Velocity Correlations of a Brownian Particle

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A new derivation of the velocity correlations of a thermally fluctuating Brownian particle is shown by direct calculation from a stochastic hydrodynamic model in which the fluid-particle coupling is treated in a simple manner. The model significantly simplifies the calculation of statistics of a particle and has the virtue of being readily amenable to numerical simulation. To show that the model correctly captures physical features of a Brownian particle the diffusion coefficient in three dimensions is computed and shown to have the correct scaling in the physical parameters. The velocity correlation function for both short and long times scales is then discussed. It is found for short times that the velocity correlation of a particle satisfies an equipartition principle. For long times the autocorrelation function is shown to have non-exponential decay of algebraic order $\tau^{-3/2}$ capturing well-known hydrodynamic effects [1]. The results are then compared with numerical simulations of the hydrodynamic model using the computational method proposed in [2].

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I. INTRODUCTION

With advances in optical traps, in which single particles of only a few microns or smaller can be manipulated and tracked at high spatial and temporal resolution, there has been a renewed interest in attempting to observe the velocity correlations of Brownian particles [3, 11]. Classical models of Brownian motion [4, 6–8, 14, 19] treat thermal fluctuations of a particle as "white noise" which yields a velocity autocorrelation function which decays exponentially in time.

Brownian particles however are immersed in a fluid which serves both as a source of the thermal fluctuations driving the particle and as a source of viscous damping. As a consequence, it has been shown in molecular dynamics simulations that memory effects associated with the dynamics of the fluid play an important role with the velocity correlations of a Brownian particle having a slow non-exponential decay for long times of algebraic order $\tau^{-3/2}$ [1]. Experimental observations also indicate long-time velocity correlations of Brownian particles consistent with this power law [9].

A number of models have been proposed that account for hydrodynamic effects of a Brownian particle [5, 17, 20, 21]. In many of these models the particles are coupled to the fluid through stresses at the particle surface. To derive statistics of a Brownian particle a number of asymptotic approximations are made in the limit of small particle size. In this work we introduce a stochastic model for the hydrodynamics and treat the fluid-particle coupling in a novel manner allowing for direct calculation of the velocity autocorrelation function.

To check that this model captures physical features of a Brownian particle the diffusion coefficient is computed and shown to scale correctly in the physical parameters. The autocorrelation function for short times is then investigated and shown to satisfy an equipartition principle. The autocorrelation function for long times is then analyzed and shown to decay with algebraic order $\tau^{-3/2}$ correctly capturing the power law associated with hydrodynamic memory effects. The results are then compared with numerical simulations performed using the computational method proposed in [2].

II. THE HYDRODYNAMIC MODEL

For water at room temperature the radius of a particle observed to undergo physical Brownian motion is on the order of tens of microns or smaller. To model the fluid an approximation of the Navier-Stokes equations will be considered. The amplitude of the velocity fluctuations is sufficiently small, relative to the viscosity of the fluid and length scale of the particle, that the Reynolds number is very small. This allows in the Navier-Stokes equations for the nonlinear advection term to be neglected. However, the derivative in time will not be dropped as a consequence of the fast time scales associated with the thermal fluctuations of the fluid. Therefore, the hydrodynamics will be modeled by the time-dependent Stokes equations:

$$\rho\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} = \mu\Delta\mathbf{u}(\mathbf{x},t) - \nabla p + \mathbf{f}_{\mathrm{thm}}(\mathbf{x},t) \qquad (1)$$

$$\nabla\cdot\mathbf{u} = 0, \qquad (2)$$

where p is the pressure arising from the incompressibility constraint, ρ is the fluid density, μ is the dynamic viscosity, and $\mathbf{f}_{\mathrm{thm}}$ is a force density acting on the fluid which models the thermal fluctuations of the fluid. The details of the thermal force $\mathbf{f}_{\mathrm{thm}}$ will be discussed below. For concreteness we shall consider the fluid equations in

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three dimensions on a cubic domain Λ having sides L with periodic boundary conditions.

A particle of size a immersed in the fluid is modeled by a Lagrangian coordinate $\mathbf{X}(t)$ with the fluid-particle coupling handled by treating the particle as part of the fluid body. In particular, the Stokes equation are viewed as conservation equations for the total momentum of both the particle and fluid. The momentum associated with a particle is obtained by averaging the fluid momentum in the vicinity of the center of mass of the particle $\mathbf{X}(t)$. The following equation of motion is used to model the particle dynamics:

$$\frac{d\mathbf{X}(t)}{dt} \;=\; \mathbf{U}(\mathbf{X}(t),t) \tag{3}$$

with $\mathbf{U}$ defined by:

$$\mathbf{U}(\mathbf{x},t) \;:=\; \int_\Lambda \delta_a(\mathbf{y}-\mathbf{x})\mathbf{u}(\mathbf{y},t)d\mathbf{y} \tag{4}$$

where δ_a is an approximation to the Dirac δ-function spread over a ball of radius a and Λ denotes the periodic domain of the fluid. This fluid-particle coupling is a special case of what is referred to as the "immersed boundary method" and has been demonstrated to be an effective approach in modeling many systems in which a fluid interacts with immersed particles or moving boundaries [10, 15, 16].

III. HYDRODYNAMIC THERMAL FLUCTUATIONS

To derive the forcing which models the thermal fluctuations of the system we shall consider the Fourier transform of the fluid equations. The equations 1 - 3 become:

$$\frac{d\hat{\mathbf{u}}_\mathbf{k}}{dt} \;=\; -\alpha_\mathbf{k}\hat{\mathbf{u}}_\mathbf{k} + \rho^{-1}\wp_\mathbf{k}^{\perp}\hat{\mathbf{f}}_{\mathrm{thm},\mathbf{k}} \tag{5}$$

$$\hat{\mathbf{g}}_\mathbf{k}\cdot\hat{\mathbf{u}}_\mathbf{k} \;=\; 0, \tag{6}$$

where

$$\alpha_\mathbf{k} := \frac{4\pi^2\mu}{\rho L^2}|\mathbf{k}|^2 \tag{7}$$

$$\hat{\mathbf{g}}_\mathbf{k} := \frac{2\pi\mathbf{k}}{L}. \tag{8}$$

The projection operator which enforces incompressibility is defined by

$$\wp_\mathbf{k}^{\perp} := \left(\mathcal{I} - \frac{\hat{\mathbf{g}}_\mathbf{k}\hat{\mathbf{g}}_\mathbf{k}^T}{|\hat{\mathbf{g}}_\mathbf{k}|^2}\right). \tag{9}$$

In the case that $\hat{\mathbf{g}}_\mathbf{k} = 0$ the incompressibility constraint becomes trivial and we define $\wp_\mathbf{k}^{\perp} = \mathcal{I}$.

The requirement that the Fourier coefficients represent a real-valued velocity field gives the extra constraint

$$\overline{\hat{\mathbf{u}}_{-\mathbf{k}}} = \hat{\mathbf{u}}_\mathbf{k}. \tag{10}$$

We shall model the thermal force by Fourier modes proportional to "white noise":

$$\hat{\mathbf{f}}_{\mathrm{thm},\,\mathbf{k}}(t) = \sqrt{2D_\mathbf{k}}\frac{d\tilde{\mathbf{B}}_\mathbf{k}(t)}{dt} \tag{11}$$

where the coefficients $D_\mathbf{k}$ are to be determined. The factors $\tilde{\mathbf{B}}_\mathbf{k}$ are complex-valued Brownian motions. To ensure that the thermal forcing is real-valued the constraint:

$$\overline{d\tilde{\mathbf{B}}_{-\mathbf{k}}} = d\tilde{\mathbf{B}}_\mathbf{k} \tag{12}$$

is imposed.

By equilibrium statistical mechanics the hydrodynamics should exhibit fluctuations governed by Boltzmann's distribution. By Parseval's Lemma, the total kinetic energy can be expressed in terms of the Fourier modes of the fluid as:

$$\begin{aligned}\mathcal{E}[\{\hat{\mathbf{u}}_\mathbf{k}\}] \;&=\; \frac{\rho}{2}\int_\Lambda |\mathbf{u}(\mathbf{x})|^2 d\mathbf{x} \\ &=\; 2\frac{\rho}{2}\sum_{\mathbf{k}\in\mathcal{A}} |\hat{\mathbf{u}}_\mathbf{k}|^2 L^3\end{aligned} \tag{13}$$

where we have restricted the sum over the set $\mathcal{A}$ consisting of only one pair of the wavenumbers appearing in constraint 10. For concreteness, the set $\mathcal{A}$ is defined as those wavenumbers $\mathbf{k} = (k_1, k_2, k_3)$ which have at least one positive component and two or more non-negative components $k_1 \geq 0, k_2 \geq 0, k_3 \geq 0$. To obtain the expression we use the constraint 10 to set the terms associated with the inadmissible wavenumbers to their admissible wavenumber counter-parts, which gives the additional factor of 2.

Each degree of freedom of the fluid contributes a quadratic term to the energy of the system, giving a Boltzmann distribution which is Gaussian. Therefore, the Equipartition Theorem holds and each independent degree of freedom contributes on average $\frac{1}{2}k_BT$ to the kinetic energy.

For a particular wavenumber $\mathbf{k}$, equation 5 can be solved exactly by the method of integrating factors and expressed in terms of Ito integrals [12] to obtain:

$$\hat{\mathbf{u}}_\mathbf{k}(t) \;=\; \sqrt{2D_\mathbf{k}}\wp_\mathbf{k}^{\perp}\int_{-\infty}^{t} e^{-\alpha_\mathbf{k}(t-s)}d\tilde{\mathbf{B}}_\mathbf{k}(s). \tag{14}$$

To determine the mean contribution of $\hat{\mathbf{u}}_\mathbf{k}$ to the energy we use:

$$E\left(|\hat{\mathbf{u}}_\mathbf{k}|^2\right) \;=\; E\left(\mathrm{trace}\left(\hat{\mathbf{u}}_\mathbf{k}\overline{\hat{\mathbf{u}}_\mathbf{k}^T}\right)\right) \tag{15}$$

and

$$\mathrm{trace}\left(\wp_\mathbf{k}^{\perp}\right) \;=\; 2. \tag{16}$$

From the properties of Brownian motion we also have:

$$E\left(d\tilde{\mathbf{B}}_\mathbf{k}(w)\overline{d\tilde{\mathbf{B}}_\mathbf{k}(q)^T}\right) \;=\; 2\mathcal{I}\delta(w-q)dwdq. \tag{17}$$

From 14 - 17 it follows that the mean contribution of $\hat{\mathbf{u}}_{\mathbf{k}}$ to the energy is:

$$2\frac{\rho L^3}{2}E\left(|\hat{\mathbf{u}}_{\mathbf{k}}|^2\right) \;=\; 4\rho L^3\frac{D_{\mathbf{k}}}{\alpha_{\mathbf{k}}}. \tag{18}$$

Since after projection by $\wp_{\mathbf{k}}^{\perp}$ there are 4 independent degrees of freedom associated with each wavenumber $\mathbf{k}$ the Equipartition Theorem requires:

$$4\rho L^3\frac{D_{\mathbf{k}}}{\alpha_{\mathbf{k}}} = \frac{4}{2}k_BT. \tag{19}$$

This determines $D_{\mathbf{k}}$ through the following fluctuation-dissipation relation [13, 18]:

$$D_{\mathbf{k}} \;=\; \frac{k_BT}{2\rho L^3}\alpha_{\mathbf{k}}. \tag{20}$$

For a derivation of the corresponding fluctuation-dissipation relation when the fluid equations are discretized for numerical integration see [2].

IV. DERIVATION OF THE VELOCITY AUTOCORRELATION FUNCTION OF A BROWNIAN PARTICLE

In the hydrodynamic model the velocity autocorrelation function of an immersed particle can be readily computed from the autocorrelation function of the fluid which can be expressed as:

$$\begin{aligned} R(\mathbf{x}-\mathbf{y},\tau) \;&:=\; E\left(\text{trace }(\mathbf{u}(\mathbf{x},\tau)\overline{\mathbf{u}(\mathbf{y},0)^T})\right) \\ &=\; \sum_{\mathbf{k}} E\left(\text{trace }(\hat{\mathbf{u}}_{\mathbf{k}}(\tau)\overline{\hat{\mathbf{u}}_{\mathbf{k}}(0)^T})\right)\cdot \\ &\qquad \cdot\exp(i2\pi\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})/L). \end{aligned} \tag{21}$$

Equation 5 can be solved exactly by the method of integrating factors and expressed in terms of Ito integrals [12] as in equation 14. Plugging this into equation 21 gives the following expression for the velocity autocorrelation function of the fluid:

$$\begin{aligned} &E\left(\text{trace }(\hat{\mathbf{u}}_{\mathbf{k}}(\tau)\overline{\hat{\mathbf{u}}_{\mathbf{k}}(0)^T})\right) \\ &= \text{trace }\left(2D_{\mathbf{k}}\wp_{\mathbf{k}}^{\perp}\int_{-\infty}^{s}\int_{-\infty}^{r} e^{-\alpha_{\mathbf{k}}(r+s-w-q)}\right. \\ &\qquad\left. E\left(d\tilde{\mathbf{B}}_{\mathbf{k}}(w)\overline{d\tilde{\mathbf{B}}_{\mathbf{k}}(q)^T}\right)\right). \end{aligned} \tag{22}$$

From properties of the incompressibility projection operator in equation 16, Brownian motion in equation 17, and from equation 22 we have the velocity autocorrelation function for the fluid:

$$\begin{aligned} &R(\mathbf{x}-\mathbf{y},\tau) = \\ &\frac{2k_BT}{\rho L^3}\sum_{\mathbf{k}} e^{-a_{\mathbf{k}}|s-r|}\exp\left(i2\pi\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})/L\right). \end{aligned} \tag{23}$$

The velocity autocorrelation of an immersed particle can be computed from 23 and the Fourier Convolution Theorem to obtain:

$$\begin{aligned} Q(\tau) \;&:=\; E\left(\text{trace}(\mathbf{U}(\mathbf{X}(\tau),\tau)\overline{\mathbf{U}(\mathbf{X}(0),0)^T})\right) \\ &=\; \int_\Lambda\int_\Lambda E\left(\delta_a(\mathbf{y}-\mathbf{X}(\tau))\delta_a(\mathbf{z}-\mathbf{X}(0))\cdot\right. \\ &\qquad\left.\cdot\text{ trace }(\mathbf{u}(\mathbf{y},\tau)\overline{\mathbf{u}(\mathbf{z},0)^T})\right)d\mathbf{y}d\mathbf{z} \\ &\approx\; \frac{2k_BTL^3}{\rho}\sum_{\mathbf{k}}|\hat{\delta}_{a,\mathbf{k}}|^2e^{-a_{\mathbf{k}}|\tau|} \end{aligned} \tag{24}$$

where $\hat{\delta}_{a,\mathbf{k}}$ is the Fourier coefficient of the function δ_a. To obtain the last expression the approximation $\delta_a(\mathbf{x}-X(\tau)) \approx \delta_a(\mathbf{x}-X(0))$ was made for the regime in which the immersed particle is assumed to move only a small distance relative to its size a over the time scale τ of the correlations considered. If the particle moves a significant distance the full expectation expression must be computed. The diffusion coefficient of the particle can be used to determine which of the regimes is relevant for an immersed particle. To avoid computing the full expectation in this work we shall restrict ourselves to Brownian particles of size $10\mu\text{m} - 10\text{nm}$ for which this is a good approximation.

V. THE DIFFUSION COEFFICIENT OF AN IMMERSED PARTICLE

The diffusion coefficient can be computed from the autocorrelation function in equation 24 by use of the Kubo formula [13]:

$$D \;=\; \frac{1}{3}\int_0^\infty Q(r)dr. \tag{25}$$

This gives

$$D \;\approx\; \frac{2k_BTL^3}{3\rho}\sum_{\mathbf{k}}\frac{|\hat{\delta}_{a,\mathbf{k}}|^2}{\alpha_{\mathbf{k}}}. \tag{26}$$

The absence of a time-dependent term confirms that the mean squared displacement of a particle scales linearly in time in three dimensions [5]. To investigate the scaling in the other physical parameters we use equation 7 and express equation 26 as:

$$D \;\approx\; \frac{k_BT}{C_1\mu L\lambda} \tag{27}$$

where $C_1 = 12\pi^2$ and

$$\lambda \;:=\; \left(L^6\sum_{\mathbf{k}}\frac{|\hat{\delta}_{a,\mathbf{k}}|^2}{|\mathbf{k}|^2}\right)^{-1}. \tag{28}$$

We shall assume that the function δ_a approximates the Dirac δ-function over a ball of radius a with Fourier coefficients $\hat{\delta}_{a,\mathbf{k}}$ approximately $1/L^3$ for $|\mathbf{k}| \ll L/a$, and 0 for $|\mathbf{k}| \gg L/a$. The coefficient λ can then be approximated by:

$$\lambda \;\approx\; C_2 \frac{a}{L} \tag{29}$$

where C_2 denotes a non-dimensional constant.

With this approximation the diffusion coefficient is given by:

$$D \;\approx\; \frac{k_B T}{C_3 \mu a} \tag{30}$$

where $C_3 = C_1 C_2$ denotes a non-dimensional constant.

Expression 30 agrees up to a constant with classical models of Brownian particles with Stokesian drag. This shows that the diffusion coefficient of an immersed particle in the hydrodynamic model has the correct scaling in the physical parameters. The constant factor differs somewhat from the results obtained from Stokesian drag as a consequence of the way particles are handled in the hydrodynamic model. In particular, the parameter a which controls the effective size of a particle is less straight-forward to interpret then in models involving spherical particles with sharply delineated fluid-particle boundaries.

VI. SCALING OF THE VELOCITY AUTOCORRELATION FUNCTION

We now discuss the scaling of the autocorrelation function in the physical parameters for various time regimes. For short times an immersed particle is found to undergo a ballistic motion with t^2 scaling in the mean squared displacement. In this regime the velocity correlations are approximately constant and obey an equipartition principle. For long times an immersed particle has diffusive trajectories with order t scaling in the mean squared displacement. The velocity correlations in this regime are shown to decay non-exponentially with algebraic order $\tau^{-3/2}$ as a consequence of the hydrodynamics. In figure 1 the velocity autocorrelation function is compared with numerical simulations.

A. Short-Time Regime

We shall assume throughout that the function δ_a approximates the Dirac δ-function over a ball of radius a with Fourier coefficients $\hat{\delta}_{a,\mathbf{k}}$ approximately $1/L^3$ for $|\mathbf{k}| \ll L/a$, and 0 for $|\mathbf{k}| \gg L/a$. From equation 24 the time scale on which the velocity correlation remains approximately constant is $\tau \ll 1/\alpha_{[L/a]} \sim \rho a^2/\mu$.

In this regime the sum in equation 24 can be approximated by:

$$\sum_{\mathbf{k}} |\hat{\delta}_{a,\mathbf{k}}|^2 \;\approx\; \frac{L^3}{a^3}. \tag{31}$$

This gives for the velocity autocorrelation function:

$$Q(\tau) \;\approx\; \frac{k_B T}{\rho a^3} \tag{32}$$

when $\tau \ll \rho a^2/\mu$. The average kinetic energy of an immersed particle of mass ρa^3 in this regime satisfies the equipartition principle:

$$\frac{1}{2}\rho a^3 E\left(|\mathbf{U}|^2\right) \;=\; \frac{1}{2} k_B T \tag{33}$$

where $Q(\tau) \approx E\left(|\mathbf{U}|^2\right)$ from equation 24 when $\tau \ll \rho a^2/\mu$.

Since the velocity correlation is approximately constant immersed particles in the hydrodynamic model have ballistic trajectories in this regime. The mean squared displacement of a particle scales as:

$$E\left(|\mathbf{X}(t) - \mathbf{X}(0)|^2\right) \;\approx\; \frac{k_B T}{\rho a^3} t^2, \quad \text{for } t \ll \rho a^2/\mu. \tag{34}$$

The diffusive behavior of a particle occurs in the hydrodynamic model only on sufficiently long time scales $\tau \gg \rho a^2/\mu$ so that the particle velocity decorrelates.

B. Long-Time Regime

For immersed particles diffusing in a viscous fluid, the particle movements are strongly coupled to the motion of the fluid. As a particle moves along a particular direction, fluid is dragged along with it. When the particle changes direction, it is resisted by a viscous force arising from its motion relative to the nearby fluid with momentum related to the recent past of the particle's motion. This induces a somewhat stronger memory in the particle velocity than a standard model based on a constant Stokes drag would predict.

To estimate the long time behavior of the autocorrelation function given by expression 24 a number of approximations will be made. As discussed in the previous section the function δ_a is assumed to satisfy:

$$\hat{\delta}_{a,\mathbf{k}} \approx \frac{1}{L^3} \text{ for } |\mathbf{k}| \ll L/a, \tag{35}$$

with $\hat{\delta}_{a,\mathbf{k}}$ decaying rapidly with respect to $|\mathbf{k}|a/L$. From this it follows from the Fourier series representation in equation 24 that the sum will be dominated by terms with $|\mathbf{k}| \lesssim L/a$.

For $\rho a^2/\mu \ll \tau \ll \rho L^2/\mu$ the time τ is small compared to the decay time $1/\alpha_{\mathbf{k}} \sim \rho L^2/\mu$ of the low wavenumber modes $|\mathbf{k}| \sim 1$, but large compared to the decay time $1/\alpha_{\mathbf{k}} \sim \rho a^2/\mu$ of the (relatively high) wavenumber modes $|\mathbf{k}| \sim L/a$ corresponding to the length scale of the particle. Combining these observations, there exists a time-dependent wavenumber $k_c(t)$ such that $e^{-\alpha_{\mathbf{k}} t} \approx 1$ for $|\mathbf{k}| \ll k_c(t)$ and $e^{-\alpha_{\mathbf{k}} t} \approx 0$ for wavenumbers such that $|\mathbf{k}| \gg k_c(t)$. Consequently, over the intermediate asymptotic time interval, the Fourier series in equation 24 is dominated by contributions from wavenumbers $1 \leq |\mathbf{k}| \lesssim k_c(t)$. These observations allow us to make the following simplifying approximations over the time interval $\rho a^2/\mu \ll t \ll \rho L^2/\mu$:

- The prefactors multiplying the exponential in each Fourier series term may be approximated by their low wavenumber limits:

$$|\hat{\delta}_{a,\mathbf{k}}|^2 \approx 1/L^6 \text{ for all } \mathbf{k} \tag{36}$$

- This Fourier sum over the integer lattice can be approximated by an integral over continuous $\mathbf{k}$, because the dominant contribution comes from a large number of lattice sites $1 \leq |\mathbf{k}| \lesssim k_c(t)$, with $k_c(t) \gg 1$.

Applying these simplifications and then changing to spherical coordinates with radial variable $k = |\mathbf{k}|$, we obtain:

$$\begin{aligned} Q(\tau) &\approx \int_{\mathbb{R}^3} \frac{2k_BT}{\rho L^3} \exp(-\alpha|\mathbf{k}|^2\tau)\, d\mathbf{k} \\ &= \frac{8\pi k_BT}{\rho L^3} \int_0^\infty k^2 \exp(-\alpha k^2 \tau)\, dk \\ &= \frac{8\pi k_BT}{\rho L^3} \frac{1}{2} \left(\sqrt{2\pi \frac{1}{2\alpha\tau}} \frac{1}{2\alpha\tau} \right), \end{aligned}$$

where we use the notation $\alpha = 4\pi^2\mu\rho^{-1}L^{-2}$. From this the velocity autocorrelation function of a particle can be expressed as:

$$Q(\tau) \approx \left[C_{\text{IB}} \frac{k_BT\rho^{1/2}}{\mu^{3/2}} \right] \tau^{-3/2} \text{ for } \rho a^2/\mu \ll \tau \ll \rho L^2/\mu, \tag{37}$$

where $C_{\text{IB}} = \frac{1}{4\pi^{3/2}}$.

This agrees up to an order one non-dimensional prefactor with previous results obtained for Brownian motion of a particle immersed in a fluid when $D \ll \mu/\rho$ [11, 17]:

$$\tilde{Q}(\tau) \approx \frac{k_BT\rho^{1/2}}{4\mu^{3/2}} \tau^{-3/2} \text{ for } \tau \gg \rho a^2/\mu. \tag{38}$$

The condition $D \ll \mu/\rho$ can readily be checked to hold for Brownian particles with sizes ranging from $10\mu\text{m} - 10\text{nm}$ immersed in water at room temperature. The constant prefactor in expression 37 differs slightly from equation 38 due to the different way particles are represented in the previous models relative to the hydrodynamic model of this work.

The restriction that $\tau \ll \rho L^2/\mu$ for the $\tau^{-3/2}$ scaling in the hydrodynamic model is a finite size effect of the domain Λ with periodic boundary conditions. For very long times with $\tau \gg \rho L^2/\mu$ the correlation function $Q(\tau)$ in fact decays exponentially with rate $Q(\tau) \approx \exp\left(-(4\pi^2\mu/\rho L^2)\tau\right)$. This rate is associated with the smallest positive value of $\alpha_{\mathbf{k}}$ over all wavenumbers. By making L sufficiently large the time scale on which this occurs can be made arbitrarily large, suggesting that this effect is of little physical significance and can be made negligible provided the domain is taken sufficiently large.

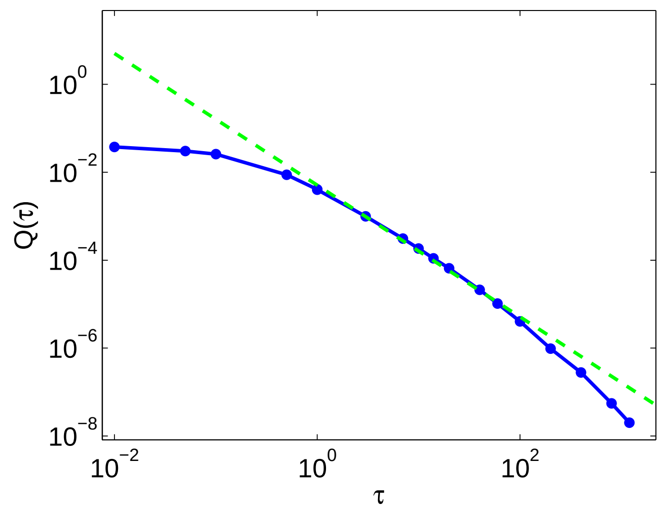

FIG. 1: Velocity Autocorrelation Function of an Immersed Particle. The solid curve denotes the velocity autocorrelation obtained from numerical simulations. The dashed curve denotes a least squares fit in log-log space of the line $Q = c\tau + b$ to the numerical data with $\tau \in [5, 100]$, corresponding to the approximate range $\rho a^2/\mu \ll \tau \ll \rho L^2/\mu$.

However, in numerical simulations this feature of the model may be non-negligible and as seen in figure 1 the finite size effects of the domain begin to manifest themselves in the numerical simulation when sufficiently long times $\tau \gg \rho L^2/\mu$ are considered for the autocorrelation function. For a more detailed discussion of the numerical implementation of the hydrodynamic model see [2].

In figure 1 a comparison is made between the numerical simulations and theoretical predictions. The solid curve denotes the velocity autocorrelation obtained from numerical simulations. The dashed curve denotes a least squares fit in log-log space of the line $Q = c\tau + b$ to the numerical data with $\tau \in [5, 100]$, corresponding to the approximate range $\rho a^2/\mu \ll \tau \ll \rho L^2/\mu$. The least squares fit yields $c = -1.497$ and $b = -5.283$. These values agree well with the theory: $c \approx -3/2 = -1.5$ and $b \approx \log\left[C_{\text{IB}} \frac{k_BT\rho^{1/2}}{\mu^{3/2}}\right] = -5.1361$. For the physical parameters used in the simulation, see table II. For details of the numerical method used for the simulations, see [2].

TABLE I: Description of the Physical Parameters

Parameter	Description
k_B	Boltzmann's constant
T	Temperature
L	Period Length of Fluid Domain
μ	Fluid Dynamic Viscosity
ρ	Fluid Density
N	Number of Grid Points in each Dimension
Δt	Time Step
Δx	Space Between Grid Points
a	Brownian Particle Size Parameter

VII. CONCLUSION

It has been shown that the simple fluid-particle coupling model captures correctly a number of physical features of Brownian particles. It was found that the diffusion coefficient of a Brownian particle has the correct scaling in the physical parameters. For the autocorrelation function it was shown that for short-times an equipartition principle holds for the particle velocity. For long times it was found that the velocity autocorrelation function has slow decay of algebraic order $\tau^{-3/2}$ capturing well-known hydrodynamic effects.

TABLE II: Physical Parameters

Parameter	Description
T	300 K
L	1000 nm
μ	6.0221×10^5 amu/(nm $\cdot$ ns)
ρ	602.2142 amu/nm^3
a	62.5 nm
N	32

[1] B. J. Alder and T. E. Wainwright, *Decay of the Velocity Autocorrelation Function*, Phys. Rev. A, vol. 1 num. 1, pp. 18–21, (1970).

[2] P. J. Atzberger, P, R. Kramer, and C. S. Peskin, *A Stochastic Immersed Boundary Method for Microscopic Biological Fluid Dynamics*, (submitted J. Comp. Phys), (2005).

[3] K. C. Neuman and S. M. Block, *Optical trapping*, Review of Scientific Instruments, volume 75, number 9, (2004).

[4] J. F. Brady and G. Bossis, *Stokesian dynamics*, in Annual review of fluid mechanics, vol. 20 of Annu. Rev. Fluid Mech., Annual Reviews, Palo Alto, CA, pp. 111–157, (1988).

[5] J. R. Dorfman and E. G. D. Cohen, *Velocity Correlation Functions in Two and Three Dimensions*, Phys. Rev. Let., Vol. 25. Num. 18, (1970).

[6] A. Einstein, *Investigations on the Theory of the Brownian Movement*, Dover Publications, New-York (1926).

[7] A. Einstein, *On the movement of small particles suspended in stationary liquids required by the molecular-kinetic theory of heat*, Ann. Phys. 17, 1905, appearing in The Collected Papers of Albert Einstein, English translation by Anna Beck Princeton U.P., Princeton, NJ, Vol. 2, pp. 123–134, (1989).

[8] D. L. Ermak and J. A. McCammon, *Brownian dynamics with hydrodynamic interactions*, J. Chem. Phys., 69, pp. 1352–1360, (1978).

[9] G. L. Paul and P. N. Pusey, *Observation of a long-time tail in Brownian motion*, J. Phys. A: Math. Gen. 14, pp. 3301–3327. Printed in Great Britain. (1981)

[10] C. S. Peskin, *The immersed boundary method*, Acta Numerica, 11, pp. 1–39, (2002).

[11] K. Berg-Sorensen and H. Flyvbjerg, *The colour of thermal noise in classical Brownian motion: a feasibility study of direct experimental observation*, New Journal of Physics, 7, (2005)

[12] B. Oksendal, *Stochastic Differential Equations: An Introduction with Applications.* Springer, (2000)

[13] R. Kubo, M. Toda, and N. Hashitsume, *Statistical physics. II*, Springer-Verlag, Berlin, second ed., section 4. Nonequilibrium statistical mechanics, (1991).

[14] D. S. Lemonsa, *Paul Langevins 1908 paper On the Theory of Brownian Motion [Sur la theorie du mouvement brownien, C. R. Acad. Sci. (Paris) 146, 530533 (1908)]*, Am. J. Phys., Vol. 65, No. 11, November (1997).

[15] L. Miller and C. Peskin, *When vortices stick: an aerodynamic transition in tiny insect flight*, J Exp Biol., 207, pp. 3073–3088, (2004).

[16] X. Meng, *A computational model of flow through porous media at the microscale*, Ph.D. thesis, Department of Mathematics, Tulane University, New Orleans, Louisiana 70118. July (1998).

[17] Y. Pomeau and P. Résibois, *Time Dependent Correlation Functions and Mode-Mode Coupling Theories*, Phys. Rep. vol.19C, num. 2, pp.63–139, (1975).

[18] L. E. Reichl, *A modern course in statistical physics*, John Wiley & Sons Inc., New York, second ed., (1998).

[19] M. von Smoluchowski, Ann. Phys. (Leipzig) 21, 756780, (1906).

[20] A. Widom, *Velocity Fluctuations of a Hard-Core Brownian Particle*, Phys. Rev. A., Vol. 3 Num. 4, (1971).

[21] R. Zwanzig and M. Bixon, *Hydrodynamic Theory of the Velocity Correlation Function*, Phys. Rev. A., Vol. 2 Num. 5, (1970).

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