavior. In [27], an approximate semianalytical calculation shows that in fact the IB equations do generate correct physical scaling behavior for various statistical features of multiparticle Brownian motion. Several of these results are corroborated and extended in the present work by the rigorous application of the MTV stochastic mode reduction procedure. In particular, a reduced set of stochastic differential equations describing the dynamics of the immersed structures is derived, with the role of the weak advective nonlinearity operating over long time scales and the nonlinear interaction between the immersed structures rigorously assessed. Such nonlinear effects are neglected in [27].

The immersed structures in the IB method are shown, through the stochastic mode reduction procedure, to obey effective drift-diffusive dynamics at long times, with both the drift coefficient and diffusion coefficient explicitly presented in section 4. Through a study of how the drift of the structures is related to the forces they feel, the structure of the self-diffusion coefficient, and the correlations between the diffusive motion of different particles, we explore to what extent the IB method, in ideal form

without numerical discretization issues, can capture various statistical physical aspects of thermally fluctuating systems. We find that many statistical physical features are properly described by the IB method, but identify a discrepancy between how the correlation in the diffusion of two closely separated particles is simulated by the IB method and its physically proper form for rigid particles. The source of the difference appears to be the lack of a sense of rigidity of particles in the IB method, rather than an artifact arising from the discretization of the fluid.

A cruder physical derivation of the same results is presented in section 5 as an aid to intuitive interpretation. Next, in section 6, we show how the effective dynamics are modified under spatial discretization. We do not consider temporal discretization, since the MTV procedure is not formulated for discrete-time systems, though it would seem that the conclusions concerning the effective dynamics would not be altered substantially [14]. Here we give explicit formulas that indicate how the discrete and continuous long-time dynamics are related. This allows us to calibrate parameters in the discrete numerical simulation as a design principle. A detailed analysis and comparison with numerical simulations will be presented in [27].

We close the introduction by describing some connections of the present work with some other stochastic analytical techniques. Our main technical tool is a singular perturbation analysis of the Kolmogorov backward equation (adjoint to the Fokker–Planck equation), a deterministic second-order parabolic partial differential equation associated with the stochastic dynamics of the full system [9, 30, 39]. The solution of this equation, in the limit of small thermal Reynolds (or Kubo) number, can be shown through a theorem of Kurtz [9, 30] to approach the solution of another second-order parabolic partial differential equation in which the variables corresponding to the fluid modes have been eliminated. The effective stochastic dynamics of the immersed structures, including their drift and diffusion coefficients, can be read off from this limiting equation.

This approach allows the treatment of a system with slow and fast modes, both of which are influenced by each other, as is the case for the IB method in general when the immersed structures do exert force. If, however, the immersed structures are simply force-free particles, then the evolution of the fluid is independent of the particle dynamics. The effective particle dynamics under the IB method can then be analyzed by a variety of other techniques. For example, the dynamics of the particles can be viewed as a random evolution problem [20, 21, 40], where the fluid variables play the role of the auxiliary Markov process parametrizing the advection operator. The long-time limiting effective dynamics, averaging out the influence of the fluid variables, can then be calculated through other fast-averaging formulas [2, 20, 21, 40]. Another approach is to view the motion of the particles as tracers in a turbulent diffusion problem, with the fluid velocity field treated as a prescribed Markovian random, time-dependent field and zero "bare" molecular diffusivity [10, 33]. The long-time behavior of the immersed particles can then be treated through homogenization techniques [1, 11]. If the nonlinear advection term can be safely ignored (due to the low Reynolds number), then the fluid velocity field is nothing more than a superposition of Ornstein–Uhlenbeck processes, for which a simpler analysis is possible [4, 11, 27]. We remark though that the standard turbulent diffusion assumption of point particles must be revised to account for the finite effective size of particles in the IB method.

The derivation of effective dynamics for interacting particle systems on large scales and long times can also be approached through "hydrodynamic limit" techniques [15, 18, 38, 50]. Here, one seeks to pass rigorously from a detailed description of the individual particle dynamics to continuum field equations describing the evolution

of the density and momentum of the collective medium formed by the particles. To our knowledge, such work is primarily focused on Hamiltonian systems with small or zero noise, or on random lattice dynamics with conservation laws. We are not aware of any such applications to systems of particles with strong damping and stochastic driving from the environment, which is the mathematical context of our present study. Moreover, hydrodynamic limit techniques seem most suited for systems in which the constituent particles interact with all other particles according to a universal law governed by their separation distance. It is not clear how to adapt these methods to polymer systems with a variety of bonded interactions. And if hydrodynamic limit techniques could be applied in certain circumstances to the IB method at low thermal Reynolds (or Kubo) number, the results would be complementary. Rather than preserving the Lagrangian framework which accounts for arbitrary N-particle interactions, the hydrodynamic limit would generally be expressed in an Eulerian framework in terms of number densities and correlation functions of the immersed particles.

2. Variables and equations for the IB method. In the IB method [42], the entire system of the fluid with immersed structures is treated as a constant density fluid. We moreover assume that the fluid domain Ω is a cube of side length L with periodic boundary conditions. This is typical for applications of the IB method, because it permits the use of a fast Fourier transform [42]. For the moment, though, we will still consider the space-time domain as continuous.

The evolution of the fluid is given by the incompressible Navier–Stokes equations

$$\begin{aligned} \rho\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t)\right) &= \mu\nabla^2\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \mathbf{f}(\mathbf{x},t), \\ \nabla\cdot\mathbf{u}(\mathbf{x},t) &= 0, \end{aligned} \tag{2.1}$$

where $\mathbf{u}(\mathbf{x},t)$ is the fluid velocity, ρ is the density, μ is the dynamic viscosity, p is the pressure, and $\mathbf{f}(\mathbf{x},t)$ is a force density. We decompose the force density into a sum,

$$\mathbf{f}(\mathbf{x},t) = \mathbf{f}_{\mathrm{IS}}(\mathbf{x},t) + \mathbf{f}_T(\mathbf{x},t),$$

with $\mathbf{f}_{\mathrm{IS}}(\mathbf{x},t)$ representing the contribution arising from the immersed structures and $\mathbf{f}_T(\mathbf{x},t)$ representing thermally fluctuating forces from microscopic processes. We next describe how these contributions to the force density are expressed concretely.

The collection of immersed structures will be modelled as a finite collection of Lagrangian particles, located at positions $\mathbf{X} = \{\mathbf{X}_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathcal{A}}$, where $\boldsymbol{\alpha}$ is a Lagrangian labelling index taking values from some finite set $\mathcal{A}$. The various stresses exerted by the immersed structures in response to deformations will be modelled in general through gradients of some interparticle potential $\Phi(\mathbf{X})$. Note that stresses such as those arising from bending resistance can be modelled by n-body interactions with $n > 2$, and still fall within our scope. We assume that there are no external forces, so that the total momentum of the system is conserved ($\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}}\Phi(\mathbf{X}) = 0$, where $\nabla_{\boldsymbol{\alpha}}$ denotes a gradient with respect to the position of the Lagrangian particle $\mathbf{X}_{\boldsymbol{\alpha}}$). By choosing an appropriate inertial frame, we can then assume that the total system momentum is always zero. (We briefly discuss in section 4.3 how the results would be modified if external forces were allowed to be present.)

With the potential prescribed, we can then describe the force density exerted on the fluid by applying the force exerted on each Lagrangian particle at its current position $\mathbf{X}_{\boldsymbol{\alpha}}(t)$, spread out via a smoothed delta function $\delta_a(\mathbf{x})$ with length scale a.

The choice of smoothing is dictated by numerical considerations, such as compact support and the minimization of oscillations in the fluid-particle interaction as the particles move with respect to the fluid grid [42]. We therefore write

$$\mathbf{f}_{\mathrm{IS}}(\mathbf{x},t) = -\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}}\Phi(\mathbf{X}(t))\delta_a(\mathbf{x}-\mathbf{X}_{\boldsymbol{\alpha}}(t)). \tag{2.2}$$

The parameter a acts as an effective particle size.

The thermal force density is obtained using a fluctuation-dissipation theorem from statistical hydrodynamics [27, 31] and is most clearly expressed in terms of its Fourier series expansion:

$$\begin{aligned} \mathbf{f}_T(\mathbf{x},t) &= \sum_{\mathbf{k}\in S} \mathbf{f}_{T,\mathbf{k}}(t) e^{2\pi i \mathbf{k}\cdot\mathbf{x}/L}, \\ \mathbf{f}_{T,\mathbf{k}}(t) &= \sqrt{\frac{8\pi^2 k^2 \mu k_B T}{L^5}}\,\frac{d\tilde{\mathbf{W}}_{\mathbf{k}}(t)}{dt}, \end{aligned} \tag{2.3}$$

where k_B is Boltzmann's constant, T is the absolute temperature, and $\{\tilde{\mathbf{W}}_{\mathbf{k}}(t)\}_{\mathbf{k}\in S}$ are a collection of standard complex Brownian processes, which are mutually independent except for the complex conjugacy relation

$$\tilde{\mathbf{W}}_{-\mathbf{k}}(t) = \overline{\tilde{\mathbf{W}}_{\mathbf{k}}(t)}, \tag{2.4}$$

which arises from the need to keep $\mathbf{f}_T(\mathbf{x},t)$ real-valued. By a "standard complex Brownian motion," we refer to a mean-zero Gaussian process with stationary increments satisfying

$$\langle d\tilde{\mathbf{W}}(t)\otimes d\tilde{\mathbf{W}}(t')\rangle = 0, \qquad \langle d\tilde{\mathbf{W}}(t)\otimes \overline{d\tilde{\mathbf{W}}(t')}\rangle = \mathcal{I}\delta(t-t')\,dt\,dt', \tag{2.5}$$

where $\mathcal{I}$ is the identity matrix. Please note that the definition of complex Brownian motion processes used in MTV [36] differs by a factor of two in normalization of the variance. In (2.3) and elsewhere in the paper, for simplicity in exposition, we occasionally use the formal notation $d\tilde{\mathbf{W}}(t)/dt$ for the white noise derivative of Brownian motion. Of course, the equations can be given a rigorous interpretation through use of the more proper Itô stochastic differential notation [37]. The set of wavenumbers is just the lattice of integers in three dimensions, with the zero mode excluded since it will always vanish: $S = \mathbb{Z}^3 \setminus \{\mathbf{0}\}$.

We note that the continuum formulation in which all these modes are retained requires care in a serious interpretation, because the velocity field induced by the thermal forcing in (2.3) exhibits an ultraviolet catastrophe due to singular small scale structure. We will not concern ourselves with such subtleties here, because in any numerical implementation the number of modes simulated is finite. Therefore, we will proceed just as if S were a finite collection of modes corresponding to some symmetric Galerkin truncation. However, in our actual discretized implementation, the IB equations are not simply crudely cut off in this way, and we show in section 6 how the results and arguments should be modified to apply to the actual numerical discretization.

With the Navier–Stokes equations (2.1) and the equations (2.2) and (2.3) for the force density, we have defined how the fluid evolves. The particle positions are updated by simple advection by the fluid at a locally interpolated fluid velocity:

$$\frac{d\mathbf{X}_{\boldsymbol{\alpha}}(t)}{dt} = \mathbf{u}_a(\mathbf{X}_{\boldsymbol{\alpha}}(t),t).$$

The same smoothed delta function that was used to spread force is used to interpolate velocity:

$$\mathbf{u}_a(\mathbf{x},t) = \int_\Omega \mathbf{u}(\mathbf{x}',t)\delta_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}'; \tag{2.6}$$

this choice (along with the enforced reflection symmetry $\delta_a(\mathbf{x}) = \delta_a(-\mathbf{x})$) conserves energy in the particle-fluid interactions [42]. Note that, particularly in this integration, the delta function δ_a should be viewed as periodic (with its spikes centered at every point of the form (n_1L, n_2L, n_3L) with n_1, n_2, and n_3 integers). Equivalently, the convolution in (2.6) should be viewed as convolution on a torus [25].

2.1. Summary of IB equations in dimensional form. Summarizing, we have the following system of equations for the IB method:

$$\begin{aligned}
\rho\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t)\right) &= \mu\nabla^2\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \mathbf{f}_T(\mathbf{x},t) \\
&\quad - \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}}\Phi(\mathbf{X}(t))\delta_a(\mathbf{x}-\mathbf{X}_{\boldsymbol{\alpha}}(t)), \\
\nabla\cdot\mathbf{u}(\mathbf{x},t) &= 0, \\
\frac{d\mathbf{X}_{\boldsymbol{\alpha}}(t)}{dt} &= \mathbf{u}_a(\mathbf{X}_{\boldsymbol{\alpha}}(t),t), \\
\mathbf{u}_a(\mathbf{x},t) &= \int_\Omega \mathbf{u}(\mathbf{x}',t)\delta_a(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}',
\end{aligned} \tag{2.7a}$$

with the thermal forcing given by the following random process:

$$\mathbf{f}_T(\mathbf{x},t) = \sum_{\mathbf{k}\in S}\sqrt{\frac{8\pi^2k^2\mu k_BT}{L^5}}\,e^{2\pi i\mathbf{k}\cdot\mathbf{x}/L}\frac{d\tilde{\mathbf{W}}_{\mathbf{k}}(t)}{dt}. \tag{2.7b}$$

These equations are supplemented with initial conditions

$$\mathbf{X}_{\boldsymbol{\alpha}}(t=0) = \mathbf{X}_{0,\boldsymbol{\alpha}}, \qquad \mathbf{u}(\mathbf{x},t=0) = \mathbf{u}^0(\mathbf{x}).$$

2.2. Nondimensionalization. To prepare for the asymptotic results and calculations in subsequent sections, we nondimensionalize the IB equations. This will make manifest the role of the relevant Kubo number as a small parameter. We choose to nondimensionalize with respect to a length and time scale associated with the thermal forcing.

2.2.1. Parameters of externally specified functions. To facilitate the parametrization of the contributions from the initial data and the prescribed force law of the immersed structures, we express each in terms of dimensionless functions.

The initial velocity field will be described by a magnitude U_0 and length scale ℓ_v, and we write

$$\mathbf{u}^0(\mathbf{x}) = U_0\tilde{\mathbf{u}}^0(\mathbf{x}/\ell_v),$$

where $\tilde{\mathbf{u}}^0$ is a dimensionless function.

We identify ψ as a *force density* induced by the immersed structures, and ℓ_f as a length scale on which the immersed structure forces vary. More explicitly, we assume

$$\Phi(\mathbf{X}) = \psi\ell_f a^3\tilde{\Phi}(\mathbf{X}/\ell_f)$$

for some nondimensional function $\tilde{\Phi}$ with order unity amplitude and order unity gradients of its argument. Then an elementary constituent particle (with volume a^3) will experience a force of magnitude ψa^3.

Envisioning that the immersed structures will be modelled as a collection of elementary constituent particles with effective size a and spacing on the order of a, we will nondimensionalize $\mathbf{X}_{0,\boldsymbol{\alpha}}$ with respect to a:

$$\mathbf{X}_{0,\boldsymbol{\alpha}} = a\tilde{\mathbf{X}}_{0,\boldsymbol{\alpha}}.$$

Of course, the functions described above could have various amplitudes and length scales, depending on the model, but such complications do not bear on the central point of this work.

2.2.2. Reference units. We choose the following units to normalize the equations with respect to the thermal dynamics of the particles:

(i) length scale $\ell_T = a$,
(ii) time scale $\tau_T = \sqrt{\rho a^5/k_B T}$,
(iii) mass $m_T = \rho a^3$.

For example, the mass reference unit is just the mass associated with an elementary particle in the IB formulation (a single delta function), and length and time units are chosen so that the reference velocity

$$V_T \equiv \frac{\ell_T}{\tau_T} = \sqrt{\frac{k_B T}{\rho a^3}}$$

has the order of magnitude of the thermalized velocity of an elementary particle (since the IB system with thermal forcing respects the equipartition law [27]). Note that, after nondimensionalization, the fluid density, the width of the delta function (as well as the grid spacing), and the root-mean-square of the fluid velocity averaged over an elementary particle region are all order unity.

2.2.3. Nondimensional groups. With the above nondimensionalization, the IB dynamics are governed by the following nondimensional groups:

(i) Kubo number based on thermal forcing

$$\mathrm{Ku_T} = \frac{\ell_T^2}{\nu \tau_T} = \sqrt{\frac{k_B T}{\rho \nu^2 a}}, \tag{2.8}$$

where $\nu = \mu/\rho$ is the kinematic viscosity of the fluid;

(ii) nondimensionalized measures of the effects of structural forces and initial velocity

$$\phi = \frac{\psi a^4}{k_B T}, \qquad \Upsilon = \sqrt{\frac{U_0^2 \rho a^3}{k_B T}} = \frac{U_0}{V_T};$$

(iii) length scale ratios

$$\tilde{K} = \frac{L}{a}, \qquad \tilde{\ell}_f = \frac{\ell_f}{a}, \qquad \tilde{\ell}_v = \frac{\ell_v}{a}.$$

We pause to clarify why the nondimensional group $\mathrm{Ku_T}$ is identified as a Kubo number and can also be viewed here as a thermal particle Reynolds number. A

Kubo number is generally defined as the ratio of the time scales of decorrelation of a particle's motion due to intrinsic (Eulerian) processes to that due to advection across variable spatial structure [29, 52]. In the present context, $\tau_T = \ell_T/V_T$ is the time scale on which one of the Lagrangian particles would change its velocity due to its motion (at typical speed V_T) because of its sampling of a new environment after it moves a distance equal to its size $\ell_T = a$. The time scale $\ell_T^2/\nu = a^2/\nu$, on the other hand, describes the intrinsic (Eulerian) decorrelation rate of the fluid velocity averaged over the region occupied by a particle of size a.

Alternatively, the group (2.8) can be viewed as a thermal particle Reynolds number $\mathrm{Re_T}$, since it is the product of a characteristic particle length scale ($\ell_T = a$) and the thermal velocity of the fluid $V_T = \ell_T/\tau_T$ divided by the kinematic viscosity [51]. (Note that the notion of the thermal velocity of a fluid makes sense only if it is discretized or smoothed over some finite region (here taken to be of width a).) The fact that the thermal particle Reynolds number $\mathrm{Re_T} = \mathrm{Ku_T}$ decreases with the length scale a may be surprising; the reason is that the root-mean-square velocity sampled over a region a scales as $a^{-3/2}$ because of its short-range correlations. Therefore, while $\mathrm{Re_T}$ is small, it is not as minuscule as one might expect based on macroscopic intuition. For typical parameter values $k_B = 1.4 \times 10^{-16}$erg/K, $T = 300$ K, $\nu = 0.01$ cm/s, we have

$$\mathrm{Re_T} \approx \sqrt{\frac{5 \times 10^{-4}\mu\mathrm{m}}{a}}.$$

The elementary constituent size in a numerical simulation will be of the order $a \sim 0.01 - 0.1\mu$m, and thus we see that the Reynolds number based on the thermal forcing can be expected to be on the order of 10^{-2}–10^{-1}. We emphasize the thermal Kubo number interpretation because it allows the most parallel handling of the three simulation methods discussed in the companion paper [26].

2.2.4. Nondimensionalized IB equations. We now nondimensionalize the independent and dependent variables with respect to the reference units described in section 2.2.2, but denote their nondimensional versions by the same symbols. We retain special symbols for the nondimensionalized externally prescribed functions, as defined in section 2.2.3,

$$\begin{aligned}
\left(\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla\mathbf{u}(\mathbf{x},t)\right) &= \mathrm{Ku_T}^{-1}\nabla^2\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) + \mathbf{f}_T(\mathbf{x},t) \\
&\quad - \phi\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}}\tilde{\Phi}\left(\frac{\mathbf{X}(t)}{\tilde{\ell}_f}\right)\delta_1(\mathbf{x}-\mathbf{X}_{\boldsymbol{\alpha}}(t)), \\
\nabla\cdot\mathbf{u}(\mathbf{x},t) &= 0, \\
\frac{d\mathbf{X}_{\boldsymbol{\alpha}}(t)}{dt} &= \mathbf{u}_1(\mathbf{X}_{\boldsymbol{\alpha}}(t),t), \\
\mathbf{u}_1(\mathbf{x},t) &= \int_\Omega \mathbf{u}(\mathbf{x}',t)\delta_1(\mathbf{x}-\mathbf{x}')\,d\mathbf{x}',
\end{aligned} \tag{2.9a}$$

with the thermal forcing given by the following random process

$$\mathbf{f}_T(\mathbf{x},t) = \mathrm{Ku_T}^{-1/2}\tilde{K}^{-3/2}\sum_{\mathbf{k}\in S}\sqrt{2\left(4\pi^2\left(\frac{k}{\tilde{K}}\right)^2\right)}e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}\,\frac{d\tilde{\mathbf{W}}_{\mathbf{k}}(t)}{dt} \tag{2.9b}$$

and initial data

$$\mathbf{X}_{\boldsymbol{\alpha}}(t=0) = \tilde{\mathbf{X}}_{0,\boldsymbol{\alpha}}, \qquad \mathbf{u}(\mathbf{x}, t=0) = \Upsilon \tilde{\mathbf{u}}^0 \left(\frac{\mathbf{x}}{\tilde{\ell}_v} \right). \tag{2.9c}$$

(We note that $\nabla_{\boldsymbol{\alpha}} \tilde{\Phi}(\mathbf{X}/\tilde{\ell}_f)$ is to be interpreted as the gradient with respect to the $\boldsymbol{\alpha}$ coordinate of $\tilde{\Phi}$, evaluated at $\mathbf{X}/\tilde{\ell}_f$.)

3. Stochastic mode reduction procedure. For the microscopic applications for which the IB method with thermal fluctuations has been designed, the systems are at low thermal Kubo number, so the fluid motion is strongly damped by viscosity. The positions of the immersed structures, however, have no such damping terms in their equations of motion, and should therefore evolve on a slower time scale than the fluid variables. To make these notions quantitative, we consider the Kubo number based on the thermal forcing, Ku_T, as a small parameter. Then we see from (2.9) that, at least formally, the (nondimensionalized) fluid variables evolve on the fast time scale $\mathrm{Ku}_\mathrm{T}^{-1}$, while the immersed structure positions evolve on a slower time scale of $O(1)$ or longer. The IB equations are therefore well suited for the stochastic mode reduction framework developed in MTV. That is, we can systematically eliminate the fluid variables from consideration for small Ku_T and obtain a closed stochastic equation for the immersed structure positions $\{\mathbf{X}_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathcal{A}}$ alone. We now sketch this stochastic mode reduction procedure for the IB system. The detailed calculations can be found in the appendix. The result will be presented at the beginning of section 4.

3.1. Fourier expansion of IB equations. We prepare by expanding the velocity field (which is assumed periodic) in a Fourier series:

$$\mathbf{u}(\mathbf{x}, t) = \sum_{\mathbf{k}\in S} e^{2\pi i \mathbf{k}\cdot\mathbf{x}/\tilde{K}} \hat{\mathbf{u}}_{\mathbf{k}}(t). \tag{3.1}$$

The Navier–Stokes equations now become a coupled collection of stochastic ordinary differential equations. The nondimensionalized IB system (2.9), expressed in terms of the Fourier coefficients of the velocity field, reads

$$\begin{aligned} d\hat{\mathbf{u}}_{\mathbf{k}}(t) &= -\mathcal{B}_{\mathbf{k}}(\mathbf{U}(t), \mathbf{U}(t))\, dt - 4\pi^2 (k/\tilde{K})^2 \mathrm{Ku}_\mathrm{T}^{-1} \hat{\mathbf{u}}_{\mathbf{k}}(t)\, dt \\ &\quad - \phi \mathcal{P}_{\mathbf{k}} \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}} \tilde{\Phi}(\mathbf{X}(t)/\tilde{\ell}_f) \hat{\delta}_{1,\mathbf{k}} e^{-2\pi i \mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(t)/\tilde{K}}\, dt \\ &\quad + \mathrm{Ku}_\mathrm{T}^{-1/2} \tilde{K}^{-3/2} \sqrt{2(4\pi^2 (k/\tilde{K})^2)}\, \mathcal{P}_{\mathbf{k}} d\tilde{\mathbf{W}}_{\mathbf{k}}(t), \\ d\mathbf{X}_{\boldsymbol{\alpha}}(t) &= \tilde{K}^3 \sum_{\mathbf{k}\in S} e^{2\pi i \mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(t)/\tilde{K}} \hat{\mathbf{u}}_{\mathbf{k}}(t) \hat{\delta}_{1,\mathbf{k}}\, dt, \end{aligned} \tag{3.2a}$$

with initial data

$$\mathbf{X}_{\boldsymbol{\alpha}}(t=0) = \tilde{\mathbf{X}}_{0,\boldsymbol{\alpha}}, \qquad \hat{\mathbf{u}}_{\mathbf{k}}(\mathbf{x}, t=0) = \Upsilon \hat{\tilde{\mathbf{u}}}^0_{\mathbf{k},\tilde{\ell}_v}. \tag{3.2b}$$

The Fourier expansion coefficients of the nonlinear advection term are

$$\mathcal{B}_{\mathbf{k}}(\mathbf{U}, \mathbf{U}) = 2\pi i \tilde{K}^{-1} \mathcal{P}_{\mathbf{k}} \sum_{\mathbf{k}'\in S} (\mathbf{u}_{\mathbf{k}'} \cdot \mathbf{k}) \mathbf{u}_{\mathbf{k}-\mathbf{k}'}. \tag{3.2c}$$

The effect of the pressure has been replaced in the standard way [32] through the introduction of a projection tensor which enforces incompressibility of each Fourier velocity mode:

$$\mathcal{P}_{\mathbf{k}} = \mathcal{I} - \frac{\mathbf{k} \otimes \mathbf{k}}{k^2}.$$

In our notation, variables with $\mathbf{k}$ subscripts indicate Fourier coefficients, as defined through the nondimensionalized Fourier transform (3.1). Note that $\{\hat{\tilde{\mathbf{u}}}^0_{\mathbf{k},\tilde{\ell}_v}\}_{\mathbf{k}\in S}$ are the Fourier coefficients of $\tilde{\mathbf{u}}^0(\mathbf{x}/\tilde{\ell}_v)$ and not of $\tilde{\mathbf{u}}^0(\mathbf{x})$. Finally, $\mathbf{U}$ is a shorthand for the collection of all Fourier velocity modes $\{\hat{\mathbf{u}}_{\mathbf{k}}\}_{\mathbf{k}\in S}$, though we recall that the zero mode $\mathbf{u}_0 \equiv \mathbf{0}$ because of our assumption that the global system momentum is conserved. To avoid excessive proliferation of $\mathcal{P}_{\mathbf{k}}$ symbols, we will consider the variables $\hat{\mathbf{u}}_{\mathbf{k}}$ to always be constrained to satisfy the incompressibility condition $\mathbf{k} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = 0$. We will not concern ourselves unduly with the infinite number of modes in S, an ideal continuum fluid system. Indeed, all results converge, and our main interest is really in a discretized finite version of these equations (section 6).

For the sake of integration and differentiation, it will be convenient to follow a convention in complex analysis of treating $\hat{\mathbf{u}}_{\mathbf{k}}$ and $\hat{\mathbf{u}}^*_{\mathbf{k}}$ as independent variables, each with two degrees of freedom (due to the transversality condition $\mathbf{k} \cdot \hat{\mathbf{u}}_{\mathbf{k}} = \mathbf{k} \cdot \hat{\mathbf{u}}^*_{\mathbf{k}} = \mathbf{0}$). Note, however, that because $\mathbf{u}(\mathbf{x}, t)$ is a real-valued vector field, its Fourier coefficients must satisfy the complex conjugacy relations

$$\hat{\mathbf{u}}_{-\mathbf{k}}(t) = \hat{\mathbf{u}}^*_{\mathbf{k}}(t).$$

Therefore, we can consider $\{\hat{\mathbf{u}}_{\mathbf{k}}\}_{\mathbf{k}\in S}$ as a complete set of independent fluid coordinates.

3.2. Kolmogorov backward equation formulation. The calculation is performed on the Kolmogorov backward equation associated with the nondimensionalized IB equations (3.2):

$$\begin{aligned}
-\frac{\partial \rho(s, \mathbf{X}, \mathbf{U}|t)}{\partial s} = \sum_{\mathbf{k}\in S} \Bigg[& -\mathcal{B}_{\mathbf{k}}(\mathbf{U}, \mathbf{U}) - \phi \mathcal{P}_{\mathbf{k}} \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}} \tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right) \hat{\delta}_{1,\mathbf{k}} e^{-2\pi i \mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}} \\
& - \mathrm{Ku}_{\mathrm{T}}^{-1} \left(4\pi^2 \left(\frac{k}{\tilde{K}}\right)^2\right) \hat{\mathbf{u}}_{\mathbf{k}} \Bigg] \cdot \frac{\partial \rho}{\partial \hat{\mathbf{u}}_{\mathbf{k}}} \\
& + \mathrm{Ku}_{\mathrm{T}}^{-1} \sum_{\mathbf{k}\in S} \tilde{K}^{-3} \left(4\pi^2 \left(\frac{k}{\tilde{K}}\right)^2\right) \frac{\partial}{\partial \hat{\mathbf{u}}^*_{\mathbf{k}}} \cdot \frac{\partial \rho}{\partial \hat{\mathbf{u}}_{\mathbf{k}}} \\
& + \tilde{K}^3 \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \sum_{\mathbf{k}\in S} e^{2\pi i \mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}} \hat{\delta}_{1,\mathbf{k}} \hat{\mathbf{u}}_{\mathbf{k}} \cdot \frac{\partial \rho}{\partial \mathbf{X}_{\boldsymbol{\alpha}}}, \\
\rho(s = t, \mathbf{X}, \mathbf{U}|t) = f(\mathbf{X}, \mathbf{U}).
\end{aligned} \tag{3.3}$$

The solution $\rho(s, \mathbf{X}, \mathbf{U}|t)$ to this Kolmogorov backward equation has the mathematical interpretation as the following conditional expectation:

$$\rho(s, \mathbf{X}, \mathbf{U}|t) = \mathbb{E}\left[f(\mathbf{X}(t), \mathbf{U}(t))|\mathbf{X}(s) = \mathbf{X}, \mathbf{U}(s) = \mathbf{U}\right], \tag{3.4}$$

where $\mathbf{X}(t)$ and $\mathbf{U}(t)$ evolve according to the IB equations (3.2) forward in time, conditioned on their starting at time $s < t$ from values $\mathbf{X}(s) = \mathbf{X}$ and $\mathbf{U}(s) = \mathbf{U}$,

and $\mathbb{E}$ denotes an average over the stochastic noise terms in the evolution equations. Because of the slight complication of using complex coordinates, we provide a formal derivation of the Kolmogorov backward equation in the appendix.

Some notational remarks are in order. We hope the reader will not be confused by our previous use of ρ as a symbol for fluid density; with the nondimensionalization in section 2.2, the fluid density has been removed from the problem and we have reallocated its symbol. To avoid straining the reader's eyes with numerous subscripts upon subscripts, we have used partial derivative notation to represent gradients with respect to vectorial modes when they apply to functions of both $\mathbf{U}$ and $\mathbf{X}$:

$$\frac{\partial}{\partial \hat{\mathbf{u}}_{\mathbf{k}}} = \nabla_{\hat{\mathbf{u}}_{\mathbf{k}}}, \qquad \frac{\partial}{\partial \mathbf{X}_{\boldsymbol{\alpha}}} = \nabla_{\mathbf{X}_{\boldsymbol{\alpha}}}.$$

We still use the abbreviation $\nabla_{\boldsymbol{\alpha}}$ for $\nabla_{\mathbf{X}_{\boldsymbol{\alpha}}}$ when applied to a function only of $\mathbf{X}$. Following the usual practice in complex analysis, $\hat{\mathbf{u}}_{\mathbf{k}}$ and $\hat{\mathbf{u}}_{\mathbf{k}}^*$ are considered to be independent variables in differentiation, so that, for example, $\partial g(\hat{\mathbf{u}}_{\mathbf{k}}^*)/\partial \hat{\mathbf{u}}_{\mathbf{k}} = 0$. Finally, we have suppressed the time arguments of most terms in the Kolmogorov backward equation; they are all understood to be evaluated at the running time argument s.

The Kolmogorov backward equation is not being used here to actually solve for the evolution of some expectation of some function of the system variables, but merely as a tool to cast the stochastic dynamics in terms of a deterministic PDE. Perhaps the Kolmogorov forward (or Fokker–Planck) equation, which describes the evolution of the probability density of the system variables, may be a more intuitive formulation, but rigorous theorems are generally easier to prove for the backward equation (see MTV section 4.4 and references therein).

3.3. Identification of small parameter and rescaling of time. We identify $\varepsilon = \mathrm{Ku}_{\mathrm{T}}$ as the small parameter and rescale to a longer time $t \to t/\varepsilon$. This temporal rescaling is necessary to see nontrivial dynamics in the $\varepsilon \downarrow 0$ limit, as we shall discuss in section 5. The Kolmogorov backward equation for the rescaled function

$$\rho^{\varepsilon}(s, \mathbf{X}, \mathbf{U}|t) = \rho(s/\varepsilon, \mathbf{X}, \mathbf{U}|t/\varepsilon)$$

may then be written as

$$\begin{aligned} -\frac{\partial \rho^{\varepsilon}(s, \mathbf{X}, \mathbf{U}|t)}{\partial s} &= \varepsilon^{-2}\mathcal{L}_1\rho^{\varepsilon} + \varepsilon^{-1}\mathcal{L}_2\rho^{\varepsilon}, \\ \rho^{\varepsilon}(s = t, \mathbf{X}, \mathbf{U}|t) &= f(\mathbf{X}, \mathbf{U}), \end{aligned} \tag{3.5a}$$

with differential operators

$$\begin{aligned} \mathcal{L}_1 &= \sum_{\mathbf{k}\in S}\left[-\left(4\pi^2\left(\frac{k}{\tilde{K}}\right)^2\right)\hat{\mathbf{u}}_{\mathbf{k}}\right]\cdot\frac{\partial}{\partial \hat{\mathbf{u}}_{\mathbf{k}}} + \left(4\pi^2\left(\frac{k}{\tilde{K}}\right)^2\right)\tilde{K}^{-3}\frac{\partial}{\partial \hat{\mathbf{u}}_{\mathbf{k}}^*}\cdot\frac{\partial}{\partial \hat{\mathbf{u}}_{\mathbf{k}}}, \\ \mathcal{L}_2 &= \sum_{\mathbf{k}\in S}\left[-\mathcal{B}_{\mathbf{k}}(\mathbf{U}, \mathbf{U}) - \phi\mathcal{P}_{\mathbf{k}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}}\tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\right]\cdot\frac{\partial}{\partial \hat{\mathbf{u}}_{\mathbf{k}}} \\ &\quad + \tilde{K}^3\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\sum_{\mathbf{k}\in S}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\hat{\delta}_{1,\mathbf{k}}\hat{\mathbf{u}}_{\mathbf{k}}\cdot\frac{\partial}{\partial \mathbf{X}_{\boldsymbol{\alpha}}}. \end{aligned} \tag{3.5b}$$

3.4. Computation of limiting equation. We now apply singular perturbation techniques to this problem to find the equation satisfied by $\rho_0 \equiv \lim_{\varepsilon\downarrow 0}\rho^\varepsilon$. This calculation is presented in the appendix. We find that

$$\begin{aligned} -\frac{\partial \rho_0}{\partial s} &= \bar{\mathcal{L}}\rho_0, \\ \rho_0(s=t,\mathbf{X}|t) &= f(\mathbf{X}), \end{aligned} \tag{3.6a}$$

where the limiting differential operator is given by

$$\begin{aligned} \bar{\mathcal{L}}g(\mathbf{X}) = &-\phi\tilde{K}^3 \sum_{\mathbf{k}\in S} \frac{\hat{\delta}_{1,\mathbf{k}}^2}{4\pi^2(k/\tilde{K})^2}\mathcal{P}_{\mathbf{k}} \sum_{\boldsymbol{\alpha},\boldsymbol{\alpha}'\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}'}\tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right) e^{2\pi i\mathbf{k}\cdot(\mathbf{X}_{\boldsymbol{\alpha}}-\mathbf{X}_{\boldsymbol{\alpha}'})/\tilde{K}} \cdot \frac{\partial g(\mathbf{X})}{\partial \mathbf{X}_{\boldsymbol{\alpha}}} \\ &+ \tilde{K}^3 \sum_{\boldsymbol{\alpha},\boldsymbol{\alpha}'\in\mathcal{A}} \sum_{\mathbf{k}\in S} \frac{|\hat{\delta}_{1,\mathbf{k}}|^2}{4\pi^2(k/\tilde{K})^2} e^{2\pi i\mathbf{k}\cdot(\mathbf{X}_{\boldsymbol{\alpha}}-\mathbf{X}_{\boldsymbol{\alpha}'})} \frac{\partial}{\partial \mathbf{X}_{\boldsymbol{\alpha}}} \cdot \mathcal{P}_{\mathbf{k}} \cdot \frac{\partial g(\mathbf{X})}{\partial \mathbf{X}_{\boldsymbol{\alpha}'}}. \end{aligned} \tag{3.6b}$$

3.4.1. Passage to reduced stochastic representation. We realize now that the PDE for ρ_0 is again a Kolmogorov backward equation for a Markov process, which we present in the next proposition. This relation can be checked through a stochastic Taylor expansion [22], as in the appendix. We use the fact that $\hat{\delta}_{1,\mathbf{k}} = \hat{\delta}_{1,\mathbf{k}}^*$ due to the assumed even symmetry $\delta_1(\mathbf{x}) = \delta_1(-\mathbf{x})$.

4. Effective dynamics for immersed structures at low thermal Kubo number. The outcome of the stochastic mode reduction procedure is summarized in the following proposition.

PROPOSITION 4.1 (IB dynamics at small Kubo number). *Suppose the IB system* (2.9) *conserves total momentum* ($\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}}\Phi(\mathbf{X}) = 0$). *Then, in the limit* $\mathrm{Ku_T} \to 0$, *with all other nondimensional quantities held fixed, the solution for the immersed structure dynamics* $\{\mathbf{X}_{\boldsymbol{\alpha}}(t)\}_{\boldsymbol{\alpha}\in\mathcal{A}}$, *obtained from the complete coupled fluid-structure system and rescaled in time as*

$$\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t) = \lim_{\mathrm{Ku_T}\to 0} \mathbf{X}_{\boldsymbol{\alpha}}(t/\mathrm{Ku_T}),$$

converges in law to the solution of the following simplified stochastic differential system involving only the structure variables $\{\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t)\}$:

$$\begin{aligned} d\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t) &= \bar{\mathbf{V}}_{\boldsymbol{\alpha}}(\bar{\mathbf{X}}(t))\,dt + \sum_{\mathbf{k}\in S} \mathcal{S}_{\mathbf{k}}(\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t))\,d\tilde{\mathbf{W}}_{\mathbf{k}}(t), \\ \bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t=0) &= \tilde{\mathbf{X}}_{0,\boldsymbol{\alpha}}, \end{aligned} \tag{4.1}$$

where the stochastic complex white noise terms $d\tilde{\mathbf{W}}_{\mathbf{k}}(t)$ *are defined below* (2.3) *and are given the Itô interpretation. The explicit expression for the drift term is*

$$\bar{\mathbf{V}}_{\boldsymbol{\alpha}}(\mathbf{X}) = -\phi \sum_{\boldsymbol{\alpha}'} \bar{\mathcal{M}}(\mathbf{X}_{\boldsymbol{\alpha}} - \mathbf{X}_{\boldsymbol{\alpha}'})\nabla_{\boldsymbol{\alpha}'}\tilde{\Phi}(\mathbf{X}/\tilde{\ell}_f), \tag{4.2}$$

and the matrix coefficients of the stochastic terms are

$$\mathcal{S}_{\mathbf{k}}(\mathbf{x}) = \sqrt{2\hat{\bar{\mathcal{M}}}_{\mathbf{k}}}\, e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}. \tag{4.3}$$

We have defined the mobility matrix function

$$\bar{\mathcal{M}}(\mathbf{r}) = \sum_{\mathbf{k}\in S} \hat{\bar{\mathcal{M}}}_{\mathbf{k}} e^{2\pi i \mathbf{k}\cdot\mathbf{r}/\tilde{K}} \tag{4.4}$$

and its Fourier coefficients

$$\hat{\bar{\mathcal{M}}}_{\mathbf{k}} \equiv \tilde{K}^3 \frac{\mathcal{P}_{\mathbf{k}} |\hat{\delta}_{1,\mathbf{k}}|^2}{4\pi^2 (k/\tilde{K})^2}.$$

The $\{\hat{\delta}_{1,\mathbf{k}}\}_{\mathbf{k}\in S}$ *are the Fourier coefficients of the delta function* $\delta_1(\mathbf{x})$ *(which we recall is to be viewed as a periodic smoothed delta function on the lattice generated by the fundamental cubic fluid domain),*

$$\hat{\delta}_{1,\mathbf{k}} = \frac{1}{\tilde{K}^3} \int_\Omega e^{-2\pi i \mathbf{k}\cdot\mathbf{x}/\tilde{K}} \delta_1(\mathbf{x})\, d\mathbf{x},$$

and we have introduced the projection tensor which enforces incompressibility of each Fourier velocity mode:

$$\mathcal{P}_{\mathbf{k}} = \mathcal{I} - \frac{\mathbf{k}\otimes\mathbf{k}}{k^2}.$$

The asymptotic statement in the proposition can be justified rigorously (see MTV section 4.4), provided that only a finite number of Fourier modes are retained. Later, in section 6, we modify these results to describe finite truncations which are better suited for numerical simulations. The asymptotics reported in the proposition are uniformly valid if the parameters ϕ and Υ are order unity or become small. Large values of ϕ might be of interest in structural models with some vibrational modes that may have time scales comparable to those of the fluid (or at least much faster than other translational and rotational modes of the structures). In this case, it may be desirable to apply the stochastic mode reduction procedure to eliminate some of the fast vibrational modes as well as the fluid modes. This falls outside the scope of our present results, and we leave its study for future work.

We will defer a discussion of the physical origin of the dynamics for $\bar{\mathbf{X}}(t)$ until section 5. There we will also develop the somewhat complicated formulas for the effective drift and diffusion coefficients into some more transparent consequents for one- and two-particle motion.

Here, we make only some brief remarks about the mathematical structure (section 4.1) and physical fidelity (section 4.2) of the effective dynamics, and comment on how the situation would be changed in a system which did not conserve momentum (section 4.3).

4.1. Mathematical remarks.

1. Perhaps somewhat surprisingly, in the low thermal Kubo number limit, the nonlinear advection term in the Navier–Stokes equation has no influence on the effective equation for $\bar{\mathbf{X}}(t)$. This fact is a consequence of the nonlinear advection term's having zero mean when averaged against the invariant measure (see (A.5)) for the velocity modes:

$$\langle \mathbf{u}\cdot\nabla\mathbf{u}\rangle = \langle \nabla\cdot(\mathbf{u}\otimes\mathbf{u})\rangle = \mathbf{0}.$$

A fundamental reason for the vanishing of the nonlinear advection term is the symmetry of the velocity field statistics under parity inversion:

$$\mathbf{x} \to -\mathbf{x}, \qquad \mathbf{u} \to -\mathbf{u}. \tag{4.5}$$

2. The factors of $\tilde{K}^3$ and $\tilde{K}^{3/2}$ in the drift and noise coefficients do not indicate a divergence with the size of the period cell, since $\hat{\delta}_{1,\mathbf{k}}$ scales as $O(\tilde{K}^{-3})$ and decays rapidly for $|k| \geq \tilde{K}$. Therefore, the $\tilde{K} \to \infty$ limits of the drift and noise contributions are in fact finite.

4.2. Physical fidelity of effective dynamics.

1. The drift term $\bar{\mathbf{V}}_{\boldsymbol{\alpha}}(\mathbf{X})$ is in accord with what one would expect on physical grounds, based on a low Reynolds number approximation in which the Navier–Stokes approximations are governed by a quasi-steady balance between the viscous and forcing terms (see section 5.1 below). The IB dynamics, however, do not produce a divergence-drift term, which, strictly speaking, should be present on physical grounds. We discuss this term in more detail in [26], where we can see its explicit form in the coarse-graining of particle-based dynamics. This term is small except when the elementary particles are close together (compared to their sizes); see [12, pp. 232–233].

2. The mobility matrix $\bar{\mathcal{M}}(\mathbf{r})$ describing the particle velocities in response to forces is a symmetric, nonnegative definite matrix function by Khinchin's theorem [53]. This implies that for any configuration of N particles the $3N \times 3N$ matrix relating the effective hydrodynamic velocity of each particle to the force on each particle is a symmetric, nonnegative definite matrix in the ordinary sense. This is also in accord with what one expects from physical arguments [19].

3. The random component of the IB dynamics can be shown to generate a physically appropriate absolute diffusion and relative diffusion of Lagrangian particles, provided that the particles are not too close together (relative to their sizes) [28]. In the IB dynamics, however, the motion of one particle is completely unaffected by the presence of other particles which do not generate force. In physical reality, though, the diffusion of a particle is hindered over the long run by the presence of other particles because they affect the fluid motion through a change of boundary conditions induced by rigidity of the particle, even if the particle does not induce any net force or torque [44, 45]. This correction to the motion of the particles is naturally proportional to the volume density occupied by the immersed particles.

4. The reduced system for the effective dynamics of the immersed structures obeys the Einstein relation [6, 16, 46]. The mobility matrix $\bar{\mathcal{M}}(\mathbf{r})$ in (4.4) is exactly the same as the matrix of relative diffusivities between different particles, as we show explicitly in section 5.2. The IB system should, on first principles, satisfy this Einstein relation because it is founded on statistical mechanical principles, but this fact is not at all transparent in the primitive formulation (2.9).

In summary, the IB method appears to generate physically correct dynamics of immersed structures in the presence of thermal fluctuations, provided that the particles constituting the structures are not too closely situated relative to their effective sizes. On the other hand, our analysis in the present work indicates that there is some quantitative difference between the statistical behavior of particles in the IB method and the physical behavior of rigid particles when the separation distance is comparable to the particle sizes. In practice, the structures (polymers, membranes, etc.) in the IB method are generally constructed with the elementary particles separated by a distance on the order of their effective size, so this regime is worth some scrutiny. One reason for the difference in behavior is surely that the Lagrangian particles in the IB method do not act on the fluid as rigid particles with a definite surface do. In particular, the fluid does not respond to the presence of an IB elementary particle unless that particle experiences a force, whereas a force-free rigid particle does exert

stress on the fluid to move it out of the way and to satisfy the no-slip condition on the surface. For physiological applications for which the IB method is primarily designed [42], the immersed structures are often elastic, so it may well be desirable to simulate it numerically using elementary particles that are not fully rigid. Moreover, the closely spaced IB particles will, often in applications, be modelled with some direct force interaction whose effects may dominate those of the rigidity of the particles. If some partial rigidity (or solidity) effects are still desired, however, they could perhaps be incorporated through a modification [41] of the IB approach described in [28]. A detailed exploration of theses issues is beyond the scope of this work and will be explored elsewhere.

We remark that the possible need for special handling of closely spaced particles in a fluid would not be unique to the IB method. Straightforward implementations of the particle-based method of simulations (to be described in [26]) based on Oseen (see [8]) or Rotne and Prager [47] hydrodynamic interaction approximations, which cause the divergence-drift term to cancel out, simulate rigid particle motion accurately only when their separation distance is large compared to their sizes. Only through a more elaborate introduction of lubrication forces as in Stokesian dynamics [3, 48] could the hydrodynamic interaction between closely spaced rigid particles be simulated accurately.

4.3. Changes in presence of nontrivial global system momentum. The simplified stochastic equations would require changes if the global system momentum were not a conserved quantity, such as if the system were subject to some fixed external potential. First of all, we would need to include the zero Fourier mode of the velocity,

$$\mathbf{u}_0(t) = \tilde{K}^{-3} \int_\Omega \mathbf{u}(\mathbf{x}, t)\, d\mathbf{x},$$

as a slow mode along with the immersed structure positions. The extent to which the effective dynamics are changed by the inclusion of this slow mode depends on its amplitude.

4.3.1. Weak zero velocity mode. If the slow mode $\mathbf{u}_0(t)$ has a small amplitude ($O(\mathrm{Ku_T})$ or less), then the stochastic mode reduction procedure can be carried through with simple changes, and the resulting effective equations would be changed in the following way:

1. The stochastic differential equations (4.1) for $d\mathbf{X}_{\boldsymbol{\alpha}}(t)$ would include a drift term $\mathbf{u}_0^\sharp(t)\, dt$, where $\mathbf{u}_0^\sharp = \mathrm{Ku}_\mathrm{T}^{-1}\mathbf{u}_0(t)$.

2. The following evolution equation for $\mathbf{u}_0^\sharp(t)$ would be included in the effective dynamics:

$$d\mathbf{u}_0^\sharp(t) = -\phi^\sharp \sum_{\boldsymbol{\alpha}'} \nabla_{\boldsymbol{\alpha}'} \tilde{\Phi}(\mathbf{X}/\tilde{\ell}_f)\, dt,$$

where $\phi^\sharp = \phi \mathrm{Ku}_\mathrm{T}^{-1}$.

Two situations in which the global system momentum can be expected to be weak are when

1. the forcing by the immersed structures is weak ($\phi \sim O(\mathrm{Ku_T})$), or

2. the external force couples to the system in such a way that the total force experienced self-averages to a small quantity when there are many immersed structures.

4.3.2. Strong zero velocity mode. If, on the other hand, the zero velocity mode has stronger amplitude, then more significant changes need to be made. For example, if the zero velocity mode has amplitude comparable with the (order unity) amplitudes of the other Fourier modes, then the hierarchy of significant dynamical variation is altered in the following way:

1. As before, the fluid velocity modes (other than the zero mode) vary on a fast time scale $O(\mathrm{Ku_T})$ (in the original nondimensional time coordinate).
2. The presence of a global system momentum would induce immersed structure motion on an $O(1)$ time scale and would itself vary on an $O(1)$ time scale as the structures were moved through the external potential.
3. The drift and diffusive motion due to internal forces and thermal fluctuations evolve on a slow time scale $O(\mathrm{Ku_T^{-1}})$.

Now, the fast velocity mode dynamics are unchanged by the presence of the global momentum. The evolution of the zero velocity Fourier mode and immersed structure positions on the $O(1)$ time scale is, to leading order, independent of the fast velocity modes. It is hard, however, to provide a general closed-form description for these $O(1)$ time scale dynamics for general nonlinear external potentials. Of course, the equations are easily solved for linear external potentials (such as gravity), but the resulting dynamics will be unphysical at long time scales (global system momentum growing unboundedly) unless the effects of backflow are somehow introduced. Of central interest in this paper is the effective drift-diffusive motion of the immersed structures on time scales $\mathrm{Ku_T^{-1}}$. The stochastic mode reduction procedure can be carried through to do this only if we can find an appropriate change of variables which removes the $O(1)$ time-scale motion of the particles. The formal procedure for doing so is presented in MTV section 5.3, but an explicit result requires a closed-form solution of the $O(1)$ time-scale dynamics, which is not generally available for the IB equations in the presence of a nonlinear external potential.

For simplicity, we hereafter consider only systems which conserve global system momentum, which we can arrange to be zero.

5. Physical discussion of effective dynamics. We wish here to provide some simple physical derivations of the drift and diffusion terms for the immersed structures as reported in Proposition 4.1, to provide an intuitive picture to complement the systematic mathematical derivation of section 3.

5.1. Drift term. At low Kubo number, the viscous dissipation term in the fluid momentum evolution equation in (2.9a) formally dominates the inertial terms. As the thermal forcing has mean zero, we can then suppose that the fluid motion inducing the deterministic part of the evolution of the immersed structures is given by the following simplified balance of viscous and pressure forces against the forces induced by the straining of the immersed structures:

$$\mathrm{Ku_T^{-1}}\nabla^2\mathbf{u}(\mathbf{x},t) - \nabla p(\mathbf{x},t) - \phi\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}}\tilde{\Phi}(\mathbf{X}(t)/\tilde{\ell}_f)\delta_1(\mathbf{x}-\mathbf{X}_{\boldsymbol{\alpha}}(t)) = 0,$$

$$\nabla\cdot\mathbf{u}(\mathbf{x},t) = 0.$$

Solving this linear system by a Fourier transform, we obtain

$$\mathbf{u}(\mathbf{x},t) = \sum_{\mathbf{k}\in S} e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}\hat{\mathbf{u}}_{\mathbf{k}}(t),$$

$$\hat{\mathbf{u}}_{\mathbf{k}}(t) = -\mathrm{Ku_T}\phi\sum_{\boldsymbol{\alpha}'\in\mathcal{A}}\frac{\mathcal{P}_{\mathbf{k}}\nabla_{\boldsymbol{\alpha}'}\tilde{\Phi}(\mathbf{X}(t)/\tilde{\ell}_f)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}'}(t)/\tilde{K}}}{4\pi^2(k/\tilde{K})^2},$$

with the Fourier symbols defined in section 3.1. Substituting this into the evolution equation in (3.2a) for $\mathbf{X}_{\boldsymbol{\alpha}}(t)$, we obtain the following expression for the deterministic component of the motion for the immersed structures at low Kubo number:

$$\left(\frac{d\mathbf{X}_{\boldsymbol{\alpha}}(t)}{dt}\right)_{\det} = -\mathrm{Ku}_{\mathrm{T}}\phi\tilde{K}^3 \sum_{\boldsymbol{\alpha}'\in\mathcal{A}} \frac{\mathcal{P}_{\mathbf{k}}\nabla_{\boldsymbol{\alpha}'}\tilde{\Phi}(\mathbf{X}(t)/\tilde{\ell}_f)\hat{\delta}^2_{1,\mathbf{k}}e^{2\pi i\mathbf{k}\cdot(\mathbf{X}_{\boldsymbol{\alpha}}(t)-\mathbf{X}_{\boldsymbol{\alpha}'}(t))/\tilde{K}}}{4\pi^2(k/\tilde{K})^2}.$$

Note how the velocity induced by the immersed structure is $O(\mathrm{Ku}_{\mathrm{T}})$, and so will only produce a significant displacement over a $O(\mathrm{Ku}_{\mathrm{T}}^{-1})$ time scale. Upon rescaling time in this way, we recover the systematically computed drift coefficient (4.2).

5.2. Diffusion term. The stochastic dynamics of the immersed structures are in response to the stochastic fluctuations of the fluid, which are in turn due to the thermal forcing. We ignore structural forces here since they contribute, to leading order, to the deterministic rather than the random component of the particle motion. The motion of the structures is then purely random (with zero mean drift) and is described at a basic level by the evolution of the second-order moments of the coordinates. One such measure of the random motion, which can be cleanly computed, is the diffusion correlation tensor

$$\mathcal{D}(\mathbf{r}) \equiv \frac{1}{2}\frac{d}{dt}\left\langle(\mathbf{X}_{\boldsymbol{\alpha}}(t)-\mathbf{X}_{\boldsymbol{\alpha}}(t'))\otimes(\mathbf{X}_{\boldsymbol{\alpha}'}(t)-\mathbf{X}_{\boldsymbol{\alpha}'}(t'))\,|\mathbf{X}_{\boldsymbol{\alpha}}(t')=\mathbf{x}+\mathbf{r},\mathbf{X}_{\boldsymbol{\alpha}'}(t')=\mathbf{x}\right\rangle_{t=t'}, \tag{5.1}$$

which describes the correlation in the random motion of two particles during the moment at which they are situated with relative separation $\mathbf{r}$. Note that this diffusion correlation tensor does not depend on $\mathbf{x}$ nor t', provided that the fluid is in thermal equilibrium so that the system is statistically invariant under space and time translations. The single-particle diffusivity is just given by the diagonal entries $\mathcal{D}(\mathbf{0})$ because two coincident particles will move as a single particle due to the common random flow environment.

We now provide a direct but approximate calculation for the diffusion correlation tensor and then show that it agrees with the results of Proposition 4.1. To do this, we will ignore the nonlinear advection term in the fluid equation, on the grounds that the Reynolds number is small. We have the following approximation for the evolution of the random component of the Fourier modes of the fluid velocity field:

$$d\hat{\mathbf{u}}_{\mathbf{k}}(t) = -4\pi^2(k/\tilde{K})^2\mathrm{Ku}_{\mathrm{T}}^{-1}\hat{\mathbf{u}}_{\mathbf{k}}(t)\,dt + \mathrm{Ku}_{\mathrm{T}}^{-1/2}\tilde{K}^{-3/2}\sqrt{2(4\pi^2(k/\tilde{K})^2)}\,\mathcal{P}_{\mathbf{k}}d\tilde{\mathbf{W}}_{\mathbf{k}}(t).$$

These linear stochastic differential equations can be solved explicitly when the fluid is in thermal equilibrium. We find that each Fourier mode of the velocity field is independent of the others and evolves as a mean-zero Gaussian Markov process with correlation function

$$\begin{aligned}\langle\hat{\mathbf{u}}_{\mathbf{k}}(t)\otimes\hat{\mathbf{u}}_{\mathbf{k}}(t')\rangle &= 0,\\ \langle\hat{\mathbf{u}}_{\mathbf{k}}(t)\otimes\hat{\mathbf{u}}^*_{\mathbf{k}}(t')\rangle &= \tilde{K}^{-3}e^{-\mathrm{Ku}_{\mathrm{T}}^{-1}4\pi^2(k/\tilde{K})^2|t-t'|}\mathcal{P}_{\mathbf{k}}.\end{aligned}$$

The fluctuating component of the smoothed version of the velocity field, $\mathbf{u}_1$, which advects the immersed structures, also has independent Fourier coefficients which evolve

according to mean-zero Gaussian random processes with correlation structure

$$\begin{aligned} &\langle \hat{\mathbf{u}}_{1,\mathbf{k}}(t) \otimes \hat{\mathbf{u}}_{1,\mathbf{k}}(t') \rangle = 0, \\ &\langle \hat{\mathbf{u}}_{1,\mathbf{k}}(t) \otimes \hat{\mathbf{u}}^*_{1,\mathbf{k}}(t') \rangle = \tilde{K}^3 e^{-\mathrm{Ku}_\mathrm{T}^{-1} 4\pi^2 (k/\tilde{K})^2 |t-t'|} |\hat{\delta}_{1,\mathbf{k}}|^2 \mathcal{P}_\mathbf{k}. \end{aligned} \tag{5.2}$$

It will be convenient in the following development to define the increment in the Lagrangian particle positions:

$$\Delta \mathbf{X}_{\boldsymbol{\alpha}}(t) = \mathbf{X}_{\boldsymbol{\alpha}}(t+\Delta t) - \mathbf{X}_{\boldsymbol{\alpha}}(t).$$

Suppose that at time t we have two elementary particles situated at $\mathbf{X}_{\boldsymbol{\alpha}}(t) = \mathbf{x}+\mathbf{r}$ and $\mathbf{X}_{\boldsymbol{\alpha}'}(t) = \mathbf{x}$. The second-order moments of the changes in position of these particles due to the random thermal fluctuations in the fluid are given by

$$\begin{aligned} &\langle \Delta \mathbf{X}_{\boldsymbol{\alpha}}(t) \otimes \Delta \mathbf{X}_{\boldsymbol{\alpha}'}(t) \rangle \\ &\quad = \int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' \, \langle \mathbf{u}_1(\mathbf{X}_{\boldsymbol{\alpha}}(s), s) \otimes \mathbf{u}_1(\mathbf{X}_{\boldsymbol{\alpha}'}(s'), s') \rangle \\ &\quad = \sum_{\mathbf{k}\in S} \sum_{\mathbf{k}'\in S} \int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' \, \langle \hat{\mathbf{u}}_{1,\mathbf{k}}(s) \otimes \hat{\mathbf{u}}_{1,\mathbf{k}'}(s') e^{2\pi i (\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(s) + \mathbf{k}'\cdot\mathbf{X}_{\boldsymbol{\alpha}'}(s'))/\tilde{K}} \rangle. \end{aligned} \tag{5.3}$$

Suppose now that we consider $\mathrm{Ku}_\mathrm{T} \ll \Delta t \ll 1$. The velocity field decorrelates on the short time scale Ku_T (see (5.2)), but the particle positions, which integrate this fluid velocity, will change very little over the time interval Δt. Therefore, if we condition on the position of the particles at time t, as in the definition of the diffusion correlation tensor (5.1), we can reasonably approximate $\mathbf{X}_{\boldsymbol{\alpha}}(s)$ and $\mathbf{X}_{\boldsymbol{\alpha}'}(s')$ to be frozen within the last integrand in (5.3):

$$\begin{aligned} \mathcal{D}(\mathbf{r}) &\approx \frac{1}{2\Delta t} \sum_{\mathbf{k}\in S} \sum_{\mathbf{k}'\in S} \int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' \, \langle \hat{\mathbf{u}}_{1,\mathbf{k}}(s) \otimes \hat{\mathbf{u}}_{1,\mathbf{k}'}(s') \rangle e^{2\pi i (\mathbf{k}\cdot(\mathbf{x}+\mathbf{r}) + \mathbf{k}'\cdot\mathbf{x})/\tilde{K}} \\ &= \frac{\tilde{K}^3}{2\Delta t} \sum_{\mathbf{k}\in S} |\hat{\delta}_{1,\mathbf{k}}|^2 \mathcal{P}_\mathbf{k} \int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' \, e^{-\mathrm{Ku}_\mathrm{T}^{-1} 4\pi^2 (k/\tilde{K})^2 |s-s'|} e^{2\pi i \mathbf{k}\cdot\mathbf{r}/\tilde{K}} \\ &\approx \frac{\tilde{K}^3}{\Delta t} \mathrm{Ku}_\mathrm{T} \sum_{\mathbf{k}\in S} |\hat{\delta}_{1,\mathbf{k}}|^2 \frac{\mathcal{P}_\mathbf{k}}{4\pi^2 (k/\tilde{K})^2} e^{2\pi i \mathbf{k}\cdot\mathbf{r}/\tilde{K}} \Delta t \quad \text{for } \mathrm{Ku}_\mathrm{T} \ll \Delta t \ll 1. \end{aligned}$$

Therefore, the diffusion correlation tensor in the low Kubo number limit is given by the above approximate calculation as

$$\mathcal{D}(\mathbf{r}) = \tilde{K}^3 \mathrm{Ku}_\mathrm{T} \sum_{\mathbf{k}\in S} |\hat{\delta}_{1,\mathbf{k}}|^2 \frac{\mathcal{P}_\mathbf{k}}{4\pi^2 (k/\tilde{K})^2} e^{2\pi i \mathbf{k}\cdot\mathbf{r}/\tilde{K}}. \tag{5.4}$$

Notice again that this diffusion is $O(\mathrm{Ku}_\mathrm{T})$, so the random motion is significant only on $O(\mathrm{Ku}_\mathrm{T}^{-1})$ time scales.

After this rescaling, this heuristically deduced law of coupled diffusion of the immersed structures agrees with what the noise terms of the effective dynamics in Proposition 4.1 would produce in the absence of drift. Indeed, if we have $\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t) = \mathbf{x}+\mathbf{r}$ and $\bar{\mathbf{X}}_{\boldsymbol{\alpha}'}(t) = \mathbf{x}$, then applying the rules of (Itô) stochastic calculus [37], we have over

a short time interval of duration Δt

$$\begin{aligned}\langle \Delta\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t) \otimes \Delta\bar{\mathbf{X}}_{\boldsymbol{\alpha}'}(t)\rangle &= \left\langle \left(\sum_{\mathbf{k}\in S} \mathcal{S}_{\mathbf{k}}(\mathbf{x}+\mathbf{r})\,\Delta\tilde{\mathbf{W}}_{\mathbf{k}}(t)\right) \otimes \left(\sum_{\mathbf{k}'\in S} \mathcal{S}_{\mathbf{k}'}(\mathbf{x})\,\Delta\tilde{\mathbf{W}}_{\mathbf{k}'}(t)\right)\right\rangle \\ &\quad + o(\Delta t) \\ &= \sum_{\mathbf{k},\mathbf{k}'\in S} \langle \mathcal{S}_{\mathbf{k}}(\mathbf{x}+\mathbf{r})\langle \Delta\tilde{\mathbf{W}}_{\mathbf{k}}(t)\otimes\Delta\tilde{\mathbf{W}}_{\mathbf{k}'}(t)\rangle \cdot \mathcal{S}^{\dagger}_{\mathbf{k}'}(\mathbf{x})\rangle,\end{aligned}$$

with the noise increment

$$\Delta\tilde{\mathbf{W}}_{\mathbf{k}}(t) \equiv \int_t^{t+\Delta t} d\tilde{\mathbf{W}}_{\mathbf{k}}(t).$$

Now using the statistical properties of the complex white noise processes (see (2.5) and surrounding discussion), we have

$$\begin{aligned}\langle \Delta\bar{\mathbf{X}}_{\boldsymbol{\alpha}}(t) \otimes \Delta\bar{\mathbf{X}}_{\boldsymbol{\alpha}'}(t)\rangle &= \sum_{\mathbf{k},\mathbf{k}'\in S} \langle \mathcal{S}_{\mathbf{k}}(\mathbf{x}+\mathbf{r}) \cdot \mathcal{I}\Delta t\delta_{\mathbf{k},-\mathbf{k}'} \cdot \mathcal{S}^{\dagger}_{\mathbf{k}'}(\mathbf{x})\rangle + o(\Delta t) \\ &= \sum_{\mathbf{k}\in S} \langle \mathcal{S}_{\mathbf{k}}(\mathbf{x}+\mathbf{r}) \cdot \mathcal{S}^{\dagger}_{-\mathbf{k}}(\mathbf{x})\rangle\,\Delta t + o(\Delta t).\end{aligned}$$

Substituting the expression (4.3) for $\mathcal{S}_{\mathbf{k}}(\mathbf{x})$, dividing by $2\Delta t$, and taking $\Delta t \to 0$, we obtain agreement with the heuristically deduced expression (5.4). The difference of the factor $\mathrm{Ku_T}$ is due to the fact that $\bar{\mathbf{X}}_{\boldsymbol{\alpha}}$ is defined with respect to the rescaled time $t/\mathrm{Ku_T}$.

We now directly observe the Einstein relation, which in our nondimensionalization reads $\mathcal{D}(\mathbf{r}) = \mathcal{M}(\mathbf{r}) = \mathrm{Ku_T}\bar{\mathcal{M}}(\mathbf{r})$, where $\mathcal{M}(\mathbf{r})$ is the mobility matrix (4.4) expressed in terms of the original time scale.

5.3. Discussion. The physical derivations of the drift and diffusion at low Kubo number are intended to provide some intuition for the results stated in Proposition 4.1. These formal arguments, however, involve assumptions which have varying degrees of plausibility and confidence, so the systematic and rigorous approach developed in section 3 is valuable. In particular, the systematic calculation allows precise assessment of the influence of the nonlinear advection term. Though indeed it is $O(\mathrm{Ku_T})$ weak relative to the viscous diffusion term, we are considering motion on $O(\mathrm{Ku_T^{-1}})$ time scales, so the nonlinearity could in principle have an $O(1)$ integrated influence on the particle motion. We found though, in section 3 that the nonlinear advection term does not in fact have an $O(1)$ effect due to cancellation caused by a parity symmetry (4.5) which it possesses.

6. Coarse-graining of the discretized IB method. In a numerical implementation, the velocity field can be represented by only a finite number of parameters. For a spectral code which retains the Fourier representation of the derivatives applied to the linear terms in the Navier–Stokes equations, the results of the continuum formulation would carry over by a simple Galerkin truncation. But such an abrupt spectral cutoff is usually not desirable in numerical simulations.

The version of the IB method implemented by Kramer and Peskin in [28] defines the fluid on a discrete, periodic, cubic mesh with (dimensional) spacing $h = L/K$, where K is an integer. The traditional IB method [42] has $h = a$, but there is no

difficulty in extending the numerical simulation approach for $h = ma$, where m is a nonnegative integer. An equivalent representation of the velocity field is through a finite set of Fourier coefficients $\{\hat{\mathbf{u}}_{\mathbf{k}}\}$ sufficient to resolve the velocity field on this mesh. The spatial derivatives appearing in the Navier–Stokes equations in (2.9a) must be replaced by operators with domain and range consistent with the finite-dimensional function space supported by the numerical resolution. The usual implementation is through finite-difference operators. We work out now how the effective dynamics of the particles are altered due to the discretization. These results are important for providing a benchmark against which numerical simulations can be compared more precisely. Temporal discretization lends itself less readily to the MTV framework, so we keep time continuous here.

6.1. Spatial discretization. We write the dynamical equations in the spatially discretized IB system (2.9) as

$$
\begin{aligned}
\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} + \mathcal{B}_{\mathbf{k}}^{(d)}(\mathbf{u},\mathbf{u})(\mathbf{x},t) &= \mathrm{Ku}_{\mathrm{T}}^{-1}(\Delta_{\tilde{h}}^{(d)}\mathbf{u})(\mathbf{x},t) - (\nabla_{\tilde{h}}^{(d)}p)(\mathbf{x},t) + \mathbf{f}_T(t) \\
&\quad - \phi \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}}\tilde{\Phi}\left(\frac{\mathbf{X}(t)}{\tilde{\ell}_f}\right)\delta_1(\mathbf{x}-\mathbf{X}_{\boldsymbol{\alpha}}(t)), \\
(\tilde{\nabla}_{\tilde{h}}^{(d)}\cdot\mathbf{u})(\mathbf{x},t) &= 0, \\
\frac{d\mathbf{X}_{\boldsymbol{\alpha}}(t)}{dt} &= \mathbf{u}_1(\mathbf{X}_{\boldsymbol{\alpha}}(t),t), \\
\mathbf{u}_1(\mathbf{x},t) &= \tilde{h}^3 \sum_{\mathbf{x}'\in\tilde{h}\mathbb{Z}_K^3} \mathbf{u}(\mathbf{x}',t)\delta_1(\mathbf{x}-\mathbf{x}').
\end{aligned}
\tag{6.1}
$$

In these equations, $\mathbf{x}$ is restricted to taking values on the periodic cubic lattice $\tilde{h}\times\mathbb{Z}_K^3$, where

$$\mathbb{Z}_K^3 \equiv [1,2,\ldots,K]^3,$$

and $\tilde{h}$ is a nondimensional length scale ratio:

$$\tilde{h} \equiv \frac{h}{a} = \frac{\tilde{K}}{K}.$$

$\mathcal{B}_{\mathbf{k}}^{(d)}$ is some finite-difference approximation for the nonlinear advection operator, $\Delta_{\tilde{h}}^{(d)}$ is a discrete Laplacian, $\nabla_{\tilde{h}}^{(d)}$ is a discrete gradient, and $\tilde{\nabla}_{\tilde{h}}^{(d)}$ is another discrete gradient used in defining a divergence operator. The current implementation of the IB method [42] takes the usual centered-difference approximations for the linear differential operators, namely,

$$
\begin{aligned}
\nabla_{\tilde{h}}^{(d)} &= \sum_{m=1}^{3} \hat{e}_m D_{\tilde{h},m}^{0}, \\
\Delta_{\tilde{h}}^{(d)} &= \sum_{m=1}^{3} D_{\tilde{h},m}^{+} D_{\tilde{h},m}^{-}, \\
\tilde{\nabla}_{\tilde{h}}^{(d)} &= \nabla_{\tilde{h}}^{(d)},
\end{aligned}
\tag{6.2}
$$

where

$$(D^+_{\tilde{h},m}g)(\mathbf{x}) = \frac{g(\mathbf{x}+\tilde{h}\hat{e}_m) - g(\mathbf{x})}{\tilde{h}},$$

$$(D^-_{\tilde{h},m}g)(\mathbf{x}) = \frac{g(\mathbf{x}) - g(\mathbf{x}-\tilde{h}\hat{e}_m)}{\tilde{h}},$$

$$(D^0_{\tilde{h},m}g)(\mathbf{x}) = \frac{g(\mathbf{x}+\tilde{h}\hat{e}_m) - g(\mathbf{x}-\tilde{h}\hat{e}_m)}{2\tilde{h}},$$

and $\hat{e}_m$ denotes a unit vector in the mth coordinate direction. The nonlinear term in the Navier–Stokes equation is discretized by a skew-symmetric central differencing scheme which conserves energy exactly (see [42]):

$$\mathcal{B}^{(d)}_{\mathbf{k}}(\mathbf{u},\mathbf{u})(\mathbf{x},t) \equiv \frac{1}{2}\left(\mathbf{u}(\mathbf{x},t)\cdot\nabla^{(d)}_{\tilde{h}}\mathbf{u}(\mathbf{x},t) + \nabla^{(d)}_{\tilde{h}}\cdot(\mathbf{u}(\mathbf{x},t)\otimes\mathbf{u}(\mathbf{x},t))\right).$$

Other discretizations can also be contemplated. For example, an upwind differencing scheme for the nonlinear term has often been used for numerical simulations at higher Reynolds number to provide numerical stability [43]. A purely divergence-form discretization would conserve total momentum exactly. Finally, Cowen [5] is investigating other discretizations for the divergence operator, adapted to the choice of the interpolation/spreading delta function, which improve volume conservation properties. For this reason, we will express the formulas for the effective drift and diffusion coefficients in terms of the general abstract differential operators $\nabla^{(d)}_{\tilde{h}}$, $\tilde{\nabla}^{(d)}_{\tilde{h}}$, and $\Delta^{(d)}_{\tilde{h}}$, without assuming that they take the specific form of (6.2). It is important to note, however, that the pressure term will conserve energy only if $\tilde{\nabla}^{(d)}_{\tilde{h}} = \nabla^{(d)}_{\tilde{h}}$.

Because the finite-difference derivative operators remain invariant under translations by a grid spacing $\tilde{h}$, they act diagonally as multiplication operators on Fourier modes. In this way we can define their action on Fourier modes $\mathbf{k}$ through the symbols $\mathcal{F}_{\mathbf{k}}(\cdot)$, defined in general for an operator $\mathcal{O}$ with translation invariance on the basic lattice, by

$$\mathcal{O}\mathbf{g}(\mathbf{x},t) = \sum_{\mathbf{k}\in\mathbb{Z}^3_K} e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}\mathcal{F}_{\mathbf{k}}(\mathcal{O})\hat{\mathbf{g}}(\mathbf{k},t),$$

where

$$\mathbf{g}(\mathbf{x},t) = \sum_{\mathbf{k}\in\mathbb{Z}^3_K} e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}\hat{\mathbf{g}}(\mathbf{k},t).$$

For the implemented version described in (6.2), the Fourier representation of the finite-difference operators would be

$$\mathcal{F}_{\mathbf{k}}(\Delta^{(d)}_{\tilde{h}}) = -\frac{4}{\tilde{h}^2}\sum_{m=1}^{3}\sin^2\frac{\pi k_m}{K},$$

$$\mathcal{F}_{\mathbf{k}}(\nabla^{(d)}_{\tilde{h}}) = \mathcal{F}_{\mathbf{k}}(\tilde{\nabla}^{(d)}_{\tilde{h}}) = \frac{i}{\tilde{h}}\sum_{m=1}^{3}\hat{e}_m\sin\frac{2\pi k_m}{K}.$$

Note that these Fourier representations of the discretized operators converge to the Fourier representation of the corresponding continuum operators as $K\to\infty$ (with the period cell length $\tilde{K} = K\tilde{h}$ held fixed).

The thermal forcing must be changed as follows (see [28]) in order to maintain the correct statistical mechanics for the spatially discretized system (6.1):

$$\mathbf{f}_T(\mathbf{x},t) = \mathrm{Ku}_{\mathrm{T}}^{-1/2}\tilde{K}^{-3/2}\sum_{\mathbf{k}\in S_K}\sqrt{2\mathcal{F}_{\mathbf{k}}(-\Delta_{\tilde{h}}^{(d)})}e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}\mathcal{P}_{\mathbf{k}}^{(dI)}\frac{d\tilde{\mathbf{W}}_{\mathbf{k}}(t)}{dt}, \tag{6.3}$$

where

$$S_K = \mathbb{Z}_K^3 \setminus (K,K,K) \tag{6.4}$$

and the projection tensor

$$\mathcal{P}_{\mathbf{k}}^{(dI)} = \mathcal{I} - \frac{\mathcal{F}_{\mathbf{k}}(\tilde{\nabla}_{\tilde{h}}^{(d)})\otimes\mathcal{F}_{\mathbf{k}}(\tilde{\nabla}_{\tilde{h}}^{(d)})}{\mathcal{F}_{\mathbf{k}}(\tilde{\nabla}_{\tilde{h}}^{(d)}\cdot\tilde{\nabla}_{\tilde{h}}^{(d)})} \tag{6.5}$$

must be included when $\tilde{\nabla}_{\tilde{h}}^{(d)} \neq \nabla_{\tilde{h}}^{(d)}$ for proper results. When $\tilde{\nabla}_{\tilde{h}}^{(d)} = \nabla_{\tilde{h}}^{(d)}$, the inclusion or omission of the factor $\mathcal{P}_{\mathbf{k}}^{(dI)}$ in (6.3) has no effect on the system dynamics.

6.2. Changes in drift and diffusion due to discretization. Whatever the precise forms of the discretized derivatives, the resulting drift and noise terms in the effective dynamics (4.1) have the form

$$\begin{aligned}\bar{\mathbf{V}}_{\boldsymbol{\alpha}}(\mathbf{X}) &= -\phi\sum_{\boldsymbol{\alpha}'\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}'}\tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right)\bar{\mathcal{M}}^{(d)}(\mathbf{X}_{\boldsymbol{\alpha}'},\mathbf{X}_{\boldsymbol{\alpha}}-\mathbf{X}_{\boldsymbol{\alpha}'}),\\ \mathcal{S}_{\mathbf{k}}(\mathbf{x}) &= \sqrt{2}\tilde{K}^{3/2}\frac{\mathcal{P}_{\mathbf{k}}^{(dI)}e^{2\pi i\mathbf{k}\cdot\mathbf{x}/\tilde{K}}}{\sqrt{\mathcal{F}_{\mathbf{k}}(-\Delta_{\tilde{h}}^{(d)})}}\sum_{\mathbf{p}\in\mathbb{Z}^3}\hat{\delta}_{1,K\mathbf{p}+\mathbf{k}}e^{2\pi i\mathbf{p}\cdot\mathbf{x}/\tilde{h}},\end{aligned} \tag{6.6a}$$

with the mobility matrix function given by

$$\begin{aligned}\bar{\mathcal{M}}^{(d)}(\mathbf{x}',\mathbf{r}) &= \sum_{\mathbf{q}\in S}\sum_{\mathbf{p}\in\mathbb{Z}^3}\hat{\bar{\mathcal{M}}}_{\mathbf{p},\mathbf{q}}^{(d)}e^{2\pi i\mathbf{q}\cdot\mathbf{r}/\tilde{K}}e^{2\pi i\mathbf{p}\cdot\mathbf{x}/\tilde{h}},\\ \hat{\bar{\mathcal{M}}}_{\mathbf{p},\mathbf{q}}^{(d)} &= \tilde{K}^3\frac{\mathcal{P}_{\mathbf{q}}^{(dII)}\hat{\delta}_{1,K\mathbf{p}+\mathbf{q}}\hat{\delta}_{1,\mathbf{q}}^{*}}{\mathcal{F}_{\mathbf{q}}(-\Delta_{\tilde{h}}^{(d)})}.\end{aligned} \tag{6.6b}$$

Note that in general we must distinguish two versions of the projection tensor $\mathcal{P}_{\mathbf{k}}$ in the discretized formalism:

$$\mathcal{P}_{\mathbf{k}}^{(dII)} = \mathcal{I} - \frac{\mathcal{F}_{\mathbf{k}}(\nabla_{\tilde{h}}^{(d)})\otimes\mathcal{F}_{\mathbf{k}}(\tilde{\nabla}_{\tilde{h}}^{(d)})}{\mathcal{F}_{\mathbf{k}}(\nabla_{\tilde{h}}^{(d)}\cdot\tilde{\nabla}_{\tilde{h}}^{(d)})},$$

and $\mathcal{P}_{\mathbf{k}}^{(dI)}$ as given in (6.5). In the discretized formalism, the projection tensors $\mathcal{P}_{\mathbf{k}}$ appearing in the dynamical equation for the velocity modes in (3.2a), except in front of the noise term, are to be replaced by $\mathcal{P}_{\mathbf{k}}^{(dII)}$. On the other hand, the projection tensor $\mathcal{P}_{\mathbf{k}}$ appearing in front of the noise term and in (A.11) should be replaced by $\mathcal{P}_{\mathbf{k}}^{(dI)}$.

The effective drift and random terms for the discretized IB formalism have the same form as those appearing in the continuum IB formalism (Proposition 4.1), with the following key differences:

1. The mobility matrix function depends not only on the relative separation of the location of applied force and the responding particle, but also on the absolute location of the applied force relative to the fluid grid. Indeed, the mobility matrix function is readily seen to be periodic in the force location $\mathbf{x}'$ along the grid axes with period equal to the grid spacing $\tilde{h}$. This implies that the dynamics of the particles will depend somewhat on their position relative to the fluid grid. The grid-induced oscillations of the mobility matrix function are quantified by the $\mathbf{p} \neq \mathbf{0}$ terms in (6.6b) and will be studied quantitatively in [27].

2. The formulas involve a clear aliasing of wavenumbers separated by integer vector multiples of K, the number of grid points in each direction.

3. The mobility matrix function $\bar{\mathcal{M}}^{(d)}(\mathbf{r})$ is a symmetric, nonnegative definite matrix function if and only if the discretized derivatives obey $\nabla_{\tilde{h}}^{(d)} = \tilde{\nabla}_{\tilde{h}}^{(d)}$. In this case, the effective dynamics still obey the Einstein relation between the mobility matrix and the relative diffusivities of particles, though we no longer have a simple relation between the Fourier coefficients of the noise and the mobility matrix as in (4.3). The violation of the Einstein relation when $\nabla_{\tilde{h}}^{(d)} \neq \tilde{\nabla}_{\tilde{h}}^{(d)}$ occurs because the discretized pressure term does not conserve energy in this case.

4. The dissipation factor for each mode is naturally changed from the continuum value $4\pi^2(k/\tilde{K})^2$ to the value $\mathcal{F}_{\mathbf{k}}(-\Delta_{\tilde{h}}^{(d)})$ appropriate to the discretized viscous diffusion operator.

5. The sum is taken over a finite set of modes S_K (6.4), and there is no issue of ultraviolet divergence.

As we emphasize in section A.6, the nonlinear advection term in the continuum formulation makes no contribution to the effective structure dynamics in the low $\mathrm{Ku_T}$ limit due to a parity symmetry (4.5). This symmetry is also preserved under the implemented discretization (6.2) or if the nonlinear advection term is alternatively discretized by upwind differencing. In general, provided the discretization scheme respects the parity symmetry (4.5), the presence of the discretized weak nonlinear advection term does not change the effective dynamics of the particles on nondimensional time scales $O(\mathrm{Ku_T^{-1}})$ to leading order. If, however, the discretization violates this symmetry, there may be spurious contamination from the discretized nonlinearity.

The effective immersed structure dynamics derived for the immersed structures evolving according to the discretized IB method can be used as a design criterion for a numerical procedure. For example, the single-particle diffusivity (which is the same as $\mathcal{D}(\mathbf{0})$ given by a discretized modification of the formula (5.4) following the above discussion) may be used as a means to identify the effective size of the simulated particle. Of course this size will be order unity in our nondimensionalized units, but since the elementary particles are represented as smoothed delta functions rather than objects with rigid boundaries, it is not a priori clear how to associate a definite size value to the particles. The general Stokes–Einstein formula [16, 46] relating the diffusivity of a particle to its size, along with the explicit formulas for the effective diffusion of the IB particles, gives us a quantitative way to associate the simulation parameters with the effective particle sizes which are desired in a simulation. The above formulas for the coarse-grained discretized IB dynamics are used extensively in [28, 27] to explore how well the IB method replicates the correct statistical physics of immersed structure motion and to provide a benchmark for the results of numerical simulations.

7. Conclusions. We have demonstrated how the stochastic mode reduction framework developed by Majda, Timofeyev, and Vanden-Eijnden (MTV) can be ap-

plied to obtain coarse-grained approximations for the equations underlying the IB method for the simulation of microfluid systems with thermal fluctuations. In this way we were able to characterize rigorously the effective drift and diffusion behavior of immersed structures in the IB method. In particular, with full rigor, the equations governing the coarse-grained spatially continuous and discrete IB methods have been compared with each other and also with the desired physical behavior. Provided that the pressure gradient is discretized in an energy-conserving way and the nonlinear advection term is discretized in a manner (such as a central difference approximation) which respects the parity symmetry (4.5), the continuous and spatially discretized IB methods have structurally similar coarse-grained dynamics with explicit formulas identifying the drift and diffusion coefficients. The main difference between the structural form of the coarse-grained dynamics of the elementary particles in the IB method and those of physically proper rigid particles (as well as the particle-based simulation methods discussed in [26]) is the absence of the "divergence-drift" term for the IB method, which is significant only for Lagrangian particles spaced closely compared to their effective sizes. As discussed in section 4.2, one source of this discrepancy is lack of rigidity of the Lagrangian particles in the IB method, which may be desirable for physiological systems with flexible and elastic structures. Incorporation of rigidity into the IB method [41] might bring its effective dynamics into closer agreement with those of rigid particle-based methods [3, 8, 26, 48] at small separation distances. Finally, the explicit formulas for the effective diffusion of the Lagrangian particles under spatial discretization provide a means for choosing the size parameter precisely in applications so as to match desired diffusion coefficients.

Appendix. Details of computations for stochastic mode reduction. The details of the calculation from section 3 are presented here.

A.1. Derivation of Kolmogorov backward equation. We provide here a formal derivation of the Kolmogorov backward equation (3.3) based on a stochastic Taylor expansion [22, 37]. Consider the change of $\rho(s, \mathbf{X}, \mathbf{U}|t)$ over a small time interval Δs, using its definition (3.4) and the law of total expectation (see [49]):

$$\begin{aligned}
&\rho(s+\Delta s, \mathbf{X}, \mathbf{U}|t) - \rho(s, \mathbf{X}, \mathbf{U}|t) \\
&\quad = \rho(s+\Delta s, \mathbf{X}, \mathbf{U}|t) \\
&\qquad\qquad - \mathbb{E}\left[f(\mathbf{X}(t), \mathbf{U}(t))|\mathbf{X}(s) = \mathbf{X}, \mathbf{U}(s) = \mathbf{U}\right] \\
&\quad = \rho(s+\Delta s, \mathbf{X}, \mathbf{U}|t) \\
&\qquad\qquad - \mathbb{E}\left[\mathbb{E}\left(f(\mathbf{X}(t), \mathbf{U}(t))|\mathbf{X}(s+\Delta s), \mathbf{U}(s+\Delta s)\right)\big|\mathbf{X}(s) = \mathbf{X}, \mathbf{U}(s) = \mathbf{U}\right] \\
&\quad = \rho(s+\Delta s, \mathbf{X}, \mathbf{U}|t) \\
&\qquad\qquad - \mathbb{E}\left[\rho(s+\Delta s, \mathbf{X}(s+\Delta s), \mathbf{U}(s+\Delta s)|t)|\mathbf{X}(s) = \mathbf{X}, \mathbf{U}(s) = \mathbf{U}\right] \\
&\quad = \mathbb{E}\left[\rho(s+\Delta s, \mathbf{X}, \mathbf{U}|t) - \rho(s+\Delta s, \mathbf{X}(s+\Delta s), \mathbf{U}(s+\Delta s)|t)\right. \\
&\qquad\qquad\qquad \left.\big|\mathbf{X}(s) = \mathbf{X}, \mathbf{U}(s) = \mathbf{U}\right].
\end{aligned}$$

Now we will want to perform a stochastic Taylor expansion of the second term, using the following expressions for the increments in the system variables during the small time step Δs:

$$\mathbf{X}_{\boldsymbol{\alpha}}(s+\Delta s) - \mathbf{X}_{\boldsymbol{\alpha}}(s) = \tilde{K}^3 \sum_{\mathbf{k}\in S} e^{2\pi i \mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(s)} \hat{\mathbf{u}}_{\mathbf{k}}(s) \hat{\delta}_{1,\mathbf{k}} \Delta s + O((\Delta s)^2),$$

$$\begin{aligned}\Delta\hat{\mathbf{u}}_{\mathbf{k}}(s) \equiv \hat{\mathbf{u}}_{\mathbf{k}}(s+\Delta s) - \hat{\mathbf{u}}_{\mathbf{k}}(s) &= -\mathcal{B}_{\mathbf{k}}(\mathbf{U}(s),\mathbf{U}(s))\Delta s - 4\pi^2(k/\tilde{K})^2\mathrm{Ku}_{\mathrm{T}}^{-1}\hat{\mathbf{u}}_{\mathbf{k}}(s)\Delta s \\ &\quad - \phi\mathcal{P}_{\mathbf{k}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}}\tilde{\Phi}(\mathbf{X}_{\boldsymbol{\alpha}}(s)/\tilde{\ell}_f)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(s)}\Delta s \\ &\quad + \mathrm{Ku}_{\mathrm{T}}^{-1/2}\tilde{K}^{-3/2}\sqrt{2(4\pi^2(k/\tilde{K})^2)}\,\mathcal{P}_{\mathbf{k}}\Delta\tilde{\mathbf{W}}_{\mathbf{k}}(s) + o(\Delta s),\end{aligned}$$

which arise upon integrating the equations of motion (3.2) over the short time interval Δs and using the Itô property of the noise [37]. The noise increments $\Delta\tilde{\mathbf{W}}_{\mathbf{k}}(s) = \int_s^{s+\Delta s} d\tilde{\mathbf{W}}_{\mathbf{k}}(s)$ are Gaussian, mean-zero complex random variables, which are independent except for the complex conjugacy property

$$\Delta\tilde{\mathbf{W}}_{-\mathbf{k}} = \overline{\Delta\tilde{\mathbf{W}}_{\mathbf{k}}}. \tag{A.1}$$

Their covariances are given by integration of (2.5):

$$\langle\Delta\tilde{\mathbf{W}}_{\mathbf{k}}\otimes\Delta\tilde{\mathbf{W}}_{\mathbf{k}}\rangle = 0, \qquad \langle\Delta\tilde{\mathbf{W}}_{\mathbf{k}}\otimes\overline{\Delta\tilde{\mathbf{W}}_{\mathbf{k}}}\rangle = \Delta s\mathcal{I}. \tag{A.2}$$

Now we can compute

$$\begin{aligned}&\rho(s+\Delta s,\mathbf{X},\mathbf{U}|t) - \rho(s,\mathbf{X},\mathbf{U}|t) \\ &\quad = \mathbb{E}\Bigg[\rho(s+\Delta s,\mathbf{X},\mathbf{U}|t) - \Bigg(\rho(s+\Delta s,\mathbf{X},\mathbf{U}|t) + \sum_{\boldsymbol{\alpha}\in\mathcal{A}}(\Delta\mathbf{X}_{\boldsymbol{\alpha}})\cdot\frac{\partial\rho(s,\mathbf{X},\mathbf{U}|t)}{\partial\mathbf{X}_{\boldsymbol{\alpha}}} \\ &\qquad + \sum_{\mathbf{k}\in S}(\Delta\hat{\mathbf{u}}_{\mathbf{k}})\cdot\frac{\partial\rho(s,\mathbf{X},\mathbf{U}|t)}{\partial\hat{\mathbf{u}}_{\mathbf{k}}} \\ &\qquad + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'\in S}(\Delta\hat{\mathbf{u}}_{\mathbf{k}})\cdot\frac{\partial^2\rho(s,\mathbf{X},\mathbf{U}|t)}{\partial\hat{\mathbf{u}}_{\mathbf{k}}\partial\hat{\mathbf{u}}_{\mathbf{k}'}}\cdot(\Delta\hat{\mathbf{u}}_{\mathbf{k}'})\Bigg)\Bigg|\,\mathbf{X}(s)=\mathbf{X},\mathbf{U}(s)=\mathbf{U}\Bigg] \\ &\qquad + o(\Delta s) \\ &\quad = -\tilde{K}^3\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\sum_{\mathbf{k}\in S}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(s)}\hat{\delta}_{1,\mathbf{k}}\hat{\mathbf{u}}_{\mathbf{k}}(s)\cdot\frac{\partial\rho(s,\mathbf{X},\mathbf{U}|t)}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\Delta s \\ &\qquad + \sum_{\mathbf{k}\in S}\Bigg[\mathcal{B}_{\mathbf{k}}(\mathbf{U}(s),\mathbf{U}(s)) + 4\pi^2\left(\frac{k}{\tilde{K}}\right)^2\mathrm{Ku}_{\mathrm{T}}^{-1}\hat{\mathbf{u}}_{\mathbf{k}}(s) \\ &\qquad\qquad + \phi\mathcal{P}_{\mathbf{k}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}}\tilde{\Phi}\left(\frac{\mathbf{X}_{\boldsymbol{\alpha}}(s)}{\tilde{\ell}_f}\right)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}(s)}\Bigg]\cdot\frac{\partial\rho(s,\mathbf{X},\mathbf{U}|t)}{\partial\hat{\mathbf{u}}_{\mathbf{k}}}\Delta s \\ &\qquad - \sum_{\mathbf{k}\in S}\mathrm{Ku}_{\mathrm{T}}^{-1}\tilde{K}^{-3}\left(4\pi^2\left(\frac{k}{\tilde{K}}\right)^2\right)\mathcal{P}_{\mathbf{k}} : \frac{\partial^2\rho(s,\mathbf{X},\mathbf{U}|t)}{\partial\hat{\mathbf{u}}_{\mathbf{k}}\partial\hat{\mathbf{u}}_{\mathbf{k}}^*}\Delta s + o(\Delta s).\end{aligned} \tag{A.3}$$

We used (A.1) and (A.2) to collapse the sum over $\mathbf{k}$ and $\mathbf{k}'$ in the last term to a single sum (with $\mathbf{k}' = -\mathbf{k}$). Dividing the final relation by Δs, then sending $\Delta s \to 0$, leads to the Kolmogorov backward equation (3.3). The $\mathcal{P}_{\mathbf{k}}$ can be dropped from the term involving second derivatives of $\hat{\mathbf{u}}_{\mathbf{k}}$ because $\mathbf{k}\cdot\partial/(\partial\hat{\mathbf{u}}_{\mathbf{k}}) = 0$ follows automatically from the fact that $\hat{\mathbf{u}}_{\mathbf{k}}$ is understood to always be restricted so that $\mathbf{k}\cdot\hat{\mathbf{u}}_{\mathbf{k}} = 0$.

A.2. Asymptotic expansion of solution. We show now how to derive the limiting equation (3.6) from the original Kolmogorov backward equation (3.5) with the small parameter ε. We expand the solution in powers of ε:

$$\rho^\varepsilon = \rho_0 + \varepsilon\rho_1 + \varepsilon^2\rho_2 + \cdots.$$

Then, writing out the first three equations of the asymptotic hierarchy, we have

$$\begin{aligned} \mathcal{L}_1\rho_0 &= 0, \\ \mathcal{L}_1\rho_1 &= -\mathcal{L}_2\rho_0, \\ \mathcal{L}_1\rho_2 &= -\frac{\partial\rho_0}{\partial s} - \mathcal{L}_2\rho_1. \end{aligned} \tag{A.4}$$

We will now solve these in succession; all three must be considered to obtain a full description of the evolution of ρ_0. Our presentation will take the form of a formal calculation, but the results find rigorous support from the theorem of Kurtz [9, 30] for any finite truncation of the set of modes S.

Since we are interested in deriving effective equations for only the (slow) particle coordinates $\mathbf{X}$, we can restrict attention to initial data which depends only on $\mathbf{X}$:

$$f = f(\mathbf{X}).$$

In the solvability conditions that will follow after consideration of the second- and higher-order equations of the hierarchy, it will be helpful to explicitly identify some analytical properties of $\mathcal{L}_1$. Since $\mathcal{L}_1$ is the generator of the Ornstein–Uhlenbeck process, the projection $\mathcal{P}_N$ onto its null space can be identified with the operation of averaging against its invariant measure (MTV):

$$\begin{aligned} (\mathcal{P}_N g)(\mathbf{X}) = (\mathbb{E}_{OU} g)(\mathbf{X}) &\equiv \int_{\mathbb{C}^S} d\mathbf{U}\, \pi_{OU}(\mathbf{U}) g(\mathbf{X},\mathbf{U}), \\ \pi_{OU}(\mathbf{U}) &= \left(\prod_{\mathbf{k}\in S} \frac{\tilde{K}^3}{4\pi}\right) \exp\left(-\frac{1}{2}\tilde{K}^3 \sum_{\mathbf{k}\in S} |\hat{\mathbf{u}}_{\mathbf{k}}|^2\right). \end{aligned} \tag{A.5}$$

Also, the null space of $\mathcal{L}_1^*$ is exactly spanned by π_{OU}, so in applying the solvability conditions, it is helpful to note that (see [13])

$$g \in \operatorname{Ran}\mathcal{L}_1 \Leftrightarrow g \in (\operatorname{Ker}\mathcal{L}_1^*)^\perp \Leftrightarrow \mathbb{E}_{OU} g = 0. \tag{A.6}$$

A.3. First equation in asymptotic hierarchy. The leading-order equation in (A.4) implies simply that ρ_0 does not depend on the fast variables $\mathbf{U}$:

$$\rho_0 = \rho_0(s, \mathbf{X}|t).$$

Another way of expressing this is

$$\mathbb{E}_{OU}\rho_0 = \rho_0.$$

A.4. Second equation in asymptotic hierarchy. The solvability condition for the second equation in (A.4) is

$$\mathbb{E}_{OU}\mathcal{L}_2\rho_0 = \mathbb{E}_{OU}\mathcal{L}_2\mathbb{E}_{OU}\rho_0 = 0,$$

which is trivially satisfied because $\mathbb{E}_{OU}\mathcal{L}_2\mathbb{E}_{OU} = 0$.

Therefore, the equation may be solved directly by writing

$$\rho_1 = -\mathcal{L}_1^{-1}\mathcal{L}_2\mathbb{E}_{OU}\rho_0 + \tilde{\rho}_1. \tag{A.7}$$

Since $\mathcal{L}_1$ has a one-dimensional null-space, the inverse operator $\mathcal{L}_1^{-1}$ should be thought of as a particular continuous choice of an inverse image associated with each function in the range of $\mathcal{L}_1$. We make a specific choice in section A.6. The function $\tilde{\rho}_1 = \tilde{\rho}_1(\mathbf{X}, s|t)$ is a function in the null space of $\mathcal{L}_1$; its presence reflects the one-dimensional indeterminacy of the inversion of $\mathcal{L}_1$.

A.5. Third equation in asymptotic hierarchy. Substituting the solution (A.7) into the third equation in (A.4) and applying the solvability condition, we obtain the desired evolution equation for ρ_0 in operator-theoretic form:

$$\begin{aligned} -\frac{\partial \rho_0}{\partial s} &= -\mathbb{E}_{OU}\mathcal{L}_2\mathcal{L}_1^{-1}\mathcal{L}_2\mathbb{E}_{OU}\rho_0, \\ \rho_0(s=t, \mathbf{X}|t) &= f(\mathbf{X}). \end{aligned} \tag{A.8}$$

The arbitrary function $\tilde{\rho}_1 \in \operatorname{Ker}\mathcal{L}_1$ has now disappeared because $\mathbb{E}_{OU}\mathcal{L}_2\tilde{\rho}_1 = 0$. Therefore, we see that the evolution equation for ρ_0 will not depend on the particular way in which we choose to invert $\mathcal{L}_1$.

A.6. Explicit computation of limiting PDE. To express the differential operator

$$\bar{\mathcal{L}} \equiv -\mathbb{E}_{OU}\mathcal{L}_2\mathcal{L}_1^{-1}\mathcal{L}_2\mathbb{E}_{OU},$$

appearing on the right-hand side of (A.8), in a concrete form, we follow the development in Appendix B of MTV. To map the formulas appearing there to the present problem, we write

$$\mathcal{L}_1 = \sum_{\mathbf{k}\in S}\left(-\gamma_{\mathbf{k}}\hat{\mathbf{u}}_{\mathbf{k}}\cdot\frac{\partial}{\partial\hat{\mathbf{u}}_{\mathbf{k}}} + \frac{\sigma_{\mathbf{k}}^2}{2}\frac{\partial}{\partial\hat{\mathbf{u}}_{\mathbf{k}}}\cdot\frac{\partial}{\partial\hat{\mathbf{u}}_{\mathbf{k}}^*}\right),$$

with

$$\gamma_{\mathbf{k}} \equiv 4\pi^2(k/\tilde{K})^2, \qquad \sigma_{\mathbf{k}} \equiv \sqrt{2\tilde{K}^{-3}(4\pi^2(k/\tilde{K})^2)}. \tag{A.9}$$

We pass to the representation of $\mathcal{L}_2$ acting on Fourier transformed functions of the fast variables $\mathbf{U}$. We must be careful in defining this Fourier transform, however, because the variables constituting $\mathbf{U}$ are complex and are constrained by the complex conjugacy relations $\hat{\mathbf{u}}_{-\mathbf{k}} = \hat{\mathbf{u}}_{\mathbf{k}}^*$. Therefore, we define the Fourier transform of functions $g(\mathbf{U})$ by

$$\hat{g}(\mathbf{P}) = \int_{\mathbb{C}^S}\exp\left[\frac{1}{4}i\sum_{\mathbf{k}\in S}\left(\hat{\mathbf{u}}_{\mathbf{k}}\cdot(\mathbf{p}_{\mathbf{k}} + \mathbf{p}_{-\mathbf{k}}^*) + \hat{\mathbf{u}}_{\mathbf{k}}^*\cdot(\mathbf{p}_{-\mathbf{k}} + \mathbf{p}_{\mathbf{k}}^*)\right)\right] g(\mathbf{U})\,d\mathbf{U},$$

where $\mathbf{P} = \{\mathbf{p}_{\mathbf{k}}\}_{\mathbf{k}\in S}$. This artifice first ensures that the exponent is purely imaginary (so that the Fourier integration is at least well defined in each mode), and second allows us to identify $\mathbf{p}_{-\mathbf{k}}$ with $\mathbf{p}_{\mathbf{k}}^*$ just as we have been identifying $\hat{\mathbf{u}}_{-\mathbf{k}}$ with $\hat{\mathbf{u}}_{\mathbf{k}}^*$. Indeed, $\hat{g}$ must perforce depend on $\mathbf{p}_{\mathbf{k}}$ and $\mathbf{p}_{-\mathbf{k}}^*$ in the same way, and thus these

variables can be identified with each other. Also, we can and will restrict the domain of definition of the variables $\mathbf{p_k}$ to the hyperplane $\mathbf{p_k} \cdot \mathbf{k} = 0$; the component of $\mathbf{p_k}$ parallel to $\mathbf{k}$ is irrelevant because of the restriction $\hat{\mathbf{u}}_\mathbf{k} \cdot \mathbf{k} = 0$. Finally, it can be readily checked that the Fourier transform rules for derivatives carry over to our present definition of the Fourier transform in a straightforward way:

$$\hat{\mathbf{u}}_\mathbf{k} \to -i\frac{\partial}{\partial \mathbf{p_k}}, \qquad \frac{\partial}{\partial \hat{\mathbf{u}}_\mathbf{k}} \to -i\mathbf{p_k}.$$

Proceeding, then, we write down the Fourier transform of the operator $\mathcal{L}_2$ as

$$\begin{aligned}\hat{\mathcal{L}}_2 = \sum_{\mathbf{k}\in S}\Bigg[&-2\pi\tilde{K}^{-1}\mathcal{P}_\mathbf{k}\sum_{\mathbf{k}'\in S}\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{p}_{\mathbf{k}'}}\frac{\partial}{\partial\mathbf{p}_{\mathbf{k}-\mathbf{k}'}}\\ &+ i\phi\mathcal{P}_\mathbf{k}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}}\tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\Bigg]\cdot\mathbf{p_k}\\ &- i\tilde{K}^3\sum_{\mathbf{k}\in S}\hat{\delta}_{1,\mathbf{k}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial}{\partial\mathbf{p_k}}\cdot\frac{\partial}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}.\end{aligned}$$

We can now adapt relation (B.4) of MTV to our present case with complex-valued variables:

$$\begin{aligned}&-\mathbb{E}_{OU}\mathcal{L}_2\mathcal{L}_1^{-1}\mathcal{L}_2\mathbb{E}_{OU}g(\mathbf{X})\\ &\quad=\int_{\mathbb{C}^S}d\mathbf{P}\,\hat{\tilde{P}}_{OU}(\mathbf{P})\hat{\mathcal{L}}_2\int_0^\infty dt\\ &\quad\exp\left(\sum_{\mathbf{k}\in S}\gamma_\mathbf{k}t-\frac{1}{4}\sum_{\mathbf{k}\in S}\frac{\sigma_\mathbf{k}^2|\mathbf{p_k}|^2}{\gamma_\mathbf{k}}(e^{2\gamma_\mathbf{k}t}-1)\right)\left[\hat{\mathcal{L}}_2(g(\mathbf{X})\delta(\mathbf{P}'))\right]_{\mathbf{P}'=\boldsymbol{\beta}(\mathbf{P},t)},\end{aligned}$$

where $\mathbf{P}$ is shorthand notation for the collection $\{\mathbf{p_k}\}_{\mathbf{k}\in S}$ (similarly for $\mathbf{P}'$),

$$\hat{\tilde{P}}_{OU}(\mathbf{P}) = \exp\left(-\frac{1}{4}\sum_{\mathbf{k}\in S}\frac{\sigma_\mathbf{k}^2|\mathbf{p_k}|^2}{\gamma_\mathbf{k}}\right)$$

is the Fourier transform of the invariant measure $\pi_{OU}(\mathbf{U})$ in (A.5), and

$$\boldsymbol{\beta}(\mathbf{P},t) = \{e^{\gamma_\mathbf{k}t}\mathbf{p_k}\}_{\mathbf{k}\in S}.$$

We have here chosen to define $\mathcal{L}_1^{-1}$ in terms of its Fourier transform:

$$(\hat{\mathcal{L}}_1^{-1}b)(\mathbf{P}) = -\int_0^\infty \exp\left(-\frac{1}{4}\sum_{\mathbf{k}\in S}\frac{\sigma_\mathbf{k}^2|\mathbf{p_k}|^2}{\gamma_\mathbf{k}}(e^{2\gamma_\mathbf{k}t}-1)\right)\exp\left(\sum_{\mathbf{k}\in S}\gamma_\mathbf{k}t\right)\hat{b}(\boldsymbol{\beta}(\mathbf{P},t))\,dt.$$

Computing now the action of the rightmost $\hat{\mathcal{L}}_2$, we obtain

$$\begin{aligned}&\exp\left(\sum_{\mathbf{k}\in S}\gamma_\mathbf{k}t\right)\left(\left[\hat{\mathcal{L}}_2(g(\mathbf{X})\delta(\mathbf{P}'))\right]_{\mathbf{P}'=\boldsymbol{\beta}(\mathbf{P},t)}\right)\\ &\qquad= -i\tilde{K}^3\sum_{\mathbf{k}\in S}\hat{\delta}_{1,\mathbf{k}}e^{-\gamma_\mathbf{k}t}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial g}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\frac{\partial\delta(\mathbf{P})}{\partial\mathbf{p_k}}.\end{aligned}$$

Continuing,

$$
\begin{aligned}
&\hat{\mathcal{L}}_1^{-1}\hat{\mathcal{L}}_2(g(\mathbf{X})\delta(\mathbf{P})) \\
&\quad = -\int_0^\infty dt\, \exp\left(-\frac{1}{4}\sum_{\mathbf{k}\in S}\frac{\sigma_{\mathbf{k}}^2|\mathbf{p}_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}}(e^{2\gamma_{\mathbf{k}}t}-1)\right) \\
&\qquad\qquad \times\left[-i\tilde{K}^3\sum_{\mathbf{k}\in S}\hat{\delta}_{1,\mathbf{k}}e^{-\gamma_{\mathbf{k}}t}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial g}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\frac{\partial\delta(\mathbf{P})}{\partial\mathbf{p}_{\mathbf{k}}}\right] \\
&\quad = i\tilde{K}^3\sum_{\mathbf{k}\in S}\hat{\delta}_{1,\mathbf{k}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial g}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\frac{\partial\delta(\mathbf{P})}{\partial\mathbf{p}_{\mathbf{k}}}\int_0^\infty e^{-\gamma_{\mathbf{k}}t}\,dt \\
&\quad = i\tilde{K}^3\sum_{\mathbf{k}\in S}\frac{\hat{\delta}_{1,\mathbf{k}}}{\gamma_{\mathbf{k}}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial g}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\frac{\partial\delta(\mathbf{P})}{\partial\mathbf{p}_{\mathbf{k}}}.
\end{aligned}
$$

Next, using the distribution identity $\mathbf{p}_{\mathbf{k}}\otimes\frac{\partial\delta(\mathbf{p}_{\mathbf{k}})}{\partial\mathbf{p}_{\mathbf{k}}} = -\mathcal{I}\delta(\mathbf{p}_{\mathbf{k}})$, we have

$$
\begin{aligned}
&\hat{\mathcal{L}}_2\hat{\mathcal{L}}_1^{-1}\hat{\mathcal{L}}_2(g(\mathbf{X})\delta(\mathbf{P})) \\
&\quad = -i\tilde{K}^3\sum_{\mathbf{k}\in S}\left[-2\pi\tilde{K}^{-1}\mathcal{P}_{\mathbf{k}}\sum_{\mathbf{k}'\in S}\mathbf{k}\cdot\frac{\partial}{\partial\mathbf{p}_{\mathbf{k}'}}\frac{\partial}{\partial\mathbf{p}_{\mathbf{k}-\mathbf{k}'}}\right. \\
&\qquad\qquad \left. + i\phi\mathcal{P}_{\mathbf{k}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}}\tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\right] \\
&\qquad\qquad \cdot\left[\frac{\hat{\delta}_{1,\mathbf{k}}}{\gamma_{\mathbf{k}}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial g(\mathbf{X})}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\delta(\mathbf{P})\right] \\
&\quad + \tilde{K}^6\sum_{\mathbf{k},\mathbf{k}'\in S}\frac{\hat{\delta}_{1,\mathbf{k}}\hat{\delta}_{1,\mathbf{k}'}}{\gamma_{\mathbf{k}}}\sum_{\boldsymbol{\alpha},\boldsymbol{\alpha}'\in\mathcal{A}}e^{2\pi i(\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}+\mathbf{k}'\cdot\mathbf{X}_{\boldsymbol{\alpha}'})/\tilde{K}}\frac{\partial^2 g(\mathbf{X})}{\partial\mathbf{X}_{\boldsymbol{\alpha}}\partial\mathbf{X}_{\boldsymbol{\alpha}'}}:\frac{\partial^2\delta(\mathbf{P})}{\partial\mathbf{p}_{\mathbf{k}}\partial\mathbf{p}_{\mathbf{k}'}} \\
&\quad + \tilde{K}^6\sum_{\mathbf{k},\mathbf{k}'\in S}\frac{\hat{\delta}_{1,\mathbf{k}}\hat{\delta}_{1,\mathbf{k}'}}{\gamma_{\mathbf{k}}}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\frac{\partial g(\mathbf{X})}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\frac{\partial^2\delta(\mathbf{P})}{\partial\mathbf{p}_{\mathbf{k}}\partial\mathbf{p}_{\mathbf{k}'}}\cdot(2\pi i\mathbf{k}).
\end{aligned}
\tag{A.10}
$$

Finally, taking the leftmost expectation defining $\bar{\mathcal{L}}$, we have

$$
\begin{aligned}
\bar{\mathcal{L}}g(\mathbf{X}) &= -\int_{\mathbb{C}^S}\hat{\bar{P}}_{OU}(\mathbf{P})\hat{\mathcal{L}}_2\hat{\mathcal{L}}_1^{-1}\hat{\mathcal{L}}_2(g(\mathbf{X})\delta(\mathbf{P})) \\
&= -\tilde{K}^3\sum_{\mathbf{k}\in S}\phi\mathcal{P}_{\mathbf{k}}\sum_{\boldsymbol{\alpha}'\in\mathcal{A}}\nabla_{\boldsymbol{\alpha}'}\tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right)\hat{\delta}_{1,\mathbf{k}}e^{-2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}'}/\tilde{K}}\hat{\delta}_{1,\mathbf{k}}\gamma_{\mathbf{k}}^{-1}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot\mathbf{X}_{\boldsymbol{\alpha}}/\tilde{K}}\cdot\frac{\partial g(\mathbf{X})}{\partial\mathbf{X}_{\boldsymbol{\alpha}}} \\
&\quad + \tilde{K}^6\sum_{\mathbf{k}\in S}\frac{|\hat{\delta}_{1,\mathbf{k}}|^2\sigma_{\mathbf{k}}^2}{2\gamma_{\mathbf{k}}^2}\sum_{\boldsymbol{\alpha},\boldsymbol{\alpha}'\in\mathcal{A}}e^{2\pi i\mathbf{k}\cdot(\mathbf{X}_{\boldsymbol{\alpha}}-\mathbf{X}_{\boldsymbol{\alpha}'})/\tilde{K}}\frac{\partial}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\mathcal{P}_{\mathbf{k}}\cdot\frac{\partial g(\mathbf{X})}{\partial\mathbf{X}_{\boldsymbol{\alpha}'}} \\
&\quad + \tilde{K}^6\sum_{\mathbf{k},\mathbf{k}'\in S}\frac{\hat{\delta}_{1,\mathbf{k}}\hat{\delta}_{1,\mathbf{k}'}\sigma_{\mathbf{k}}^2}{2\gamma_{\mathbf{k}}^2}\sum_{\boldsymbol{\alpha}\in\mathcal{A}}\frac{\partial g(\mathbf{X})}{\partial\mathbf{X}_{\boldsymbol{\alpha}}}\cdot\mathcal{P}_{\mathbf{k}}\cdot(2\pi i\mathbf{k})
\end{aligned}
$$

$$= -\phi \tilde{K}^3 \sum_{\mathbf{k}\in S} \frac{\hat{\delta}^2_{1,\mathbf{k}}}{\gamma_{\mathbf{k}}} \mathcal{P}_{\mathbf{k}} \sum_{\boldsymbol{\alpha},\boldsymbol{\alpha}'\in\mathcal{A}} \nabla_{\boldsymbol{\alpha}'} \tilde{\Phi}\left(\frac{\mathbf{X}}{\tilde{\ell}_f}\right) e^{2\pi i \mathbf{k}\cdot(\mathbf{X}_{\boldsymbol{\alpha}}-\mathbf{X}_{\boldsymbol{\alpha}'})/\tilde{K}} \cdot \frac{\partial g(\mathbf{X})}{\partial \mathbf{X}_{\boldsymbol{\alpha}}}$$

$$+ \tilde{K}^6 \sum_{\boldsymbol{\alpha},\boldsymbol{\alpha}'\in\mathcal{A}} \sum_{\mathbf{k}\in S} \frac{|\hat{\delta}_{1,\mathbf{k}}|^2 \sigma^2_{\mathbf{k}}}{2\gamma^2_{\mathbf{k}}} e^{2\pi i \mathbf{k}\cdot(\mathbf{X}_{\boldsymbol{\alpha}}-\mathbf{X}_{\boldsymbol{\alpha}'})/\tilde{K}} \frac{\partial}{\partial \mathbf{X}_{\boldsymbol{\alpha}}} \cdot \mathcal{P}_{\mathbf{k}} \cdot \frac{\partial g(\mathbf{X})}{\partial \mathbf{X}_{\boldsymbol{\alpha}'}}.$$

We have used the fact that

$$\mathbb{E}_{OU} \frac{\partial^2 \delta(\mathbf{P})}{\partial \mathbf{p}_{\mathbf{k}} \partial \mathbf{p}_{\mathbf{k}'}} = \begin{cases} -\frac{\sigma^2_{\mathbf{k}}}{2\gamma_{\mathbf{k}}} \mathcal{P}_{\mathbf{k}} & \text{if } \mathbf{k}+\mathbf{k}'=0, \\ 0 & \text{otherwise.} \end{cases} \tag{A.11}$$

We show in more detail how the contribution from the first term in brackets in (A.10), arising from the nonlinear advection term in the Navier–Stokes equations, vanishes upon averaging. From (A.11) we have

$$\mathbb{E}_{OU} \sum_{\mathbf{k}'} \frac{\partial}{\partial \mathbf{p}_{\mathbf{k}'}} \frac{\partial \delta(\mathbf{P})}{\partial \mathbf{p}_{\mathbf{k}-\mathbf{k}'}} = 0 \quad \text{unless } \mathbf{k} = \mathbf{0}.$$

However, since this expression appears in an inner product with $\mathbf{k}$ in (A.10), the term arising from nonlinear advection in the Navier–Stokes equations makes no contribution at all upon averaging.

We finally complete the calculation of $\bar{\mathcal{L}}$ by converting back to our original problem parameters, using the expressions (A.9) for $\gamma_{\mathbf{k}}$ and $\sigma_{\mathbf{k}}$. We thereby arrive at (3.6).

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