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A HYDRODYNAMIC FORMALISM FOR BROWNIAN SYSTEMS

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ABSTRACT

A formal hydrodynamic approach to Brownian motion is presented and the corresponding equations are derived. Hydrodynamic quantities are expressed in terms of the physical variables characterizing the Brownian systems. Contact is made with the hydrodynamic model of Quantum Mechanics.

RESUMEN

Se presenta una descripción hidrodinámica formal del movimiento Browniano y se derivan las ecuaciones correspondientes. Los parámetros hidrodinámicos se expresan en función de las variables físicas que caracterizan a los sistemas Brownianos. Se establece contacto con el modelo hidrodinámico de la Mecánica Cuántica.

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INTRODUCTION

It is found in some fields of Physics, that the differential equations representing a theory suggest a formal analogy with those of Hydrodynamics. In the case of Quantum Mechanics, such an analogy was recognized long ago, when Madelung[1] proposed that the motion of a quantum particle could be described as that of a highly localized inhomogeneity in a continuous fluid. The statement of hydrodynamic equations for this system from the usual definitions of the density and the current of probability[2] leads to the appearance of the so-called Bohm's potential[3,4,5] directly related to the pressure tensor of the hypothetical fluid, and to the possibility of a causal formulation of Quantum Mechanics.[6,7]

In this paper, we attempt to establish the analogy between the equations governing the motion of a brownian system and the equations of Hydrodynamics. Such an analogy is first suggested by the existence of a continuity equation for brownian systems. From this equation and a specific form for the velocity of the brownian particles, we derive Smoluchowski's and the hydrodynamic equations, including an explicit expression for the pressure tensor in terms of the quantities defining the brownian system.

The case we deal with, is that of a brownian particle acted on by an external conservative force field, and whose velocity is rotational. Therefore, the expression for its velocity includes, besides the contribution from the density gradient, a term arising from the presence of the external force and another giving place to the required rotational character.

Smoluchowski's equation, and the hydrodynamic equation of motion are obtained in Section I, where an explicit expression for the pressure tensor is given. Also, a "Hydrodynamic force" is defined through an "effective potential" in terms of the actual potential acting on the brownian system. The relationship between these potentials is examined further in Section II where we linearize it to obtain a Schrödinger-like equation solvable for the true potential. In Section III, contact is made with the hydrodynamic formulation of Quantum Mechanics, and a Bohm's potential is found. An alternative formulation of the Hydrodynamic model of Quantum Mechanics in terms of the pressure tensor is proposed in Section IV.

I. A BROWNIAN SYSTEM WITH ROTATIONAL VELOCITY IN A FORCE FIELD

Consider a closed system of brownian particles where the continuity equation,

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\vec{v}) = 0 , \qquad (1)$$

holds for the diffusion flux

$$\vec{j} = \rho\vec{v} = -D\nabla\rho - \frac{\rho}{\beta}\nabla\phi + \nabla\times\vec{a}, \qquad (2)$$

where the first term on the right hand side arises from Fick's law and contains the driving force proportional to the gradient of the density of brownian particles in a host fluid, the diffusion coefficient D being assumed constant. In the presence of an external potential field, another driving force appears such that the flux is proportional to it, with a proportionality factor $\rho\beta^{-1}$, where β is a measure of the viscosity of the brownian particles such that $\beta^{-1} \sim t_r$ (t_r is the relaxation time of the brownian system). An additional driving force is given by the last term, where $\vec{a}$ is assumed to have no explicit time dependence, but is otherwise arbitrary. This term is introduced to include the case of rotational diffusion flux.

Using expression (2) to obtain the divergence of $\rho\vec{v}$, and introducing this into Eq. (1) one gets

$$\frac{\partial\rho}{\partial t} = \nabla \cdot (D\nabla\rho - \frac{\rho}{\beta}\vec{k}), \qquad (3)$$

where $\vec{k} = -\nabla\phi$. Eq. (3) is Smoluchowski's equation[8] and describes the system for $t \gg t_r$.

The streaming and time derivatives of $\vec{v}$ can also be calculated from Eq. (2) to yield, after some lengthy but straightforward algebra, the desired hydrodynamic equation:

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = \vec{F} + \frac{1}{\rho} \nabla \cdot \overleftrightarrow{T} , \quad (4)$$

where the symmetrical tensor of the second rank $\overleftrightarrow{T}$ is given by

$$\overleftrightarrow{T} = - D^2 \left(\nabla^2 \rho (A+1) \overleftrightarrow{I} - A\nabla(\nabla\rho) - \frac{1}{\rho} \nabla\rho\nabla\rho \right.$$

$$- \frac{1}{\rho D} [(\nabla\times\vec{a})\nabla\rho + \nabla\rho(\nabla\times\vec{a})] + \frac{1}{\rho D^2} (\nabla\times\vec{a}) (\nabla\times\vec{a})$$

$$\left. + \frac{1}{\beta D} [(\nabla\times\vec{a})\nabla\phi + \nabla\phi(\nabla\times\vec{a})] \right) , \quad (5)$$

$\overleftrightarrow{I}$ being the unit tensor and A is an arbitrary constant. In order to complete the analogy, a hydrodynamic force per unit mass has been defined in Eq. (14):

$$\vec{F} = -\nabla V , \quad (6)$$

in terms of the "effective potential"

$$V = \frac{D}{\beta} \nabla^2 \phi - \frac{1}{\beta^2} (\nabla\phi)^2 + \frac{1}{\beta} \frac{\partial\phi}{\partial t} . \quad (7)$$

Hence, Eq.(4) is formally identical to the hydrodynamic equation of motion when $\vec{F}$ is identified as the external force per unit mass and $\overleftrightarrow{T}$ is made to play the role of the pressure tensor.

Hitherto, we have shown that an expression for the velocity of the brownian particles and the continuity equation are sufficient to render Smoluchowski's and the hydrodynamic motion equations, Eqs.(3) and (4). It is also possible to study particular cases of the general problem we have treated along the same line we used here or, alternatively, modifying our previous results according to appropriate physical conditions. These particular cases are:

a) A brownian system whose particles have irrotational velocity and are acted on by a force field. The velocity can then be written as

$$\vec{v} = - D \frac{1}{\rho} \nabla\rho - \frac{1}{\beta} \nabla\phi ,$$

and the hydrodynamical force $\vec{F}$ is seen to coincide with that of the general case, Eqs. (6) and (7). The pressure tensor, on the other hand, takes on the simple form

$$\overset{\rightrightarrows}{T}_o = -D^2 \left(\nabla^2\rho(A+1)\overset{\rightrightarrows}{I} - A\nabla(\nabla\rho) - \frac{1}{\rho}\nabla\rho\nabla\rho \right), \tag{8}$$

and the hydrodynamic equation of motion is Eq.(4) with $\overset{\rightrightarrows}{T}_o$ instead of $\overset{\rightrightarrows}{T}$.

b) A force-free brownian system of particles with rotational velocity, the expression for which is

$$\vec{v} = -D\frac{1}{\rho}\nabla\rho + \frac{1}{\rho}\nabla\times\vec{a} .$$

The hydrodynamic force vanishes as expected, an the pressure tensor is obtained from Eq.(5) as

$$\overset{\rightrightarrows}{T}_1 = \overset{\rightrightarrows}{T}_o - \frac{1}{\rho}(\nabla\times\vec{a})(\nabla\times\vec{a}) + \frac{D}{\rho}[\nabla\rho(\nabla\times\vec{a}) + (\nabla\times\vec{a})\nabla\rho] ,$$

when $\overset{\rightrightarrows}{T}_o$ is given by Eq.(8). The hydrodynamic equation of motion for the force-free case reduces to

$$\frac{\partial\vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v} = \frac{1}{\rho}\nabla\cdot\overset{\rightrightarrows}{T}_1 . \tag{9}$$

c) A force-free brownian system of particles with irrotational velocity, the expression of which is

$$\vec{v} = -D\frac{1}{\rho}\nabla\rho ,$$

with vanishing hydrodynamic force and a presure tensor given by $\overset{\rightrightarrows}{T}_o$ in Eq.(8). The hydrodynamic equation of motion is that given by Eq.(9) when $\overset{\rightrightarrows}{T}_o$ is used in the place of $\overset{\rightrightarrows}{T}_1$.

In the last two cases a diffusion equation,

$$\frac{\partial\rho}{\partial t} = -D\nabla^2\rho ,$$

is obtained instead of the usual Smoluchowski's. This is an expected result, since the latter reduces to the former for force-free brownian systems.

II. RELATIONSHIP BETWEEN THE ACTUAL AND THE EFFECTIVE POTENTIALS

From the definition of the effective potential per unit mass V, Eq.(7), it is seen that a relationship exists between this and the actual external potential ϕ. Whenever ϕ is known, V can be easily computed from this equation but, if V happens to be known, then ϕ can in principle be obtained by solving the differential equation (7); however, this is non-linear and its solution is not easy to get. In order to linearize this equation we assume that a function $f(\phi)$ exists such that Eq.(7) is a linear differential equation in $f(\phi)$. Using this function we get that

$$\nabla^2 f(\phi) = f'(\phi)\nabla^2\phi + f''(\phi)(\nabla\phi)^2.$$

Comparison with Eq.(7) shows that

$$\frac{f'(\phi)}{f''(\phi)} = -2D\beta$$

or

$$\frac{df'(\phi)}{f'(\phi)} = -\frac{1}{2D\beta}\,d\phi \quad ,$$

and integrating this last equation twice we arrive at the desired expression for $f(\phi)$, namely

$$f(\phi) = -2D\beta\exp(-\phi/2D\beta)$$

and the equivalent linear differential equation reads

$$2D^2\nabla^2\Psi + V\Psi = -2D\frac{\partial\Psi}{\partial t} \quad , \tag{10}$$

where

$$\Psi = \sqrt{n_o}\, \exp(-\phi/2D\beta). \tag{11}$$

Let us examine this equation: It is known[8] that

$$2D\beta = \frac{2kT}{m},$$

where k is Boltzmann's constant, m is the mass of a particle of the system and T is the absolute temperature of the system. Therefore, Eq.(11) can be written in the form

$$\Psi = \sqrt{n_o}\, \exp(-m\phi/2kT) . \tag{12}$$

On the other hand, Boltzmann's law of Statistical Mechanics predicts[9] the distribution function

$$n(\vec{r}) = n_o \exp(-m\phi(\vec{r})/kT) \tag{13}$$

for the number of particles around $\vec{r}$, belonging to a system of n_o particles at temperature T and acted on by the external potential $\phi(\vec{r})$. Comparing Eqs. (12) and (13) we conclude that

$$\Psi = \sqrt{n} .$$

Hence, Eq.(10) and the meaning of Ψ resemble the Schrödinger equation and the wave function of Quantum Mechanics, since in both cases $|\Psi|^2$ produces a probability density. It must be noted, however, that Eq.(10) differs from Schrödinger's in that the coefficient of the time derivative is real, which makes Ψ a (decreasing) monotonic function of time instead of having the oscillatory behaviour of the wave function. A difference also appears in the coefficient of the Laplacian operator which has a different sign from that of Quantum Mechanics.

III. BOHM'S POTENTIAL

Consider the tensor

$$\overleftrightarrow{T}_o = -D^2 \left(\nabla^2\rho(A+1)\overleftrightarrow{I} - A\nabla(\nabla\rho) - \frac{1}{\rho}\nabla\rho\nabla\rho \right) .$$

Since it enters the hydrodynamic equation of motion through its divergence, and since

$$\nabla \cdot [\nabla^2 \rho \overleftrightarrow{I} - \nabla(\nabla\rho)] = 0 ,$$

it follows that we have only to consider the remaining term

$$- D^2 (\nabla^2 \rho \overleftrightarrow{I} - \frac{1}{\rho} \nabla\rho\nabla\rho) ;$$

the i-th component of its divergence being

$$Q_i = - D^2 \frac{\partial}{\partial x_j} \left(\frac{\partial}{\partial x_j} \frac{\partial}{\partial x_k} \rho \, \delta_{ik} - \frac{1}{\rho} \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j} \right)$$

(repeated indices indicate summation from 1 to 3).

Using the fact that

$$\frac{\partial (f \delta_{ik})}{\partial x_k} = \frac{\partial f}{\partial x_i}$$

for an arbitrary function f, and interchanging the differentiation order in the first term, differentiating the second term with respect to x_k and rearranging terms we are lead to the equation

$$\vec{Q} = - \nabla U , \qquad (14)$$

where

$$U = D^2 \left(\frac{1}{\rho} \nabla^2 \rho - \frac{1}{2\rho^2} \nabla\rho \cdot \nabla\rho \right) \qquad (15)$$

has the same density dependence as Bohm's potential[3,4,5] obtained in the hydrodynamic formulation of Quantum Mechanics. The difference between Eq.(15) and its quantum mechanical analogue is the sign of the right hand side. This result has the same origin as the difference discussed when dealing with Eq.(10) and the Schrödinger equation.

IV. ALTERNATIVE FORMULATION OF THE HYDRODYNAMIC MODEL OF QUANTUM MECHANICS

In the usual hydrodynamic model of Quantum Mechanics[3,4,5] one deals with the force $\vec{Q}$ defined in Eq.(14), and it is introduced in the hydrodynamic equation of motion as the gradient of Bohm's potential:

$$\frac{\partial\vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v} = \vec{f} - \nabla U$$

with

$$U = -(\hbar/2m)^2\left(\frac{1}{\rho}\nabla^2\rho - \frac{1}{2\rho^2}\nabla\rho\cdot\nabla\rho\right).$$

We have shown in the previous section, however, that such a potential can be obtained from a pressure tensor as that given in Eq.(8). Henceforth, the above procedure can be reversed and a pressure tensor,

$$\overset{\Rightarrow}{T} = (\hbar/2m)^2\left(\nabla^2\rho(A+1)\overset{\Rightarrow}{I} - A\nabla(\nabla\rho) - \frac{1}{\rho}\nabla\rho\nabla\rho\right), \qquad (16)$$

for the quantum-mechanical case can be obtained. The corresponding hydrodynamic equation of motion will include the divergence of this pressure tensor, emphasizing the formal analogy between this model and the equations of Hydrodynamics. Again, the sign difference directly related to the two Bohm's potentials is observed in Eqs.(8) and (16).

CONCLUSIONS

It has been shown that a formal analogy between the equations governing the brownian motion and those of Hydrodynamics exists, and the explicit form of the hydrodynamic force and the pressure tensor for the hypothetical fluid have been given in terms of the quantities defining the brownian ensemble.

In our approach, the equation of continuity has been assumed to hold, and Smoluchowski's equation was derived from it. It is possible, of course, to assume the latter instead, but we have chosen this view since, as we mentioned in the introduction the formal analogy we studied is first suggested by the existence of an equation of continuity for brownian systems. Smoluchowski's equation is seen to reduce naturally to a diffusion equation for force-free systems.

It has been pointed out to us that, in the approach which takes Smoluchowski's equation as the starting point, a more general expression for the diffusion flux would contain a term $\nabla f(\vec{r})$, with $f(\vec{r})$ a solution of Laplace's equation. The new flux is indeed consistent with Eqs. (1) and (3), and modifies the form of the pressure tensor. Nevertheless, our results do not seem to be substantially affected by the presence of new terms in that tensor.

We have also shown that the relationship between the effective and the actual external potentials leads to a Schrödinger-like equation for an exponential function of the latter, except that its solutions are monotonically decreasing functions of time due to the real nature of the diffusion coefficient of brownian systems.

A potential similar to Bohm's has been derived for brownian systems from the pressure tensor of the hydrodynamic model and, conversely, a pressure tensor has been proposed for the hydrodynamic model of Quantum Mechanics which so far had made use of Bohm's potential only.

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