NTNU **Institutt for fysikk**

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Exam in TFY4275/FY8907 CLASSICAL TRANSPORT THEORY

May 26, 2012
09:00–13:00

Allowed help: Alternativ **D**
Authorized calculator and mathematical formula book

This problem set consists of 4 pages.

This exam consists of two problems each containing several sub-problems. Each of the sub-problems will be given approximately equal weight during grading (if nothing else is said to indicate otherwise).

I (or a substitute) will be available for questions related to the problems themselves (though not the answers!). The first round (of two), I plan to do a round 10am, and the other one, about two hours later.

The problems are given in English only. Should you have any language problems related to the exam set, do not hesitate to ask. For your answers, you are free to use either English or Norwegian.

Good luck to all of you!

Problem 1.

This problem is dedicated to the so-called *Einstein-Green-Kubo* relation. This relation states that the diffusion constant is related to the time-integral of the velocity-velocity correlation function of the diffusing particle. This relation was used in the seminal (famous) paper on diffusion that Einstein wrote in 1905. It is one of his four *Annus Mirabilis* papers that contributed substantially to the foundation of modern physics.

In mathematical terms, the Einstein-Green-Kubo relation can be express as

$$D = \frac{1}{d}\int_0^\infty \mathrm{d}t \, \langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle_{\mathrm{eq}} \,. \tag{1}$$

Here D denotes the (spatially independent) diffusion constant; d is the dimension of space; and $\mathbf{v}(t)$ signifies the (d-dimensional) velocity vector of the particle at time t. The notation $\langle\cdot\rangle_{\mathrm{eq}}$ is used to indicate an ensemble average taken when the system is in equilibrium. On the other hand, $\langle\cdot\rangle$ (without the subscript "eq"), means general ensemble averages where the system can potentially be out of equilibrium (non-equilibrium), but it can also be in equilibrium.

In this problem, we will derive the Einstein-Green-Kubo relation, and in the next problem we will demonstrate how it can be used.

a) Write down the diffusion equation in d-dimensional space, and explain the meaning of the symbols that you use. Argue (or derive) that the fundamental solution of this equation can be written in the form

$$p(\mathbf{x},t|\mathbf{x}_0,t_0) = \prod_{i=1}^{d} p_*(x_i,t|x_{0,i},t_0), \tag{2}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ is the position vector of the particle at time t; $\mathbf{x}_0 \equiv \mathbf{x}(t=t_0)$; $x_{0,i}$ means the ith component of $\mathbf{x}_0$; and

$$p_*(y,t|y_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left(-\frac{(y-y_0)^2}{4D(t-t_0)}\right), \tag{3}$$

is the fundamental solution of the one-dimensional diffusion equation. Recall that a fundamental solution means that the solution satisfies $p_*(y,t_0|y_0,t_0) = \delta(y-y_0)$.

b) Use solution (2) of the d-dimensional diffusion equation to show that the mean-square-displacement, defined as (with $t_0 = 0$)

$$\Delta(t) = \left\langle [\mathbf{x}(t) - \mathbf{x}(0)]^2 \right\rangle, \tag{4}$$

grows with time t as

$$\Delta(t) \simeq 2dDt, \tag{5}$$

for sufficiently long time. To simplify this calculation, you my assume that the coordinate system is chosen so that $\mathbf{x}_0 \equiv \mathbf{x}(t_0) = \mathbf{x}(0) = 0$.

c) Starting from Eq. (4), derive the relation

$$\frac{\mathrm{d}\Delta(t)}{\mathrm{d}t} = 2\left\langle \mathbf{v}(t)\cdot[\mathbf{x}(t)-\mathbf{x}(0)]\right\rangle = 2\int_0^t \mathrm{d}t' \left\langle \mathbf{v}(t)\cdot\mathbf{v}(t')\right\rangle. \tag{6}$$

d) Argue that at *equilibrium*, the last ensemble average in Eq. (6) depends only on the difference between the times t and t', i.e., it only depends explicitly on $t''=t-t'$. Use this to conclude that

$$\frac{\mathrm{d}\Delta(t)}{\mathrm{d}t} = 2\int_0^t \mathrm{d}t'' \left\langle \mathbf{v}(0)\cdot\mathbf{v}(t'')\right\rangle_{\mathrm{eq}}. \tag{7}$$

e) With Eq. (7), and by taking the time limit $t\to\infty$, obtain the Einstein-Green-Kubo relation [i.e., Eq. (1)]

$$D = \frac{1}{d}\int_0^\infty \mathrm{d}t \left\langle \mathbf{v}(t)\cdot\mathbf{v}(0)\right\rangle_{\mathrm{eq}}. \tag{8}$$

Problem 2.

Consider at Brownian particle of mass, m, in a solution (or bath) kept at constant absolute temperature T. Like in the previous problem, space is assumed to be d-dimensional, and all vectors are therefore d-dimensional.

The intention of this problem is to study the stochastic properties of the velocity process that is associated with the Brownian particle. Furthermore, we will use it to obtain the diffusion constant of the particle on the basis of the Einstein-Green-Kubo relation.

Note that even if you are not able to solve sub-problems 2c and 2d correctly, it is still possible to solve the remaining sub-problems.

a) Write down the Langevin equation for the particle and state the meaning of the variables that you use. From this equation, show that the equation satisfied by the velocity $\mathbf{v}(t)$ of the Brownian particle is

$$\dot{\mathbf{v}}(t) = -\gamma\mathbf{v}(t) + \boldsymbol{\xi}(t), \tag{9}$$

where

$$\left\langle \boldsymbol{\xi}(t)\right\rangle = 0, \tag{10a}$$

$$\left\langle \boldsymbol{\xi}(t)\cdot\boldsymbol{\xi}(t')\right\rangle = C\delta(t-t'), \tag{10b}$$

with C a constant to be determined. You do not have to prove Eq. (10), only argue why $\boldsymbol{\xi}$ should satisfy these properties. What is the physical meaning of the constant γ and $\boldsymbol{\xi}(t)$?

b) Show that the solution to Eq. (9) is

$$\mathbf{v}(t) = \mathbf{v}_0 \mathrm{e}^{-\gamma t} + \int_0^t \mathrm{d}t' \mathrm{e}^{-\gamma(t-t')}\boldsymbol{\xi}(t'); \qquad \mathbf{v}_0 = \mathbf{v}(0). \tag{11}$$

c) (*Double weight*) From the velocity of the Brownian particle, Eq. (11), derive an expression for the velocity-velocity correlation function $\langle \mathbf{v}(t) \cdot \mathbf{v}(t') \rangle$. [In deriving this relation, note that the following two possibilities exist; $t \leq t'$ or $t' \leq t$].

d) Show that for sufficiently long time, $t + t' \gg 1/\gamma$, a *stationary* (or *equilibrium*) state has been reached, so that the correlation function $\langle \mathbf{v}(t) \cdot \mathbf{v}(t') \rangle$, derived in the previous subproblem, can be written in the form

$$\big\langle \mathbf{v}(t) \cdot \mathbf{v}(t') \big\rangle_{\text{eq}} = \frac{C}{2\gamma} \exp\big(-\gamma \left|t - t'\right|\big). \tag{12}$$

e) What is the stochastic process called that describes $\mathbf{v}(t)$? Obtain an expression for the constant C present in Eq. (12).

f) Use Einstein-Green-Kubo relation, Eq. (8), to obtain an expression for the diffusion constant, D, of the Brownian particle valid in d-dimensional space.