A novel approach to computing the orientation moments of spheroids in simple shear flow at arbitrary Péclet number

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(Received 28 August 2001; accepted 11 October 2001)

A Langevin approach to computing the orientation moments of a dilute suspension of spheroids in a simple shear flow at arbitrary Péclet number is presented. In this method we obtain the equations governing the time evolution of the orientation averages using a generalized Langevin equation approach and develop a computational technique for computing the evolution of the moments from these equations. These results are compared with those available in the literature obtained from other methods and show good agreement. The approach presented here can be easily generalized to a number of similar systems such as forced suspensions of dipolar particles in shear flows and can be applied to other flow problems governed by appropriate Fokker–Planck equations. [DOI: 10.1063/1.1426391]

I. INTRODUCTION

There are a number of instances, both in engineering applications and in natural phenomena, where the dynamics and bulk viscometric properties of fluid suspensions of small orientable particles have to be considered (e.g., magneto-fluidization,[1] magnetostriction of ferromagnetic particle suspensions,[2] characterization of magnetorheological suspensions,[3] bio-convection setup by swimming of certain micro-organisms[4,5]). The bulk properties of suspensions generally depend on the nature of the fluid, the properties and distribution of the particles in the fluid, and the degree of isotropy of the solution. The most important factor affecting the bulk properties is the orientation of the particles in the suspension, and an important step in any investigation of these properties is the determination of the orientation distribution function (ODF), the density function for the orientations of the particles. The spatial orientations and positions of particles in such suspensions are affected by a number of factors such as the type and strength of the flow field (if the suspending fluid is in motion), the particle–particle interactions which are a result of the disturbance that the presence of each particle produces on the behavior of nearby particles (if the suspension is concentrated), the rotary Brownian diffusion resulting from the bombardment of the suspension particles by the randomly moving fluid molecules (if the particle size is sufficiently small), and the presence of an external field which may impart an orientational torque to the particles (if the suspension particles are dipolar, e.g., ferromagnetic particles suspended in a ferro fluid). In this study we neglect the effect of the particle interactions and attempt to model the dynamics and the orientation moments of a dilute suspension of Brownian spheroids subjected to a simple shear flow using a generalized Langevin equation approach.

In the absence of particle–particle interactions and external forces the particle orientations are determined by a competition between the torques due to the shearing motion of the imposed flow and the rotational Brownian motion. The relative importance of these fluxes is expressed in terms of the rotary Péclet number $\mathrm{Pe}=\dot{\gamma}/D_r$ where $\dot{\gamma}$ is the shear rate and D_r is the rotary diffusivity of a spheroid of aspect ratio r. According to a classic result due to Jeffery,[6] in the absence of Brownian diffusion or any other particle body forces, an ellipsoidal particle subjected to a simple shear flow executes a periodic motion along a certain orbit depending on its initial orientation. Hence in this case, the steady state orientation distribution of the particles is determined by the initial conditions. Subsequently Leal and Hinch[7] showed that the presence of even very weak rotary Brownian motion can make the steady state orientations *independent* of the initial conditions. The presence of rotary Brownian motion makes the orientations of the particles a stochastic process and as such the system can be modeled either through a Fokker–Planck (diffusion) equation approach or through a Langevin equation approach. The traditional approach to modeling such systems (the diffusion equation approach) is based on expressing the bulk suspension properties in terms of suitable moments of the ODF obtained by solving an appropriate diffusion equation for the system at steady state. Since solving the diffusion equation in its full generality is difficult

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various authors have attempted different numerical schemes to approximate the solution for various ranges of shear and Brownian parameters.[8–12] If diffusion is weak compared to shear, the particles tend to spend most of the time along the flow direction and diffusion can be neglected except in a small region of the orientation space near the flow direction.[8] Hinch and Leal[8] used a regular perturbation method around 1/Pe to approximate the ODF in this regime ($\mathrm{Pe}^{1/3} \gg r$). On the other hand, if the Brownian diffusion is stronger ($\mathrm{Pe} \ll 1$), the weak flow disturbs the uniform orientation distribution caused by the randomizing effect of diffusion only slightly; hence a regular perturbation about Pe may be used to approximate the ODF.[9] When the flow strength is in between these extremes, the perturbation methods fail. Chen and Koch[11] developed a spherical harmonic method to determine the orientation distribution function of fibers of large aspect ratio in this intermediate regime where diffusion and advection are comparable. This involves expanding the steady state orientation distribution function into a double series of spherical harmonics and substituting a suitably truncated form of this series into the diffusion equation for the system, leaving a set of linear equations in the expansion coefficients. The number of terms in the truncated series and hence the number of linear equations to be solved generally increases with increasing Pe to achieve a given accuracy. Hence the procedure becomes computationally formidable for larger values of Pe, but the technique can be successfully applied for Pe up to 1000 (Chen and Jiang). Chen and Jiang[12] present another approach, in which the diffusion equation of the system is numerically solved for the steady state ODF using a finite difference scheme with a pair of boundary conditions. This method is applicable when the flow is moderate (Pe up to 1000), but even for small Pe, the numerical scheme requires a large number of mesh points to achieve a given accuracy and so the computation time is longer even in the weak flow regime. For very large Pe they suggest another method in which the diffusion equation is numerically solved for the time evolution of the ODF with a given initial state until steady state is reached. This is particularly useful for $\mathrm{Pe} > 1000$ where spherical harmonics method becomes computationally difficult.

It is clear from the above discussion that the numerical schemes currently used for solving the diffusion equation vary as the flow and Brownian parameters are changed. In this work, we present an alternate approach to computing the orientation moments without having to solve the diffusion equation. This method is based on a generalized Langevin equation approach presented recently by Coffey *et al.*[13] for nonlinear systems with noise, and provides a unified strategy for modeling such systems placing little restriction on the Péclet number of the flow. We shall consider a dilute suspension of Brownian spheroids subjected to a simple shear flow and derive suitable Langevin equations for their time evolution. Each Langevin equation is an equation of motion for the orientation of a single particle depicting the irregular part of the motion due to Brownian effects in terms of a suitable random noise term whose properties are determined only on average. An ensemble of these equations must be identical to the governing diffusion equation of the entire system. We then obtain the *exact equation of motion for any desired orientation average* using a novel idea of Coffey *et al.* A brief account of this procedure is given in Sec. III. These moment equations being ordinary differential equations are easier to handle than the original Langevin equations which are stochastic differential equations. *For each pair of averages we get a couple of ordinary differential equations which together govern their time evolution*. These equations can be solved analytically in simple cases giving earlier results in the literature. For the general case, we develop a brute-force computational technique to generate the desired averages in pairs by simulating a set of related equations with given initial conditions until steady state is reached.

The basic idea behind the Coffey *et al.* treatment of nonlinear systems with noise is that by interpreting a Langevin equation for a stochastic variable as an integral equation in the Stratanovich sense with a sharp initial condition, it is possible to express suitable time averages of the stochastic variable in terms of a deterministic equation of motion for the sharp values. Any desired ensemble average can then be generated directly from an ensemble of time-averaged Langevin equations without having to solve the diffusion equation. For the system we consider the bulk suspension properties are related to orientation averages over the particles aligned along a set of common directions. The most realistic model for such a suspension may be a set of Langevin equations starting off from sharp initial conditions in a time-averaged sense over an appropriate white noise term. Thus this system is an ideal one for applying the Coffey *et al.* approach. The technique presented here can be easily generalized and applied to other similar systems with noise.

The exact form of the noise term in the Langevin equation is obtained by comparing the moments of spherical harmonics as obtained from the diffusion equation and an ensemble of Langevin equations. We note that the spherical harmonics form a complete set for the eigenfunction expansion of any orientation average. We derive in Sec. II a differential recurrence formula for the moments of surface spherical harmonics starting from the diffusion equation and reproduce it in Sec. III from the Langevin equation method with a presumed noise term for the Langevin equations as suggested by some heuristic arguments. The exact agreement between the two formulas then justifies the form of noise we started with. Details of the relevant ideas of the Coffey *et al.* method are also given in Sec. III. Section IV is devoted to the computation of certain orientation moments from the governing evolution equations obtained by the new method. These equations are easily solved in the zero shear limit giving the familiar result that the orientations tend to a uniform distribution at equilibrium due to the randomization effect caused by the Brownian diffusion. In other cases, we transform each pair of moment equations into a pair of coupled ODEs and a set of such equations is simulated over a finite number of initial conditions until steady state is reached. The desired moments can be easily obtained from these solutions and the results are in good agreement with previously known ones. Concluding remarks are given in Sec. V. The new method has the advantage that it provides a unified strategy that can be applied over a wider range of Pe than is possible by other methods. It can be easily generalized to more complex systems like suspensions of charged particles or suspensions of dipolar particles with external forcing.

II. THE DIFFUSION EQUATION APPROACH

We begin by considering a single particle from a suspension of identical rigid, neutrally buoyant spheroids in an infinite incompressible Newtonian fluid subject to a uniform shearing motion defined by a flow field, $\mathbf{v}=\dot{\gamma}y\mathbf{i}$ where $\dot{\gamma}$ is the shear rate, y is the y-coordinate, and $\mathbf{i}$ is the unit vector in the X-direction. The suspension is assumed to be sufficiently dilute so that particle particle hydrodynamic interactions may be neglected. Since for a dilute suspension the bulk properties are generally determined by the orientations of the particles alone, we neglect any translatory motion of the particle by choosing a coordinate system that moves along with it. The particles may experience rotational torques due to the hydrodynamic force caused by the imposed flow and the Brownian force caused by the bombardment of the particles by surrounding fluid molecules. The diffusion (Fokker–Planck) equation that governs the time evolution of the particle distributions of the system is then given by[10]

$$\frac{\partial \psi}{\partial t}+\frac{\partial}{\partial \mathbf{u}}\cdot(\dot{\mathbf{u}}\psi)=D_r\frac{\partial^2\psi}{\partial \mathbf{u}^2}. \tag{1}$$

Here $\mathbf{u}$ is the vector describing the orientation of the particle and is assumed to be a unit vector fixed along the major axis of the spheroid. $\psi(\mathbf{u},t)$ is the *orientation distribution function* which is such that $\psi(\mathbf{u},t)d\mathbf{u}$ gives the probability that a particle is oriented in the solid angle $d\mathbf{u}$ about $\mathbf{u}$ at time t. The term on the right side of Eq. (1) reflects the effect of rotary Brownian diffusion, the factor D_r being the rotary diffusivity defined by $D_r=k_BT/\zeta_\perp$, where $\zeta_\perp$ represents the rotational resistance in the direction perpendicular to the particle symmetry axis, k_B is the Boltzmann constant, and T is the absolute temperature. The time derivative of the orientation vector appearing in the above equation may be expressed as $\dot{\mathbf{u}}=\omega\times\mathbf{u}$, where ω is the angular velocity of the particle, an expression for which may be obtained through an angular momentum balance equation[10]

$$\omega=\mathbf{\Omega}+C[\mathbf{u}\times(\mathbf{E}\cdot\mathbf{u})]. \tag{2}$$

In the above expression, $C=(r^2-1)/(r^2+1))$ is a shape factor for a spheroid of aspect ratio r and $\mathbf{E}$ and $\mathbf{\Omega}$ are, respectively, the rate of deformation tensor and vorticity vector for the flow defined thus:

$$\mathbf{E}=\tfrac{1}{2}(\nabla\mathbf{v}+\nabla\mathbf{v}^T),\quad \mathbf{\Omega}=\tfrac{1}{2}(\nabla\times\mathbf{v}).$$

The resulting expression for the evolution of the orientation vector becomes

$$\dot{\mathbf{u}}=\mathbf{\Omega}\times\mathbf{u}+C[\mathbf{u}\times(\mathbf{E}\cdot\mathbf{u})]\times\mathbf{u}. \tag{3}$$

Writing $\mathbf{u}=u_1\mathbf{i}+u_2\mathbf{j}+u_3\mathbf{k}$ the last equation may be written in Cartesian coordinates as follows:

$$\begin{aligned}\dot{u}_1&=\dot{\gamma}Cu_2(1-u_1^2)+\dot{\gamma}\left(\frac{1-C}{2}\right)u_2,\\ \dot{u}_2&=-\dot{\gamma}Cu_1u_2^2-\dot{\gamma}\left(\frac{1-C}{2}\right)u_1,\\ \dot{u}_3&=-\dot{\gamma}Cu_1u_2u_3.\end{aligned} \tag{4}$$

Equation (3) gives the regular part of the evolution of the orientation vector in the complete absence of Brownian diffusion, while the effect of Brownian diffusion is taken care of by the diffusive term on the right of Eq. (1). In the Langevin equation, on the other hand, the random behavior due to Brownian effects is incorporated by an additional noise term to Eq. (3) whose properties are determined only by an ensemble of such equations. In the next section we shall be mainly concerned with the exact form of the noise term in the Langevin equation that makes an ensemble of such equations identical to the diffusion equation (1). We do this by requiring that the diffusion equation (1) and the system of Langevin equations with noise generate the same set of orientation averages. Equivalently, since any orientation average can be expanded in terms of suitable spherical harmonics, we may require that both the methods give rise to the same evolution equations for spherical harmonics and use this as a matching condition for obtaining the noise term. Towards this end, we derive a set of differential recurrence relations for surface spherical harmonics for the system governed by Eq. (1) and compare them in Sec. III with a similar set of equations to be obtained from a set of Langevin equations for the same system.

The transformations $u_1=\sin\theta\cos\phi$, $u_2=\sin\theta\sin\phi$, $u_3=\cos\theta$ convert Eq. (4) into their spherical coordinates counterparts,

$$\begin{aligned}\dot{\theta}&=\dot{\gamma}C\sin\theta\cos\theta\sin\phi\cos\phi,\\ \dot{\phi}&=-\dot{\gamma}C\sin^2\phi-\dot{\gamma}\left(\frac{1-C}{2}\right).\end{aligned} \tag{5}$$

We can use the above expressions in Eq. (1) to write it in spherical coordinates thus:

$$\frac{\partial\psi}{\partial t}+\dot{\gamma}C\overline{\Omega}(\psi)-\frac{\dot{\gamma}}{2}(1-C)\frac{\partial\psi}{\partial\phi}=D_r\overline{\Lambda}(\psi). \tag{6}$$

The $\overline{\Omega}$ and $\overline{\Lambda}$ appearing in the above equation are linear operators defined by

$$\overline{\Omega}(\psi)=\frac{\sin\phi\cos\phi}{\sin\theta}\frac{\partial}{\partial\theta}(\psi\sin^2\theta\cos\theta)-\frac{\partial}{\partial\phi}(\psi\sin^2\phi),$$

$$\overline{\Lambda}(\psi)=\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}.$$

We may now expand ψ into a double series of eigenfunctions assuming that $\psi(\theta,\phi,t)$ satisfies the boundary conditions $\psi|^{\theta=\pi,\phi=2\pi}=\psi|^{\theta=0,\phi=0}$

$$\psi=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}a_{n,m}(t)Y_{n,m}.$$

$Y_{n,m}$ are the normalized spherical harmonics[14] defined by

$$Y_{n,m}=N_{n,m}P_n^m(\cos\theta)e^{im\phi},\quad -n\leqslant m\leqslant n.$$

The normalization constants $N_{n,m}$ are given by

$$N_{n,m}=(-1)^m\sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}}.$$

P_n^m are associated Legendre functions defined for non-negative m by

$$P_n^m(x)=(1-x^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}x^m}(P_n(x)),\quad -1\leqslant x\leqslant 1,$$

where $P_n(x)$ is the Legendre polynomial, and for negative m by

$$P_n^{-m}(x)=(-1)^m\frac{(n-m)!}{(n+m)!}P_n^m(x).$$

$Y_{n,m}$ therefore satisfy the relation $Y_{n,m}=(-1)^mY^*_{n,-m}$ where $*$ denotes the complex conjugate. Since ψ is to be real the expansion coefficients $a_{n,m}$ also satisfy a similar relation viz., $a_{n,-m}=(-1)^m a^*_{n,m}$. The spherical harmonics $Y_{n,m}$ form an orthonormal set satisfying the orthogonality relation

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}Y_{q\cdot p}Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi=\delta_{qn}\delta_{pm}. \tag{7}$$

Since ψ is a probability density function it must satisfy the normalization condition,

$$\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\psi(\theta,\phi,t)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi=1.$$

This constrains the first term in the expansion for ψ to satisfy $a_{0,0}Y_{0,0}=1/(4\pi)$ due to orthogonality. We shall denote by $\langle B\rangle$ the ensemble average of any quantity B and evaluate it thus:

$$\langle B\rangle=\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}B\psi\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi.$$

Using the expansion for ψ and Eq. (6) we can now obtain the following differential recurrence relation for $Y^*_{n,m}$:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle Y^*_{n,m}\rangle&=\dot\gamma C\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2}b^{m,j}_{n,k}\langle Y^*_{k,j}\rangle\\&\quad+\frac{3}{2}\dot\gamma C\langle\sin^2\theta\sin(2\phi)Y^*_{n,m}\rangle\\&\quad+\dot\gamma\left(\frac{1-C}{2}\right)im\langle Y^*_{n,m}\rangle-D_r n(n+1)\langle Y^*_{n,m}\rangle,\end{aligned} \tag{8}$$

where $b^{m,j}_{n,k}$ are suitable multiples of the Bird–Warner coefficients (see Appendix A). The details of the calculations leading to Eq. (8) are left to Appendix A. We note that in the absence of shear ($\dot\gamma=0$) or when the particles are spheres ($C=0$), the above recurrence relation is easy to solve, giving $a_{n,m}(t)=\langle Y^*_{n,m}\rangle\rightarrow 0$ as $t\rightarrow\infty$ except $a_{0,0}$ which by normalization is $1/\sqrt{4\pi}$. This is the familiar result that in these cases the randomization effect due to Brownian motion leads to a uniform distribution of the suspension at equilibrium.

III. THE LANGEVIN APPROACH

Before deriving the Langevin equation for the orientation of the particle in the system we consider, we give a brief mathematical description of the Coffey *et al.* approach.[13] Let $\xi=(\xi_1,\xi_2,\ldots\xi_n)$ be an n-dimensional stochastic variable whose components satisfy a set of Langevin equations with multiplicative noise terms,

$$\dot\xi_i(t)=h_i(\boldsymbol\xi(t),t)+g_{ij}(\boldsymbol\xi(t),t)\Gamma_j(t),\quad 1\leqslant i\leqslant n,\quad 1\leqslant j\leqslant m, \tag{9}$$

where Γ_j are Gaussian random variables with zero mean and autocorrelation functions proportional to the δ function:

$$\overline{\Gamma_j(t)}=0,\quad \overline{\Gamma_i(t)\Gamma_j(t')}=2D\delta_{ij}\delta(t-t'), \tag{10}$$

where δ_{ij} is the Kronecker delta, $\delta(t)$ is the Dirac delta function, and D is the spectral density. The overbars denote statistical time averages over a large number of random variables. We start with interpreting Eq. (9) as an integral equation (in the Stratonovich sense) for the values of ξ at a later time $t+\delta t$,

$$\begin{aligned}\xi_i(t+\delta t)=x_i(t)+\int_t^{t+\delta t}&[h_i(\boldsymbol\xi(t'),t')\\&+g_{ij}(\boldsymbol\xi(t'),t')\Gamma_j(t')]\mathrm{d}t',\end{aligned} \tag{11}$$

where $x_i(t)$ is the sharp starting values for $\xi_i(t)$ at the instant t. Let x_i (without the time argument) denote the time average of a large number of random variables $\xi_i(t)$ all starting from the sharp value $x_i(t)$, calculated by the Stratonovich rule. Then the time averages can be expressed as a *deterministic* equation of motion for the set of sharp starting values $\mathbf{x}$,

$$\begin{aligned}\dot x_i&=\lim_{\delta t\rightarrow 0}\frac{\overline{[\xi_i(t+\delta t)-x_i(t)]}}{\delta t}\\&=h_i(\mathbf{x})+Dg_{kj}(\mathbf{x},t)\frac{\partial}{\partial x_k}(g_{ij}(\mathbf{x},t)),\\&\quad 1\leqslant i\leqslant n,\quad 1\leqslant j,k\leqslant m.\end{aligned} \tag{12}$$

In the above we have used Einstein's summation convention so that the second term on the right represents a sum over j and k. Similarly it can also be proved that for any well behaved function $f_i(\mathbf{x})$,[13]

$$f_i(\mathbf{x})\dot x_i=f_i(\mathbf{x})h_i(\mathbf{x})+Dg_{kj}(\mathbf{x},t)\frac{\partial}{\partial x_k}(f_i(\mathbf{x})g_{ij}(\mathbf{x},t)), \tag{13}$$

where again the summation over j and k is understood.

To obtain the appropriate Langevin equation for the orientation of the spheroids in a simple shear flow, we heuristically suppose that the rotary Brownian motion causes the angular velocity of the particle to change and we incorporate this effect by superposing on Eq. (2) for ω a white noise vector term:

$$\omega=\mathbf{\Omega}+C[\mathbf{u}\times(\mathsf{E}\cdot\mathbf{u})]+\mathbf{\Gamma}(t),$$

where the Cartesian components $\Gamma_i(t)$ of $\mathbf{\Gamma}$ satisfy Eq. (10) with $D=D_r$. The expression for $\dot{\mathbf{u}}$ then changes into

$$\dot{\mathbf{u}} = \mathbf{\Omega}\times\mathbf{u} + C[\mathbf{u}\times(\mathbf{E}\cdot\mathbf{u})]\times\mathbf{u} + \mathbf{\Gamma}\times\mathbf{u}. \tag{14}$$

When converted into spherical coordinates the equation becomes [cf. Eq. (5)]

$$\begin{aligned} \dot{\theta} &= \dot{\gamma}C \sin\theta\cos\theta\sin\phi\cos\phi \\ &\quad -\sin\phi\Gamma_1(t) + \cos\phi\Gamma_2(t), \\ \dot{\phi} &= -\dot{\gamma}C\sin^2\phi - \dot{\gamma}\left(\frac{1-C}{2}\right) - \cot\theta\cos\phi\Gamma_1(t) \\ &\quad -\sin\phi\cot\theta\Gamma_2(t) + \Gamma_3(t). \end{aligned} \tag{15}$$

These equations are now in the form of Eq. (9), with h_1 and h_2 corresponding to the deterministic parts of $\dot{\theta}$ and $\dot{\phi}$ in Eq. (15), repectively, and with

$$g_{11} = -\sin\phi, \quad g_{12} = \cos\phi, \quad g_{13} = 0,$$

$$g_{21} = -\cot\theta\cos\phi, \quad g_{22} = -\cot\theta\sin\phi, \quad g_{23} = 1.$$

To obtain the differential recurrence relations for the spherical harmonics $Y^*_{n,m}$ for $m \geqslant 0$ note first that

$$\frac{\mathrm{d}}{\mathrm{d}t}(Y^*_{n,m}) = \frac{\partial}{\partial\theta}(Y^*_{n,m})\dot{\theta} + \frac{\partial}{\partial\phi}(Y^*_{n,m})\dot{\phi}. \tag{16}$$

Writing $f_1 = \partial Y^*_{n,m}/\partial\theta$, $f_2 = \partial Y^*_{n,m}/\partial\phi$, $\theta_1 = \theta$, and $\theta_2 = \phi$ and applying the results of Eq. (12) in Eq. (15) and of Eq. (13) in Eq. (16) we get the equation of motion for the sharp values $Y^*_{n,m}$ as

$$\frac{\mathrm{d}}{\mathrm{d}t}(Y^*_{n,m}) = f_1h_1 + f_2h_2 + D_r g_{kj}\frac{\partial}{\partial\theta_k}(f_1g_{1j} + f_2g_{2j}), \tag{17}$$

where the last term represents a sum over j and k. Simplifying the deterministic and noise parts of Eq. (17) separately (the details are left to Appendix B), we get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}Y^*_{n,m} &= \dot{\gamma}C\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2} b^{m,j}_{n,k}Y^*_{k,j} \\ &\quad + \frac{3}{2}\dot{\gamma}C\sin^2\theta\sin(2\phi)Y^*_{n,m} \\ &\quad + \dot{\gamma}\left(\frac{1-C}{2}\right) imY^*_{n,m} - D_r n(n+1)Y^*_{n,m}. \end{aligned} \tag{18}$$

Taking now a second average over the probability density of the sharp values (θ,ϕ) we finally get

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle Y^*_{n,m}\rangle &= \dot{\gamma}C\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2} b^{m,j}_{n,k}\langle Y^*_{k,j}\rangle \\ &\quad + \frac{3}{2}\dot{\gamma}C\langle\sin^2\theta\sin(2\phi)Y^*_{n,m}\rangle \\ &\quad + \dot{\gamma}\left(\frac{1-C}{2}\right) im\langle Y^*_{n,m}\rangle - D_r n(n+1)\langle Y^*_{n,m}\rangle, \end{aligned} \tag{19}$$

which is in the same form as Eq. (8) which was obtained through the diffusion equation. The extension to negative m is obvious as before. This demonstrates that an ensemble of Eqs. (18) for the sharp $Y^*_{n,m}$ has the same dynamics as the moments $\langle Y^*_{n,m}\rangle$ as determined by the Fokker–Planck equation. Further, the equivalence between the two formulas justifies the form of the noise term we started with and makes the system of Langevin equations (14) identical to the diffusion equation (1). It also demonstrates that in the Brownian regime we can use the time averaged Langevin equations to generate averages using the new method.

IV. THE COMPUTATION OF MOMENTS

In this section we obtain the equations governing the time evolution of the orientation moments based on the methods of the previous section and develop methods for computing the moments from these equations. We shall generate the moments $\langle u_3^2\rangle = \langle\cos^2\theta\rangle$, $\langle u_1u_2\rangle = \langle\sin^2\theta\sin\phi\cos\phi\rangle$, and $\langle u_1^2u_2^2\rangle = \langle\sin^4\theta\sin^2\phi\cos^2\phi\rangle$ for a wide range of parameters using the new method and compare our results with those of Chen and Jiang[12] and Chen and Koch.[11]

Each term in Eq. (14) has dimension (1/time) and may be scaled with respect to D_r. The scaled form of the Langevin equation, in Cartesian coordinates is as follows:

$$\begin{aligned} \dot{u}_1 &= \mathrm{Pe}\,C\,u_2(1-u_1^2) + \mathrm{Pe}\left(\frac{1-C}{2}\right)u_2 \\ &\quad + \Gamma_2(t)u_3 - \Gamma_3(t)u_2, \\ \dot{u}_2 &= -\mathrm{Pe}\,C\,u_1u_2^2 - \mathrm{Pe}\left(\frac{1-C}{2}\right)u_1 + \Gamma_3(t)u_1 - \Gamma_1(t)u_3, \\ \dot{u}_3 &= -\mathrm{Pe}\,Cu_1u_2u_3 + \Gamma_1(t)u_2 - \Gamma_2(t)u_1, \end{aligned} \tag{20}$$

where $\mathrm{Pe} = \dot{\gamma}/D_r$ is the Péclet number introduced earlier. Note that in the scaled form the Γ_i satisfy Eq. (10) with $D = 1$. When converted into spherical coordinates these equations become

$$\begin{aligned} \dot{\theta} &= \mathrm{Pe}\,C\sin\theta\cos\theta\sin\phi\cos\phi - \sin\phi\Gamma_1(t) \\ &\quad + \cos\phi\Gamma_2(t), \\ \dot{\phi} &= -\mathrm{Pe}\,C\sin^2\phi - \mathrm{Pe}\left(\frac{1-C}{2}\right) - \cot\theta\cos\phi\Gamma_1(t) \\ &\quad -\sin\phi\cot\theta\Gamma_2(t) + \Gamma_3(t). \end{aligned} \tag{21}$$

The above equations may now be time-averaged using Eq. (13) to express it as an equation of motion for the sharp starting values. We retain the same notation of the random variables θ, ϕ for their sharp values at t. Following a procedure similar to that leading to Eq. (17) we obtain for any orientation moment $\langle B(\theta,\phi)\rangle$, the following expression for the sharp values $B(\theta,\phi)$:

$$\frac{\mathrm{d}}{\mathrm{d}t}B(\theta,\phi) = f_1h_1 + f_2h_2 + g_{kj}\frac{\partial}{\partial\theta_k}(f_1g_{1j} + f_2g_{2j}), \tag{22}$$

where $f_1 = \partial B/\partial\theta$, $f_2 = \partial B/\partial\phi$, $\theta_1 = \theta$, and $\theta_2 = \phi$ and h_1 and h_2 are the deterministic parts in Eq. (21). A set of these equations averaged over the density of the sharp values has the same evolution dynamics as $\langle B(\theta,\phi)\rangle$. We thus get the governing equations for the time evolution of the moments $\langle u_3^2\rangle$, $\langle u_1u_2\rangle$, and $\langle u_1^2u_2^2\rangle$:

$$\begin{aligned}
\frac{d}{dt}\langle u_3^2\rangle &= -\frac{d}{dt}\langle\cos^2\theta\rangle = \left(\frac{\mathrm{Pe}}{4}\right)C\langle\sin^2 2\theta\sin 2\phi\rangle \\
&\quad -2(3\langle\cos^2\theta\rangle-1), \\
\frac{d}{dt}\langle u_1u_2\rangle &= \frac{d}{dt}\langle\sin^2\theta\sin\phi\cos\phi\rangle \\
&= 2C\,\mathrm{Pe}\langle\sin^2\theta\cos^2\theta\sin^2\phi\cos^2\phi\rangle \\
&\quad - C\,\mathrm{Pe}\langle\sin^2\theta\sin^2\phi\cos 2\phi\rangle - \mathrm{Pe}\left(\frac{1-C}{2}\right) \\
&\quad \times\langle\sin^2\theta\cos 2\phi\rangle - 3\langle\sin^2\theta\sin 2\phi\rangle, \qquad (23) \\
\frac{d}{dt}\langle u_1^2u_2^2\rangle &= \frac{d}{dt}\langle\sin^4\theta\sin^2\phi\cos^2\phi\rangle \\
&= 4C\,\mathrm{Pe}\langle\sin^4\theta\cos^2\theta\sin^3\phi\cos^3\phi\rangle \\
&\quad -2C\,\mathrm{Pe}\langle\sin^4\theta\sin^3\phi\cos\phi\cos 2\phi\rangle \\
&\quad -\mathrm{Pe}\left(\frac{1-C}{2}\right)\langle\sin^4\theta\sin^2\phi\cos 2\phi\rangle \\
&\quad +2\langle\sin^2\theta\rangle - 20\langle\sin^4\theta\sin^2\phi\cos^2\phi\rangle.
\end{aligned}$$

For $\mathrm{Pe}\neq 0$ the above system of equations is not closed, but for $\mathrm{Pe}=0$ (i.e., in the absence of shear), they have a simple form, namely.

$$\frac{d}{dt}\langle u_3^2\rangle = -2(3\langle u_3^2\rangle-1),$$

$$\frac{d}{dt}\langle u_1u_2\rangle = -\frac{3}{2}\langle u_1u_2\rangle,$$

$$\frac{d}{dt}\langle u_1^2u_2^2\rangle = 2-2\langle u_3^2\rangle-20\langle u_1^2u_2^2\rangle.$$

Solving them we get the following results in the zero shear limit:

$$\langle u_3^2\rangle = \tfrac{1}{3}+k_1e^{-6t},$$

$$\langle u_1u_2\rangle = k_2e^{-(3/2)t},$$

$$\langle u_1^2u_2^2\rangle = \frac{1}{15}+k_3e^{-2t}+k_4e^{-20t},$$

where the k_i are constants depending on the initial conditions. In the limit $t\to\infty$, the solutions approach, as expected, the values of the moments when the orientation distribution is uniform ($\psi=1/4\pi$). An advantage of Eqs. (23) for moments is that they are ordinary differential equations unlike the original Langevin equations for the orientations.

We now discuss a computational technique for solving the moment equations in the general case. We note that in general the evolution of the moments is governed by two variables θ and ϕ and not by the moment itself. This necessitates considering two moment equations simultaneously for generating the averages. Our computational procedure is based on the fact that the dynamics of any moment $\langle B(\theta,\phi)\rangle$ can be captured by simulating an ensemble of Eqs. (22) for the sharp values $B(\theta,\phi)$. Equivalently, we may set up the equations of motion for the tracer variables θ and ϕ and compute the averages by iterating a set of such equations. For the sharp values $B_1(\theta,\phi)$ and $B_2(\theta,\phi)$ of any two desired orientation averages, we may write from Eq. (22)

$$\begin{aligned}
f_1\dot{\theta}+f_2\dot{\phi} &= f_1h_1+f_2h_2+g_{kj}\frac{\partial}{\partial\theta_k}(f_1g_{1j}+f_2g_{2j}), \\
f_1'\dot{\theta}+f_2'\dot{\phi} &= f_1'h_1+f_2'h_2+g_{kj}\frac{\partial}{\partial\theta_k}(f_1'g_{1j}+f_2'g_{2j}),
\end{aligned} \tag{24}$$

where f_i are the partial derivatives of B_1 and f_i' those of B_2. We can solve the above system for $\dot{\theta}$ and $\dot{\phi}$ assuming that the coefficient determinant $\Delta=f_1f_2'-f_1'f_2$ is not zero,

$$\begin{aligned}
\dot{\theta} &= h_1+\frac{1}{\Delta}\Big[f_2'g_{kj}\frac{\partial}{\partial\theta_k}(f_1g_{1j}+f_2g_{2j}) \\
&\quad - f_2g_{kj}\frac{\partial}{\partial\theta_k}(f_1'g_{1j}+f_2'g_{2j})\Big], \\
\dot{\phi} &= h_2-\frac{1}{\Delta}\Big[f_1'g_{kj}\frac{\partial}{\partial\theta_k}(f_1g_{1j}+f_2g_{2j}) \\
&\quad - f_1g_{kj}\frac{\partial}{\partial\theta_k}(f_1'g_{1j}+f_2'g_{2j})\Big].
\end{aligned} \tag{25}$$

This gives a system of two coupled ODEs and an ensemble of such systems for the sharp values θ and ϕ collectively determine the pair of averages B_1 and B_2. Thus for each pair of averages for which Δ is nonzero, we consider an ensemble of systems of coupled ODEs of the type of Eq. (25) over a set of sharp initial conditions.

To carry out the computations, we start with a finite but large number of sharp initial conditions for the random variables (θ,ϕ) with each initial condition representing a large number of random variables starting from there. The $\theta\phi$ space is first divided into n^2 bins by the points (θ_i,ϕ_i) where $\theta_i=\cos^{-1}[(2i/n)-1]$, and $\phi_i=2\pi/n$ $i=0,1,\ldots n$. We consider n^2 initial conditions (θ_i,ϕ_i) directed along the centers of these bins and let each of them evolve according to Eqs. (25). This choice of θ and ϕ corresponds to a set of nearly uniform initial conditions for the sharp values over the $\theta\phi$ space. The trajectory of the vector (θ,ϕ) is obtained by integration using the integrator *odeint* of Press *et al.*[15] with adaptive step-size control. The sharp values (θ,ϕ) may themselves be considered a random variable with density $\psi(\theta,\phi,t)$ with sharp peaks at the sites of the vectors (θ,ϕ) at any instant. This gives the following estimate for any moment $\langle B(\theta,\phi)\rangle$ at that instant t:

TABLE I. The steady state values of the moments for various initial conditions at different values of Pe.

No. of initial conditions	Pe=0.0		Pe=1.0		Pe=100.0		Pe=500.0	
	$\langle u_3^2\rangle$	$\langle u_1u_2\rangle$	$\langle u_3^2\rangle$	$\langle u_1u_2\rangle$	$\langle u_3^2\rangle$	$\langle u_1u_2\rangle$	$\langle u_3^2\rangle$	$\langle u_1u_2\rangle$
64	0.3333	0.0000	0.3293	0.0532	0.2376	0.1325	0.1763	0.0950
81	0.3333	0.0000	0.3280	0.0473	0.2082	0.1199	0.1537	0.0778
100	0.3333	0.0000	0.3288	0.0322	0.1730	0.0910	0.1285	0.0576
121	0.3333	0.0000	0.3283	0.0321	0.1721	0.0907	0.1294	0.0598
144	0.3333	0.0000	0.3285	0.0317	0.1728	0.0911	0.1277	0.0568

$$\langle B(\theta,\phi)\rangle=\frac{\int\int B(\theta,\phi)\,\delta(\theta-\theta_i)\,\delta(\phi-\phi_j)\mathrm{d}(\cos\theta)\mathrm{d}\phi}{\int\int\delta(\theta-\theta_i)\,\delta(\phi-\phi_j)\mathrm{d}(\cos\theta)\mathrm{d}\phi}$$
$$=\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}B(\theta_i,\phi_j). \tag{26}$$

The values of the moments $\langle B_1(\theta,\phi)\rangle$, $\langle B_2(\theta,\phi)\rangle$ at any instant are computed from the iterates of the n^2 instances of the corresponding pair of Eqs. (25) using the above formula. These computations are repeated for successive time steps using, at each step, the values (θ_i,ϕ_j) obtained from numerical integration, and continued until the values of the moments stabilize.

We generated the moments in pairs of $\langle u_3^2\rangle$ and $\langle u_1^2u_2^2\rangle$, $\langle u_1u_2\rangle$ and $\langle u_2^2\rangle$, and $\langle u_3^2\rangle$ and $\langle u_1u_2\rangle$ for various values of Pe, keeping the number of initial conditions at $n^2=100$. Note that the coefficient determinant Δ does not vanish for this choice of moments. The simulations may run into trouble if any of the subsequent iterations approach a singularity of Eq. (25), but our computations did not lead to any such problems. The computations were repeated changing the number of initial conditions from 64 to 2500, but the results practically stabilized for $n^2=100$ onward and so n^2 was fixed at 100 in subsequent computations. Table I shows the variation of the moments with the number of initial conditions for typical values of the parameters. With Pe=0, the computations reproduced the theoretical values 1/3, 0, and 1/15 for $\langle u_3^2\rangle$, $\langle u_1u_2\rangle$, and $\langle u_1^2u_2^2\rangle$, respectively. Also we had scaled time with respect to $1/D_r$, which makes the right side of Eq. (25) large for larger values of Pe. Hence to minimize the round of errors we changed the scaling to $1/\dot{\gamma}$ for Pe>10 while for Pe<10 the earlier scaling was retained. The results obtained for Pe between 0 and 1000 are plotted in Fig. 1. These results are in good agreement with those obtained from other methods, spherical harmonics method of Chen and Koch[11] and finite difference method of Chen and Jiang[12] (compare Fig. 3 of Chen and Jiang[12]). An advantage of this method is the internal check it provides on the computations by way of making one average common to each pair of averages. Thus in our simulations we paired $\langle u_3^2\rangle$ with both $\langle u_1u_2\rangle$ and $\langle u_2^2u_3^2\rangle$ and found that the results were consistent.

With a given number of initial conditions, the time taken by the simulations to settle down to steady values depends both on the Péclet number and the pair of averages chosen. Table II summarizes the time data for our computations on a Pentium III, 500 MHz, 128 MB RAM PC, with 100 initial conditions for typical values of Pe. It seems that the current method offers significant improvement in terms of the computation time of various moments compared to the other methods.[12]

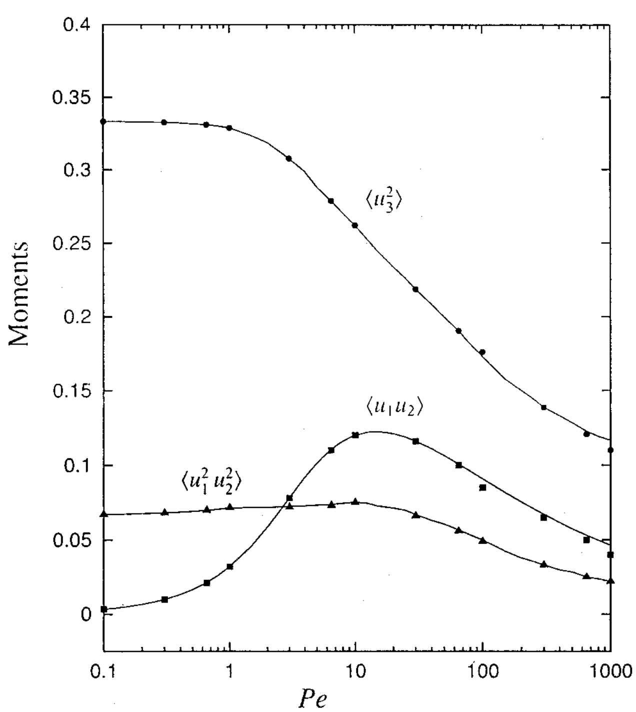

FIG. 1. Plot of the orientation moments vs Péclet number. The symbols are the results from the finite difference method and the spherical harmonics method.

TABLE II. Time taken to compute the moments on a 500 MHz, 128 RAM, Pentium III PC for two different pairs at various Pe.

Pe	$\langle u_3^2\rangle$ and $\langle u_1u_2\rangle$	$\langle u_3^2\rangle$ and $\langle u_1^2u_2^2\rangle$
0.0	1 s	1 s
1.0	2 s	2 s
10.0	4 s	10 s
50.0	7 s	823 s
100.0	10 s	1920 s
250.0	28 s	2030 s
500.0	86 s	2800 s

V. CONCLUSIONS

We have developed the Langevin equations for the orientation dynamics of the spheroids in a dilute suspension under simple shear flow. A method for calculating the evolution of the moments of the orientation distribution function from a set of appropriately time averaged Langevin equations is also developed. This presents a unified approach to computing the orientation moments over a wide range of Péclet number. An advantage of the present approach is that it provides an internal check on the computations by keeping one average common in any couple of pairs of averages that is generated. It also does not require solving the diffusion equation with all its attendant complications. Another advantage is that it can be easily generalized to study more complex systems such as suspensions of dipolar particles with external forcing or suspensions of charged particles. This involves only modifying the governing Eqs. (3) with terms corresponding to the additional effects.

Kumar and Ramamohan[16] have recently demonstrated that in a *periodically forced* suspension of dipolar particles, the moments of the ODF may evolve chaotically in the weak Brownian motion regime. This observation has some important implications for certain concepts in chaos theory such as the nontrivial collective behavior of spatially extended systems.[17] The method developed in this paper is ideal for studying the possibility of moments evolving chaotically under periodic forcing in the strong Brownian motion regime. In this case, the moment equations for each pair of averages would be a couple of nonlinear coupled nonautonomous ODEs.[16] These points are being currently investigated and will be discussed in future work.

ACKNOWLEDGMENTS

The authors wish to thank Dr. G. Vijay Nair, Director, Regional Research Laboratory (CSIR), Thiruvananthapuram-695019, India, for constant encouragement. One of the authors (K.A.) wishes to acknowledge CSIR, India, for financial support.

APPENDIX A

We give here the details of the calculations leading to Eq. (8) from the diffusion equation. Fixing $m \geqslant 0$ and multiplying Eq. (6) through by $Y^*_{n,m}$ and integrating over the unit sphere we get

$$\begin{aligned}&\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\frac{\partial\psi}{\partial t}Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\quad+\dot\gamma C\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\overline{\Omega}(\psi)Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\quad-\dot\gamma\left(\frac{1-C}{2}\right)\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\frac{\partial\psi}{\partial\phi}\sin\theta Y^*_{n,m}\,\mathrm{d}\theta\mathrm{d}\phi\\&\quad=D_r\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\overline{\Lambda}(\psi)Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi.\end{aligned}\tag{A1}$$

The first term on the left side of Eq. (A1) is evidently $(\mathrm{d}/\mathrm{d}t)\langle Y^*_{n,m}\rangle$. To evaluate the second term on the left we first note that

$$\begin{aligned}&\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\overline{\Omega}(\psi)Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\quad=\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\frac{\sin\phi\cos\phi}{\sin\theta}\frac{\partial}{\partial\theta}(\psi\sin^2\theta\cos\theta)\\&\qquad\times Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\qquad-\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\frac{\partial}{\partial\phi}(\psi\sin^2\phi)\sin\theta Y^*_{n,m}\,\mathrm{d}\theta\mathrm{d}\phi\\&\quad=-\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\sin\phi\cos\phi\frac{\partial}{\partial\theta}(Y^*_{n,m})\\&\qquad\times\psi\sin^2\theta\cos\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\qquad+\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\sin\theta\frac{\partial}{\partial\phi}(Y^*_{n,m})\psi\sin^2\phi\,\mathrm{d}\theta\mathrm{d}\phi.\end{aligned}\tag{A2}$$

In the foregoing expressions the last step follows by integrating the first term of the previous step by parts with respect to θ and the second term with respect to ϕ. Now using the relations

$$\begin{aligned}\frac{\partial}{\partial\theta}(Y^*_{n,m})\sin^2\theta\cos\theta&=\frac{\partial}{\partial\theta}(Y^*_{n,m}\sin^2\theta\cos\theta)\\&\quad-\frac{\partial}{\partial\theta}(\sin^2\theta\cos\theta)Y^*_{n,m},\\\frac{\partial}{\partial\phi}(Y^*_{n,m})\sin^2\phi&=\frac{\partial}{\partial\phi}(Y^*_{n,m}\sin^2\phi)-Y^*_{n,m}\sin(2\phi)\end{aligned}\tag{A3}$$

in Eq. (A2) and simplifying we get

$$\begin{aligned}&\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\overline{\Omega}(\psi)Y^*_{n,m}\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\quad=-\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\overline{\Omega}(Y^*_{n,m})\psi\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi\\&\qquad-\frac{3}{2}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}Y^*_{n,m}\sin^3\theta\sin(2\phi)\psi\,\mathrm{d}\theta\mathrm{d}\phi.\end{aligned}\tag{A4}$$

The effects of $\overline{\Omega}$ on $P_n^m(\cos\theta)$ and $P_n^m(\sin\theta)$ have been evaluated previously[18] [here and in what follows we have abbreviated $P_n^m(\cos\theta)$ by P_n^m, etc.]:

$$\overline{\Omega}(P_n^m\sin(m\phi))=\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2}a_{n,k}^{m,j}P_k^j\cos(j\phi),\quad m\geqslant 0,$$

$$\overline{\Omega}(P_n^m\cos(m\phi))=-\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2}a_{n,k}^{m,j}P_k^j\sin(j\phi),\quad m>0.$$

The constants $a_{n,k}^{m,j}$ are the Bird–Warner coefficients.[18] Hence it follows that

$$\bar{\Omega}(Y_{n,m}^*)=\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2} b_{n,k}^{m,j}Y_{k,j}^*, \tag{A5}$$

where we have written $b_{n,k}^{m,j}=-i(N_{n,m}/N_{k,j})a_{n,k}^{m,j}$. This can now be used in Eq. (A4) to complete the evaluation for the second term on the left of Eq. (A1):

$$\begin{aligned}\dot\gamma C\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\bar{\Omega}(\psi)Y_{n,m}^*\sin\theta\,d\theta d\phi\\ =-\dot\gamma C\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2} b_{n,k}^{m,j}\langle Y_{k,j}^*\rangle\\ -\frac{3}{2}\dot\gamma C\langle\sin^2\theta\sin(2\phi)Y_{n,m}^*\rangle.\end{aligned} \tag{A6}$$

The integral in the third term on the left of Eq. (A1) can be integrated by parts with respect to ϕ and the boundary conditions for ψ applied to show that

$$\begin{aligned}-\dot\gamma\left(\frac{1-C}{2}\right)\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\frac{\partial\psi}{\partial\phi}\sin\theta Y_{n,m}^*\,d\theta d\phi\\ =-\dot\gamma\left(\frac{1-C}{2}\right)im\langle Y_{n,m}^*\rangle.\end{aligned} \tag{A7}$$

To evaluate the right side of Eq. (A1) we use the known effects of $\bar\Lambda$ on real spherical harmonics:[18]

$$\bar\Lambda(P_n^m\cos(m\phi))=-n(n+1)P_n^m\sin(m\phi),$$

$$\bar\Lambda(P_n^m\sin(m\phi))=-n(n+1)P_n^m\cos(m\phi).$$

Hence using the linearity of $\bar\Lambda$ we have $\bar\Lambda(Y_{n,m}^*)=-n(n+1)Y_{n,m}^*$ and then invoking the eigenfunction expansion of ψ:

$$\begin{aligned}\bar\Lambda(\psi)&=\bar\Lambda\left(\sum_{q=0}^{\infty}\sum_{p=-q}^{q}a_{q,p}Y_{q,p}\right)\\ &=\sum_{q=0}^{\infty}\sum_{p=-q}^{q}(-q)(q+1)a_{q,p}Y_{q,p}.\end{aligned}$$

This result together with the orthogonality relation for the spherical harmonics, Eq. (7), and term by term integration yields

$$\begin{aligned}&\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\bar\Lambda(\psi)\sin\theta Y_{n,m}^*\,d\theta d\phi\\ &=\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\left(\sum_{q=0}^{\infty}\sum_{p=-q}^{q}(-q)(q+1)a_{q,p}Y_{q,p}\right)\\ &\quad\times Y_{n,m}^*\sin\theta\,d\theta d\phi\\ &=\sum_{q=0}^{\infty}\sum_{p=-q}^{q}\Bigg(-q(q+1)\\ &\quad\times a_{q,p}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}Y_{q,p}Y_{n,m}^*\sin\theta\,d\theta d\phi\Bigg)\\ &=(-n)(n+1)a_{n,m}.\end{aligned}$$

In a similar fashion, using the orthogonality relation Eq. (7) and the expansion for ψ, we can prove that the expansion coefficients $a_{n,m}$ are related to $Y_{n,m}^*$ by $a_{n,m}=\langle Y_{n,m}^*\rangle$. The final expression for the right side of Eq. (A1), therefore, becomes

$$D_r\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\bar\Lambda(\psi)\sin\theta Y_{n,m}^*\,d\theta d\phi=D_r n(n+1)\langle Y_{n,m}^*\rangle. \tag{A8}$$

Putting together Eqs. (A6), (A7), and (A8) in Eq. (A1) we get Eq. (8). The recurrence relation Eq. (8) has been derived on the assumption that m is non-negative. If m is negative $-m$ is positive and the Bird–Warner coefficients $a_{n,k}^{-m,j}$ are defined. We will then get a similar recurrence relation by complex conjugation using $Y_{n,m}=(-1)^mY_{n,-m}^*$ with appropriate modifications.

APPENDIX B

The calculations leading to Eq. (19) from Eq. (17) are detailed here. We first write out the deterministic part of Eq. (17) using Eq. (15):

$$\begin{aligned}f_1h_1+f_2h_2=\dot\gamma C\Bigg[\frac{\partial}{\partial\theta}(Y_{n,m}^*)\sin\theta\cos\theta\sin\phi\cos\phi\\ -\frac{\partial}{\partial\phi}(Y_{n,m}^*)\sin^2\phi\Bigg]\\ -\dot\gamma\left(\frac{1-C}{2}\right)\frac{\partial}{\partial\phi}(Y_{n,m}^*).\end{aligned} \tag{B1}$$

Now multiply the first of the relations in Eq. (A3) by $(\dot\gamma C\sin\phi\cos\phi)/\sin\theta$ and the second by $\dot\gamma C$ and subtract to get

$$\begin{aligned}&\dot\gamma C\left[\frac{\partial}{\partial\theta}(Y_{n,m}^*)\sin\theta\cos\theta\sin\phi\cos\phi-\frac{\partial}{\partial\phi}(Y_{n,m}^*)\sin^2\phi\right]\\ &=\dot\gamma C\Bigg[\frac{\sin\phi\cos\phi}{\sin\theta}\frac{\partial}{\partial\theta}(Y_{n,m}^*\sin^2\theta\cos\theta)\\ &\quad-\frac{\partial}{\partial\phi}(Y_{n,m}^*\sin^2\phi)\Bigg]+\dot\gamma C\Bigg[Y_{n,m}^*\sin(2\phi)\\ &\quad-\frac{Y_{n,m}^*\sin\phi\cos\phi}{\sin\theta}\frac{\partial}{\partial\theta}(\sin^2\theta\cos\theta)\Bigg]\\ &=\dot\gamma C\bar\Omega(Y_{n,m}^*)+\frac{3}{2}\dot\gamma C\sin^2\theta\sin(2\phi)Y_{n,m}^*.\end{aligned} \tag{B2}$$

Substituting Eq. (B2) in Eq. (B1) and using Eq. (A5), we get the following form for the deterministic part of Eq. (17):

$$\begin{aligned}f_1h_1+f_2h_2=\dot\gamma C\sum_{j=m-2}^{m+2}\sum_{k=n-2}^{n+2}b_{n,k}^{m,j}Y_{k,j}^*\\ +\frac{3}{2}\dot\gamma C\sin^2\theta\sin(2\phi)Y_{n,m}^*\\ +\dot\gamma\left(\frac{1-C}{2}\right)imY_{n,m}^*.\end{aligned} \tag{B3}$$

Now the noise part of Eq. (17) simplifies as follows:

$$
\begin{aligned}
D_r g_{kj}\frac{\partial}{\partial\theta_k}(f_1 g_{1j}+f_2 g_{2j})
&= D_r\bigg[g_{11}\frac{\partial}{\partial\theta}(f_1 g_{11}+f_2 g_{21})+g_{12}\frac{\partial}{\partial\theta}(f_1 g_{12}+f_2 g_{22})\\
&\quad +g_{13}\frac{\partial}{\partial\theta}(f_1 g_{13}+f_2 g_{23})+g_{21}\frac{\partial}{\partial\phi}(f_1 g_{11}+f_2 g_{21})\\
&\quad +g_{22}\frac{\partial}{\partial\phi}(f_1 g_{12}+f_2 g_{22})+g_{23}\frac{\partial}{\partial\phi}(f_1 g_{13}+f_2 g_{23})\bigg]\\
&= D_r\bigg[\frac{\partial^2}{\partial\theta^2}(Y^*_{n,m})+\frac{1}{2\sin^2\theta}\\
&\quad\times\left(2\,\frac{\partial^2}{\partial\phi^2}(Y^*_{n,m})+\sin(2\theta)\,\frac{\partial}{\partial\theta}(Y^*_{n,m})\right)\bigg]\\
&= D_r N_{n,m}e^{-im\phi}\left[\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}(P_n^m)+\frac{\cos\theta}{\sin\theta}\,\frac{\mathrm{d}P_n^m}{\mathrm{d}\theta}-\frac{m^2}{\sin^2\theta}P_n^m\right]\\
&= D_r N_{n,m}e^{-im\phi}\left[\frac{1}{\sin\theta}\,\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\,\frac{\mathrm{d}P_n^m}{\mathrm{d}\theta}\right)-\frac{m^2}{\sin^2\theta}P_n^m\right]\\
&= -D_r n(n+1)N_{n,m}e^{-im\phi}P_n^m\\
&= -D_r n(n+1)Y^*_{n,m}.
\end{aligned}
\tag{B4}
$$

In the above we have used the fact that P_n^m satisfies

$$\frac{1}{\sin\theta}\,\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\,\frac{\mathrm{d}P_n^m}{\mathrm{d}\theta}\right)+\left[n(n+1)-\frac{m^2}{\sin^2\theta}\right]P_n^m=0.$$

Putting together Eq. (B3) and (B4) in Eq. (17) and averaging over an ensemble of random initial conditions we get Eq. (19) from the time-averaged Langevin equation.

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