Physica A 163 (1990) 804–812
North-Holland

TWO-DIMENSIONAL BROWNIAN MOTION AND FLUCTUATING HYDRODYNAMICS

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Received 13 March 1989
Revised manuscript received 31 July 1989

We derive the generalized Langevin equation for the motion of a hard disk in a two-dimensional incompressible fluid using a fluctuating hydrodynamical treatment. We show that our results are consistent with the fluctuation-dissipation theorem.

1. Introduction

The theory of Brownian motion is one of the most useful tools in statistical mechanics. One aspect of this theory is that the equation of motion of the Brownian particle can be described by the Langevin equation where the force exerted on the Brownian particle is split into a frictional force and a random force. In the usual Langevin equation, memory (non-Markovian) effects are ignored; in the more general case, one refers to the so-called generalized Langevin equation (GLE). It is now standard to use the GLE as a basis for the discussion of linear fluctuation phenomenon in non-equilibrium thermodynamics. For example, a decade ago, Mazur and Bedeaux [1], and Bedeaux and Mazur [2] published two papers. In the first paper [1], they calculated the force exerted on a spherical Brownian particle by an incompressible fluid, using the linearized stochastic Landau–Lifshitz equation by the induced force method. In the second paper [2], by the same method they derived the GLE for the sphere and showed by a direct calculation that the fluctuation–dissipation theorem is indeed true for the GLE they derived, and thus give a firm foundation for the application of the GLE to the study of linear fluctuation phenomenon. Several years ago, Varley and Zhou [3] extended the work of ref. [1] to the two-dimensional (2D) case. Using the same calculation scheme as that used in ref. [1], Varley and Zhou derived the force on a hard disk in a 2D incompressible fluid. However, no parallel study of the use of the 2D GLE for obtaining the corresponding fluctuation–dissipation theorem, analogous to that carried out by ref. [2] for the 3D case, was given.

The purpose of the present paper is two-fold. First, we want to show that the induced force method [1, 2] can be very much simplified if one solves the problem in wave-vector space. In particular, the resulting formalism is directly applicable to different dimensional cases. Secondly, in the new calculational scheme, we derive the 2D GLE and verify the corresponding fluctuation–dissipation theorem in the spirit of ref. [2].

Our formulation is presented in section 2, where we present a simple derivation of the 3D result of refs. [1, 2]. In section 3, we apply our formalism to the 2D case and derive the corresponding GLE. In section 4, we show that the 2D GLE we obtained is consistent with the fluctuation–dissipation theorem. Our results are summarized in section 5.

2. Formulation

The equation of motion for a hard sphere in an incompressible 3D fluid was written in the form of a GLE by Bedeaux and Mazur (see (3.1) of ref. [2]). Here we present an alternative and simpler approach to the problem, which is suitable for treating either the 3D or 2D situations. Consider a Brownian particle (a hard sphere for the 3D case and a hard disk for the 2D case) of radius a and mass m in an incompressible fluid. The motion of the fluid with mass density ρ and velocity field $\boldsymbol{v}(r, t)$ is described by the Navier–Stokes equations, and the force exerted by the fluid on the Brownian particle is calculated by integrating the pressure on the surface of the particle. In the linear (in terms of the velocity fields of fluid) treatment, which was done in refs. [1, 2], and is also the main interest of the present paper, one keeps only the linear terms in $\boldsymbol{v}(r, t)$ in the Navier–Stokes equations. In addition, again following refs. [1, 2], only terms linear in the velocity of the Brownian particle are retained.

The linearized equations of motion, in three dimensions, for the velocity field $\boldsymbol{v}(\boldsymbol{r}, \omega)$ of the incompressible fluid were written down by Mazur and Bedeaux (see eqs. (3.9) and (3.10) of ref. [1]). We now wish to enlarge on their work by presenting these results in wave-vector space [4] and in a form applicable to both the 3D and 2D cases. This is achieved by introducing the Fourier transform

$$\boldsymbol{v}(\boldsymbol{q}, \omega) = \int \mathrm{d}\boldsymbol{r} \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t - \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \boldsymbol{v}(\boldsymbol{r}, t) . \tag{2.1}$$

This enables us to write the equation of motion of the fluid in the form

$$(-\mathrm{i}\omega\rho + \eta q^2)\boldsymbol{v}(\boldsymbol{q},\omega) = \rho\boldsymbol{v}(\boldsymbol{q}, t=0) - \mathrm{i}\boldsymbol{q}P(\boldsymbol{q},\omega) + \boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{q},\omega)\,, \tag{2.2}$$

$$-q^2 P(\boldsymbol{q},\omega) = \mathrm{i}\boldsymbol{q}\cdot\boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{q},\omega)\,, \tag{2.3}$$

where η is the viscosity, ρ is the mass density, $\boldsymbol{v}(\boldsymbol{q},\omega)$, $P(\boldsymbol{q},\omega)$ and $F_{\mathrm{ind}}(\boldsymbol{q},\omega)$ are the Fourier transforms of $\boldsymbol{v}(\boldsymbol{r},t)$, $P(\boldsymbol{r},t)$ and $F_{\mathrm{ind}}(\boldsymbol{r},t)$, respectively. Also $P(\boldsymbol{r},t)$ is the hydrostatic pressure and $F_{\mathrm{ind}}(\boldsymbol{r},t)$ is the induced force, which is zero outside the Brownian particle and which balances the force exerted by the fluid inside the Brownian particle.

Now we turn to a discussion of the motion of the Brownian particle in the fluid. The force $F(\omega)$ exerted on a hard sphere (3D case) by the fluid was calculated by Mazur and Bedeaux (see eq. (3.16) in ref. [1], and note that we use $F(\omega)$ instead of the $K(\omega)$ used there). For our purpose, we present their result in a form suitable for both the 3D and 2D cases as

$$F(\omega) = -\mathrm{i}\omega\Omega\rho u(\omega) - \int F_{\mathrm{ind}}(\boldsymbol{r},\omega)\,\mathrm{d}\boldsymbol{r}\,, \tag{2.4}$$

where Ω is the volume of the Brownian particle, $u(\omega)$ is the Fourier transform of the velocity $u(t)$ of the Brownian particle, related to the velocity field $\boldsymbol{v}(\boldsymbol{r},t)$ of the fluid by the stick boundary condition [1]

$$\boldsymbol{v}(\boldsymbol{r},t) = \boldsymbol{u}(t) + \boldsymbol{\Omega}(t)\times[\boldsymbol{r} - \boldsymbol{R}(t)] \qquad \text{for } |r - R(t)| = a\,, \tag{2.5}$$

where $\Omega(t)$ is the angular velocity of the Brownian particle. In refs. [1, 2], a real space Green function $G(r,\omega)$ is then introduced to facilitate the calculation. We find the calculation will be simplified considerably if one uses instead the same Green function in wave vector space defined by

$$G(\boldsymbol{q},\omega) = \frac{1}{\eta(q^2+\alpha^2)}\,, \tag{2.6}$$

where $\alpha^2 = -\mathrm{i}\omega\rho/\eta$. Substitution of (2.2) and (2.6) into (2.1) yields

$$\begin{aligned}\boldsymbol{v}(\boldsymbol{q},\omega) &= \left[\rho\boldsymbol{v}(\boldsymbol{q},t=0) + \frac{\boldsymbol{q}_\perp^2}{q^2}\cdot\boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{q},\omega)\right]G(\boldsymbol{q},\omega)\\ &= \boldsymbol{v}_0(\boldsymbol{q},\omega) + \frac{\boldsymbol{q}_\perp^2}{q^2}\cdot\boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{q},\omega)G(\boldsymbol{q},\omega)\,,\end{aligned} \tag{2.7}$$

where $\boldsymbol{q}_\perp^2 = q^2 - \boldsymbol{q}\boldsymbol{q}$ and $\boldsymbol{v}_0$ is the velocity field in the absence of the induced field. We note that, by using (2.6), (2.7) can be rewritten into another form as

$$v(q, \omega) = v_0(q, \omega) - \frac{q_\perp^2}{\alpha^2} \cdot F_{ind}(q, \omega) G(q, \omega) + \frac{1}{\eta\alpha^2} \frac{q_\perp^2}{q^2} \cdot F_{ind}(q, \omega) , \tag{2.8}$$

where $v_0(q, \omega)$ is defined by (2.7).

In order to calculate the contribution due to the induced force to $F(\omega)$ of (2.4), first we perform the reverse Fourier transform with respect to q for (2.7) and (2.8), which gives the results

$$v(r, \omega) = v_0(r, \omega) + C_d \int dq\, e^{iq\cdot r} F_{ind}(q, \omega) G(q, \omega) , \tag{2.9}$$

$$v(r, \omega) = v_0(r, \omega) - \frac{C_d}{\alpha^2} \int dq\, e^{iq\cdot r} q^2 F_{ind}(q, \omega) G(q, \omega) + \frac{C_d}{\eta\alpha^2} F_{ind}(r, \omega) . \tag{2.10}$$

In obtaining (2.9) and (2.10), we have assumed that the system is isotopic, so the ratio $q_\perp^2/q^2$ contained in the q integrals of (2.7) and (2.8) will eventually contribute a constant and is written in (2.9) and (2.10) as C_d, a constant depending on the dimensionality (d), and $C_d = \frac{1}{2}, \frac{2}{3}$ for $d = 2, 3$, respectively. Next, we average (2.9) over the surface and (2.10) over the volume of the Brownian particle, respectively. The results are, after using (2.5),

$$u(\omega) = v_0^s(\omega) + C_d \int dq\, A_s(q) F_{ind}(q, \omega) G(q, \omega) , \tag{2.11}$$

$$u(\omega) = v_0^v(\omega) - \frac{C_d}{\alpha^2} \int dq\, A_v(q) q^2 F_{ind}(q, \omega) G(q, \omega) + \frac{C_d}{\eta\alpha^2} \int dr\, F_{ind}(r, \omega) , \tag{2.12}$$

where we use s for the surface area and Ω for the volume of the Brownian particle to define

$$A_s(q) = \frac{1}{s} \int_{r=a} ds\, e^{iq\cdot r} , \qquad A_v(q) = \frac{1}{\Omega} \int_{r\leq a} dr\, e^{iq\cdot r} \tag{2.13}$$

and

$$v_0^s(\omega) = \int dq\, A_s(q) v_0(q, \omega) , \qquad v_0^v(\omega) = \int dq\, A_v(q) v_0(q, \omega) . \tag{2.14}$$

By using (2.6) and (2.11)–(2.14), the explicit calculation of $F(\omega)$, given by

(2.4), is straightforward. In addition, these formulas are generally applicable to different dimensional cases, where one need only change Ω, C_d, A_v, A_s, and reevaluate the integrals contained in (2.11) and (2.12).

Here we first consider the 3D case, in which the Brownian particle is considered as a hard sphere. In this case, we use $C_d = \frac{2}{3}$ and

$$A_s(q) = \sin(qa)/qa\ , \qquad A_v(q) = 3[\sin(qa)/qa - \cos(qa)]/(qa)^2\ , \tag{2.15}$$

to calculate (2.11) and (2.12). After some algebra and cancellation we obtain from (2.11) and (2.12)

$$\int \mathrm{d}\boldsymbol{r}\, \boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{r}, \omega) = 6\pi\eta a\left[\left(1 + \alpha a + \frac{\alpha^2 a^2}{3}\right) \boldsymbol{u}(\omega) - (1 + \alpha a)v_0^{\mathrm{s}}(\omega) - \frac{\alpha^2 a^2}{3}\, v_0^{\mathrm{v}}(\omega)\right]. \tag{2.16}$$

Substituting (2.16) back to (2.4) we have the force exerted on the sphere as

$$\boldsymbol{F}(\omega) = -6\pi\eta a\left[\left(1 + \alpha a + \frac{\alpha^2 a^2}{3}\right) \boldsymbol{u}(\omega) - (1 + \alpha a)v_0^{\mathrm{s}}(\omega) - \frac{\alpha^2 a^2}{3}\, v_0^{\mathrm{v}}(\omega)\right]. \tag{2.17}$$

We note (2.16) and (2.17) were previously obtained in refs. [1, 2]. What we presented here is a much simpler calculation scheme. In the next section, we show how the same general results can be applied to the 2D case.

3. Two-dimensional Brownian motion and the generalized Langevin equation

In this section we calculate the force exerted on a hard disk in a two-dimensional incompressible fluid by using the formulas (2.4), (2.6), and (2.11)–(2.14) presented in the last section. In the 2D case, the volume Ω [appearing in (2.4), (2.13) and (2.14)] and the surface area [appearing in (2.13) and (2.14)] are πa^2 and $2\pi a$, respectively. The $A_s(q)$ and $A_v(q)$ are easily evaluated as

$$A_s(q) = J_0(qa)\ , \qquad A_v(q) = \frac{2}{qa}\, J_1(qa)\ , \tag{3.1}$$

where $J_n(x)$ is the nth order Bessel function. Substituting (2.4) and (3.1) into

(2.11) and (2.12), after some algebra they reduce to, respectively,

$$\boldsymbol{u}(\omega) = \boldsymbol{v}_0^{\mathrm{s}}(\omega) + \frac{1}{4\pi\eta} K_0(\alpha a)\boldsymbol{F}_{\mathrm{ind}}(\mathrm{i}\alpha a, \omega)\,, \tag{3.2}$$

$$\boldsymbol{u}(\omega) = \boldsymbol{v}_0^{\mathrm{v}}(\omega) - \frac{K_1(\alpha a)}{2\pi\eta\alpha a} \boldsymbol{F}_{\mathrm{ind}}(\mathrm{i}\alpha a, \omega) + \frac{1}{2\pi\eta\alpha^2 a^2}\int \mathrm{d}\boldsymbol{r}\, \boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{r}, \omega)\,, \tag{3.3}$$

where $K_n(x)$ is the nth order modified Bessel function, and $\alpha = (-\mathrm{i}\omega\rho/\eta)^{1/2}$.

Eliminating the $\boldsymbol{F}_{\mathrm{ind}}(\mathrm{i}\alpha a, \omega)$ contained in (3.2) and (3.3) we obtain

$$\int \mathrm{d}\boldsymbol{r}\, \boldsymbol{F}_{\mathrm{ind}}(\boldsymbol{r}, \omega) = 4\pi\eta\left\{\left[\frac{\alpha a K_1(\alpha a)}{K_0(\alpha a)} + \frac{\alpha^2 a^2}{2}\right]\boldsymbol{u}(\omega) - \frac{\alpha a K_1(\alpha a)}{K_0(\alpha a)}\boldsymbol{v}_0^{\mathrm{s}}(\omega) - \frac{\alpha^2 a^2}{2}\boldsymbol{v}_0^{\mathrm{v}}(\omega)\right\}. \tag{3.4}$$

Finally, combining (2.4) and (3.4) we obtain the Fourier transform of the force exerted by a 2D incompressible fluid on the disk as

$$\boldsymbol{F}(\omega) = -\mu(\omega)\boldsymbol{u}(\omega) + \boldsymbol{F}_{\mathrm{R}}(\omega)\,, \tag{3.5}$$

where the Fourier transform of the memory function is

$$\mu(\omega) = 4\pi\eta\left[\frac{\alpha a K_1(\alpha a)}{K_0(\alpha a)} + \frac{\alpha^2 a^2}{4}\right], \tag{3.6}$$

and the Fourier transform of the random force is

$$\boldsymbol{F}_{\mathrm{R}}(\omega) = 4\pi\eta\left[\frac{\alpha a K_1(\alpha a)}{K_0(\alpha a)}\boldsymbol{v}_0^{\mathrm{s}}(\omega) + \frac{\alpha^2 a^2}{2}\boldsymbol{v}_0^{\mathrm{v}}(\omega)\right]. \tag{3.7}$$

We note that (3.5)–(3.7) we previously derived by Varley and Zhou [3] using a direct extension of the calculation scheme in refs. [1, 2]. Again, our calculation is much simpler. Besides, Varley and Zhou did not present their 2D results in the form of the GLE and discuss the consistency of the fluctuation–dissipation theorem as Bedeaux and Mazur did in the 3D case. By using (3.5) and equation of motion of the disk

$$m\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = \boldsymbol{F}(t)\,, \tag{3.8}$$

the 2D GLE in the frequency space is

$$-\mathrm{i}\omega m\boldsymbol{u}(\omega) = -\mu(\omega)\boldsymbol{u}(\omega) + \boldsymbol{F}_{\mathrm{R}}(\omega)\,, \tag{3.9}$$

where the Fourier transform of the memory function $\mu(\omega)$ and the Fourier transform of the random force $\boldsymbol{F}_{\mathrm{R}}(\omega)$ are defined by (3.6) and (3.7). The basic properties of (3.9) as a GLE will be discussed in the next section. Here we show that it is convenient to use (3.9) to evaluate the velocity autocorrelation function. By using the fluctuation–dissipation theorem which we will verify in the next section, from (3.9) one has

$$\langle u_\alpha(\omega) u_\beta^*(\omega) \rangle = \delta_{\alpha\beta} \hbar\omega \coth\left(\frac{\hbar\omega}{2k_{\mathrm{B}}T} \right) \mathrm{Im}\left[\frac{1}{\omega + \mathrm{i}\mu(\omega)} \right] . \tag{3.10}$$

It follows then, from (3.6) and (3.10), that the long time tail behavior is given by $\langle u(t)u(0) \rangle \sim t^{-1}$. We note that Murphy [5] also used (3.10) in conjection with a $\mu(\omega)$ given by Stokes to get the t^{-1} behavior.

4. Fluctuation–dissipation theorem

It may be verified that the 2D GLE (3.9) derived in the last section has the following basic properties. The ensemble averaging of random force vanishes, i.e.

$$\langle F_{\mathrm{R}}(\omega) \rangle = 0 , \tag{4.1}$$

and also

$$\langle F_{\mathrm{R},\alpha}(\omega) F_{\mathrm{R},\beta}^*(\omega') \rangle = 2k_{\mathrm{B}}T\, \mathrm{Re}[\mu(\omega)] \delta_{\alpha\beta} 2\pi\delta(\omega - \omega') , \tag{4.2}$$

which is consistent with the usual fluctuation–dissipation theorem. First, we observe from (2.14) and (3.7) that (4.1) is a trivial consequence of the fact that the equilibrium average of v_0 is zero. To prove (4.2), it is convenient to rewrite (3.7) by using (2.13) and (3.1) as

$$\boldsymbol{F}_{\mathrm{R}}(\omega) \equiv \int \mathrm{d}\boldsymbol{q}\, \boldsymbol{F}_{\mathrm{R}}(\boldsymbol{q}, \omega) = \int \mathrm{d}\boldsymbol{q}\, A(q, \omega) \boldsymbol{v}_0(\boldsymbol{q}, \omega) , \tag{4.3}$$

where $\boldsymbol{v}_0(\boldsymbol{q}, \omega)$ is defined by (2.7), and

$$A(q, \omega) = 4\pi\eta \left[\frac{\alpha a K_1(\alpha a)}{K_0(\alpha a)} J_0(qa) + \alpha^2 a^2 J_1(qa) \right] . \tag{4.4}$$

Using the definitions of $G(\boldsymbol{q}, \omega)$ and $\boldsymbol{v}_0(\boldsymbol{q}, \omega)$, given by (2.6) and (2.7), respectively, it is straightforward to show that

$$\langle \boldsymbol{v}_0(\boldsymbol{q}, \omega)\boldsymbol{v}_0^*(\boldsymbol{q}', \omega')\rangle = \frac{k_B T}{\eta}\left(\frac{1}{q^2+\alpha^2} + \frac{1}{q^2-\alpha^2}\right)\left(1 - \frac{\boldsymbol{q}\boldsymbol{q}}{q^2}\right) \times (2\pi)^3\delta(\boldsymbol{q}-\boldsymbol{q}')\delta(\omega-\omega') . \tag{4.5}$$

Thus, we have

$$\langle F_{R,\alpha}(\omega)F^*_{R,\beta}(\omega')\rangle = C_d \int d\boldsymbol{q}\, |A(q, \omega)|^2 \frac{k_B T}{\eta}\left(\frac{1}{q^2+\alpha^2} + \frac{1}{q^2-\alpha^2}\right) \times 2\pi\delta(\omega-\omega')\delta_{\alpha\beta}$$
$$= 2\pi\delta(\omega-\omega')\delta_{\alpha\beta}[T_{00}(\omega) + T_{01}(\omega) + T_{11}(\omega)] , \tag{4.6}$$

where $T_{00}(\omega)$, $T_{01}(\omega)$, $T_{11}(\omega)$ represent the integral over $\boldsymbol{q}$ for the three different parts contained in $|A(q, \omega)|^2$, as can be seen from (4.4). It may be verified that they are proportional to $J_0^2(qa)$, $J_0(qa)J_1(qa)$, $J_1^2(qa)$, respectively. Carrying out these integrals we obtain

$$T_{00}(\omega) = (4\pi\eta)^2 \operatorname{Re}[I_0(\alpha a)K_0(\alpha a)]\left|\frac{\alpha a K_1(\alpha a)}{K_0(\alpha a)}\right|^2 , \tag{4.7}$$

$$T_{01}(\omega) = (4\pi\eta)^2 \operatorname{Re}\left[\frac{-I_0(\alpha a)K_1(\alpha a)}{\alpha a}\right] \operatorname{Re}\left[\frac{\alpha^3 a^3 K_1(\alpha a)}{K_0(\alpha a)}\right] , \tag{4.8}$$

$$T_{11}(\omega) = (4\pi\eta)^2 \operatorname{Re}\left[\frac{-I_1(\alpha a)K_1(\alpha a)}{\alpha^2 a^2}\right] \frac{|\alpha^2 a^2|^2}{2} , \tag{4.9}$$

where $I_n(\alpha a)$ and $K_n(\alpha a)$ are the modified Bessel functions. Substituting (4.7)–(4.9) into (4.6), we obtain (4.2).

5. Summary and discussion

In this paper, we have developed the theory of Mazur and Bedeau of Brownian motion in the fluctuating hydrodynamics calculation into a simplified and easy-to-handle formalism. By solving the linearized fluctuating hydrodynamics equations (2.1) and (2.2), we obtain the solution (2.7) for the velocity field $\boldsymbol{v}(\boldsymbol{q}, \omega)$. Then we derive the expressions for the velocity $\boldsymbol{u}(\omega)$ of the Brownian particle in the surface averaged form (2.11) and the volumed average form (2.12). From these two equations, the total force $\boldsymbol{F}(\omega)$ exerted on the Brownian particle is then obtained. Eqs. (2.11) and (2.12) are directly applicable to different dimensional cases. In the three-dimensional case we obtain $\boldsymbol{F}(\omega)$ as given in (2.17) and results of the two-dimensional calculation are given in (3.5)–(3.7) together with the 2D GLE (3.8). Our evaluation of the random force autocorrelation function, as given by (4.5), shows that the 2D GLE (3.8) we obtained for a hard disk in a 2D incompressible fluid indeed satisfies the fluctuation–dissipation theorem. We conclude that the 2D GLE (3.8) will be a convenient basis for studying the 2D Brownian motion by fluctuating hydrodynamics.

Finally, we wish to comment on a point made by Pomeau and Resibois [6], viz. that many existing theories of 2D fluids (such as fluctuating hydrodynamics theory or kinetic theory) have inherent inconsistencies. Our present theory is no exception in that as $\omega \to 0$ we conclude, from (3.6), that $\mu(0) \to 0$. But, since $\mu(0) = 1/\tau$, where τ is the relaxation time, this would imply that $\tau \to \infty$. Our feeling is that this is connected with the assumption of linearity but we hope to return to this question at a later time when we consider non-linear effects.

Acknowledgements

We thank Professor R.G. Hussey for bringing to our attention the work of ref. [3]. This research was supported in part by the U.S. Office of Naval Research under contract No. N00014-86-K-0002.

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