"Many particle systems out of equilibrium" Problems, Series 12, 2006-07.

Problem 25. Mode-coupling equations for diffusion in a random environment

(See: *M.H. Ernst, J. Machta, J.R. Dorfman and H. van Beijeren*, J. Stat. Phys. **34**, 477 (1983))

Diffusion of a tracer particle in a random environment may be descibed by the equation

$$\frac{\partial n(\boldsymbol{r},t)}{\partial t} + \nabla \cdot [\boldsymbol{j}^{av}(\boldsymbol{r},t) + \boldsymbol{j}^{r}(\boldsymbol{r},t)] = 0, \tag{1}$$

with the average and the random current satisfying

$$\begin{aligned} \boldsymbol{j}^{av}(\boldsymbol{r},t) &= -\left[\mathsf{K}(\boldsymbol{r}) \cdot \nabla \frac{n(\boldsymbol{r},t)}{n^{eq}(\boldsymbol{r})}\right] \\ < \boldsymbol{j}^{r}(\boldsymbol{r},t) > &= 0. \end{aligned} \tag{2}$$

Here $n^{eq}(\boldsymbol{r})$ and $\mathsf{K}(\boldsymbol{r})$ express the local inhomogeneity of the medium, which is independent of time. The nonuniform equilibrium density is due to a varying local potential and $\mathsf{K}(\boldsymbol{r})$ is a local *diffusion tensor* that fluctuates as function of $\boldsymbol{r}$. Set $\mathsf{K}(\boldsymbol{r}) = D_0 1 + \delta\mathsf{K}(\boldsymbol{r})$. D_0 has to be chosen such that the spatial average of $\delta\mathsf{K}(\boldsymbol{r})$ vanishes. The average $<>$ is to be taken over the realizations of the random current. Correlations between random currents should satisfy a fluctuation-dissipation theorem, but the kernel appearing in this can only be identified after applying the mode-coupling procedure. We may use the fact however, that these correlations will take care of keeping equilibrium correlations such as $< n(\boldsymbol{r}_1,t)n(\boldsymbol{r}_2,t) >$ independent of t. For small inhomogeneity we may set $n^{eq}(\boldsymbol{r}) = n_0 + \delta n^{eq}(\boldsymbol{r})$, with $n_0 =< n^{eq}(\boldsymbol{r}) >_{sp}$, where $<>_{sp}$ denotes an average over all realizations of the spatial randomness. We may assume then that $\delta\mathsf{K}(\boldsymbol{r})$ and $\delta n^{eq}(\boldsymbol{r})$ typically are small compared to D_0 and $< n^{eq}(\boldsymbol{r}) >_{sp}$ repectively. Eq. (1), with (2) substituted into it, may then be linearized in these fluctuations to

$$\begin{aligned} \frac{\partial n(\boldsymbol{r},t)}{\partial t} &= D_0 \nabla^2 n(\boldsymbol{r},t) + \nabla \cdot \frac{\delta\mathsf{K}(\boldsymbol{r})}{n_0} \cdot \nabla n(\boldsymbol{r},t) \\ &\quad - D_0 \nabla^2 \frac{n(\boldsymbol{r},t)\delta n^{eq}(\boldsymbol{r})}{n_0} - \nabla \cdot \boldsymbol{j}^{r}(\boldsymbol{r},t), \end{aligned} \tag{3}$$

with $<>_{sp}$ the average over spatial fluctuations.

If one does an additional averaging over the possible realizations of the random environment the resulting equations will be translation invariant. The Fourier components of the tracer density then will satisfy an equation of the form

$$n(\boldsymbol{k},t) = G(\boldsymbol{k},t)n(\boldsymbol{k},0) \qquad \text{or}$$

$$G(\boldsymbol{k},t) \quad = \quad \frac{< n(-\boldsymbol{k},0)n(\boldsymbol{k},t) >}{< n(-\boldsymbol{k})n(\boldsymbol{k}) >} \tag{4}$$

with a lowest order solution of the form

$$G^{(0)}(\boldsymbol{k},t) = \exp(-D_0 k^2 t). \tag{5}$$

Show that a mode coupling analysis of (1) to leading order gives rise to the result

$$\begin{aligned} G(\boldsymbol{k},t) \quad = \quad & G^{(0)}(\boldsymbol{k},t) + \int_0^t d\,t_1 \int_{t_1}^t d\,t_2\, G^{(0)}(\boldsymbol{k},t_1) \frac{1}{V} \sum_{\boldsymbol{q}} G(\boldsymbol{k}-\boldsymbol{q}, t_2 - t_1) \\ & G(\boldsymbol{k}, t-t_2) \left\langle \frac{|\boldsymbol{k}\cdot\delta\mathsf{K}(\boldsymbol{q}-\boldsymbol{k})\cdot(\boldsymbol{q}-\boldsymbol{k})|}{n_0} \right\rangle_{sp}^2 , \end{aligned} \tag{6}$$

with $\delta\mathsf{K}(\boldsymbol{k})$ the Fourier transform of $\delta\mathsf{K}(\boldsymbol{r})$ and $n_0 =< n^{eq}(\boldsymbol{r}) >_{sp}$.
(Hint: show that the third term on the right hand side of (3) only gives corrections of order k^2 to this.) Derive from this that the long-time behavior of the velocity autocorrelation function to a good approximation is given by

$$< \boldsymbol{v}(0)\cdot\boldsymbol{v}(t) > \quad = \quad -\frac{A}{V}\sum_{\boldsymbol{q}} q^2 \exp(-D_0 q^2 t) \approx -\frac{A}{4\sqrt{\pi(D_0 t)^{d+2}}} \tag{7}$$

with

$$A \quad = \quad \frac{< \delta\mathsf{K}(\boldsymbol{k}=0){:}\delta\mathsf{K}(\boldsymbol{k}=0) >_{sp}}{d n_0^2}. \tag{8}$$

Problem 26. Random walk on a disordered chain

(see: HvB, Rev. Mod. Phys. **54**, 195 (1982))

The simplest example where the results of the previous problem can be applied is that of a one-dimensional random walk on a set of points that are distributed randomly. Suppose these points are located at positions $\cdots, x_{-1}x_0, x_1, x_2, \cdots$, with $\xi_n \equiv x_n - x_{n-1} > 0$ a set of independent identically distributed random variables, with mean a and variance Δ. A tracer particle makes a continuous time random walk with average jump frequency ν on these points, as defined in problem 16 (without noticing the differences in distances between neighboring points).

a) Show that the mean square displacement of the tracer particle for long times satisfies

$$< [x(t) - x(0)]^2 >= 2\nu t a^2 + \sqrt{\frac{2\nu t}{\pi}}\Delta \tag{9}$$

and derive the long-time behavior of the velocity autocorrelation function from this. Hint: use either the recursion relation $2nI_n(x) = x[I_{n-1}(x) -$

$I_{n+1}(x)]$ or the gaussian behavior as function of n for large x of the function $\exp(-x)I_n(x)$:

$$\exp(-x)I_n(x) \approx \frac{1}{\sqrt{2\pi x}} \exp -\frac{n^2}{2x}$$

b) In this one-dimensional case $K(x)$ is defined through the relationship

$$j(x) = -K(x)\partial/\partial x\,[n(x)/n_0].$$

Therefore, for $x_{n-1} < x < x_n$ one has $K(x)/n_0 = \nu\xi(n)/2$. Now consider a system with periodic boundary conditions with N sites. The allowed k-values are $k_i = 2\pi n_i/L$ with L the length of the system. Show that for small k_1 one has the identity

$$\frac{< \delta K(k_1)\delta K(k_2) >}{n_0^2} = \delta_{n_1 n_2}\frac{\nu^2}{4}L\Delta. \tag{10}$$

Why does $L\delta_{n_1 n_2}$ reduce to $2\pi\delta(k_1 - k_2)$ in the continuum limit, $L \to \infty$?

c) Derive the long time behavior of the velocity autocorrelation function from the mode coupling equations (7) and (8) and compare with the result obtained in a).