"Many particle systems out of equilibrium" Problems, Series 4, 2006-07.

Problem 10. Projection operator formalism and the random flight model

In the random flight model of problem (6) a function $p(x, v, t)$ can be introduced, describing the probability density for finding a particle at position x with velocity v at time t. In the version considered so far, and also here, the velocity may in fact only assume the values $\pm v_0$.

a) Show that the time evolution of this function is described by

$$\frac{\partial p(x,v,t)}{\partial t} + v\frac{\partial p(x,v,t)}{\partial x} = \nu\left[\frac{1}{2}\left\{p(x,v_0,t) + p(x,-v_0,t)\right\} - p(x,v,t)\right]. \tag{1}$$

b) On taking the Fourier transform of this equation for each of the two possible velocities one obtains the matrix equation

$$\frac{\partial}{\partial t}\begin{pmatrix} \hat{p}(k,v_0,t) \\ \hat{p}(k,-v_0,t) \end{pmatrix} = \begin{pmatrix} -ikv_0 - \frac{\nu}{2} & \frac{\nu}{2} \\ \frac{\nu}{2} & ikv_0 - \frac{\nu}{2} \end{pmatrix}\begin{pmatrix} \hat{p}(k,v_0,t) \\ \hat{p}(k,-v_0,t) \end{pmatrix}. \tag{2}$$

Find the eigenvalues of this equation and show that the right eigenvectors may be chosen as

$$\begin{aligned} \hat{\boldsymbol{p}}_1(k,v) &= \begin{pmatrix} e^{-i\phi(k)} \\ e^{i\phi(k)} \end{pmatrix}; \qquad \hat{\boldsymbol{p}}_2(k,v) = \begin{pmatrix} -ie^{i\phi(k)} \\ ie^{-i\phi(k)} \end{pmatrix}, \\ \text{with } \phi &= \frac{1}{2}\arcsin\frac{2kv_0}{\nu}. \end{aligned} \tag{3}$$

Next give the solution of the distribution function for given initial value.

c) Determine the operator $\hat{\mathcal{L}}$ and use it to calculate $U(k, z)$. Does the result agree indeed with that of problem 8b? (Hint: for a system of length L with periodic boundary conditions the inner product $\langle|\rangle$ reduces to $1/L \int_0^L dx\, 1/2Tr_v$.)

d) Check if the "initial term" $\langle\Delta(0)|P_\perp e^{\hat{\mathcal{L}}t} P_\perp \hat{\mathcal{L}} n_t(\boldsymbol{k})\rangle$, which is usually ignored in evaluating the projection operator expressions, is indeed negligible for large times.

e) When transforming back the Green function $G(k, z) = \frac{1}{z+k^2U(k,z)}$ to time representation, it is common restricting oneself to the contribution of the rightmost singularity in the complex z-plane. Is this justified here in view of the neglect of the initial term one makes anyhow?

In the present case this approximation reduces the generalized diffusion equation in Fourier representation to a form

$$\frac{\partial n(k,t)}{\partial t} = -k^2 D(k) n(k,t). \tag{4}$$

Give the *dispersion relation* expressing $D(k)$ as function of k.
Can one have cases where the generalized diffusion equation cannot be reduced to the form (4)?

Problem 11. The method of images

The most common boundary conditions for the diffusion equation are

1) Reflecting boundary conditions, resulting from an inert wall at which the normal component of the current vanishes. Through Fick's first law this implies that the density gradient has zero component normal to the wall.

2) Absorbing boundary conditions. In this case all mass reaching the wall sticks to it or disappears through it. This gives rise to a vanishing density at the wall (in practice *almost* vanishing, since mass moving towards the wall will contribute to the density).

For both types of boundary conditions the diffusion equation for some appropriate geometries may be solved by the method of images. The simplest application is the diffusion in one dimension on an interval, say $[0, L]$ For a particle starting at x one adds image particles at the positions $x + 2nL$ (with $n \neq 0$) and $-x + 2nL$. In the case of reflecting boundaries all these particles have the same mass m, in the case of absorbing boundaries the "even" particles, at $x + 2nL$, have mass m and the "odd" particles, at $-x+2nL$ have mass $-m$ (what should one take if one boundary is absorbing and the other one reflecting?). The solution of the diffusion equation for one particle on $[0, L]$ is now, within this interval, identical to that of diffusion of all the particles on the real axis without boundaries; this solution satisfies the required boundary conditions for all times because of the symmetries of the particle arrangement and the symmetry properties of the diffusion equation (a solution that is even/odd initially will remain so for all times).

a) Use this method to solve the diffusion equation on $[0, L]$ with initial condition $n(x, 0) = \delta(x - x_0)$, both with reflecting and with absorbing boundary conditions.

b) Also solve the equation by expansion in terms of eigenfunctions and show the results agree. After about what time does this method become preferable?

c) In which cases can the method of images be used to describe diffusion inside a triangle?