Homework No.6, 550.695, Due April 16, 2009.

1. This problem discusses a useful exact solution of the Liouville equation starting from a local-equilibrium distribution.

(a) Consider a classical molecular dynamics system of N particles in d dimensions that has M local conservation laws of the form

$$\partial_t \widetilde{n}_m(\mathbf{x},t) + \boldsymbol{\nabla}\boldsymbol{\cdot}\widetilde{\mathbf{j}}_m(\mathbf{x},t) = 0, \quad m = 1,...,M.$$

For example, these include mass, momentum, energy and possibly others. A *local equilibrium distribution* for such a system has density of the form

$$\rho_0(\boldsymbol{\omega}) = \frac{1}{Z}\exp\left(-\sum_{m=1}^{M}\int d^dx\, \lambda_m(\mathbf{x})\widetilde{n}_m(\mathbf{x};\boldsymbol{\omega})\right).$$

Here $\boldsymbol{\omega} = (\mathbf{r}_1, \mathbf{p}_1, ..., \mathbf{r}_N, \mathbf{p}_N)$ is a point in the N-particle phase space and the dependence of $\widetilde{n}_m(\mathbf{x})$ on $\boldsymbol{\omega}$ has been made explicit. The density is with respect to the Liouville measure $d^{2Nd}\omega = \prod_{n=1}^{N} d^dr_n d^dp_n$ and the fields $\lambda_m(\mathbf{x}),\ m = 1,...,M$ are a set of local (spatially-dependent) thermodynamic potentials. Show that the exact solution of the Liouville equation with initial condition $\rho_0(\boldsymbol{\omega})$ at time $t = 0$ is

$$\rho(\boldsymbol{\omega},t) = \frac{1}{Z}\exp\left(-\sum_{m=1}^{M}\int d^dx\, \lambda_m(\mathbf{x})\widetilde{n}_m(\mathbf{x},-t;\boldsymbol{\omega})\right). \qquad (*)$$

Here $\widetilde{n}_m(\mathbf{x},t;\boldsymbol{\omega}) = \widetilde{n}_m(\mathbf{x};\boldsymbol{\omega}(t))$ and $\boldsymbol{\omega}(t)$ is the solution of the MD equations with initial condition $\boldsymbol{\omega}$ at time $t = 0$.

(b) Show that (*) can be rewritten using the fundamental theorem of calculus as

$$\begin{aligned}\rho(t) = \tfrac{1}{Z}\exp\Big(&-\textstyle\sum_{m=1}^{M}\int d^dx\, \lambda_m(\mathbf{x},t)\widetilde{n}_m(\mathbf{x}) \\ &+ \textstyle\sum_{m=1}^{M}\int_{-t}^{0} ds \int d^dx\, [\partial_t\lambda_m(\mathbf{x},t+s)\widetilde{n}_m(\mathbf{x},s) + \boldsymbol{\nabla}\lambda_m(\mathbf{x},t+s)\boldsymbol{\cdot}\widetilde{\mathbf{j}}_m(\mathbf{x},s)]\Big)\end{aligned} \qquad (**)$$

where $\lambda_m(\mathbf{x},t)$ are *any* smooth fields such that $\lambda_m(\mathbf{x},0) = \lambda_m(\mathbf{x})$ for $m = 1,...,M$.

Remark: If the potentials $\lambda_m(\mathbf{x},t)$ are chosen to correspond to the solution of the Euler hydrodynamic equation, then the time-integral term in (**) can be shown to represent a small correction $\propto$ (Knudsen number). This exact *Zubarev-McClennan solution* of the Liouville equation can be used to derive the Navier-Stokes hydrodynamic equations and the Green-Kubo formulas for the transport coefficients.

2. This problem discusses the relations between the Ito and Stratonovich definitions of stochastic differentials.

(a) Using the lecture results, show that the *Ito* stochastic differential equation

$$d\widetilde{X}_i = f_i(\widetilde{\mathbf{X}}, t)dt + g_i^a(\widetilde{\mathbf{X}}, t)dW_a(t)$$

is equivalent to the *Stratonovich* stochastic differential equation

$$d\widetilde{X}_i = \mathring{f}_i(\widetilde{\mathbf{X}}, t)dt + g_i^a(\widetilde{X}, t) \circ dW_a(t),$$

with

$$\mathring{f}_i(\widetilde{\mathbf{X}}, t) = f_i(\widetilde{\mathbf{X}}, t) - \frac{1}{2} g_k^a(\widetilde{\mathbf{X}}, t)\partial_k g_i^a(\widetilde{\mathbf{X}}, t).$$

(b) Define a new random process by

$$\widetilde{Y}(t) = \varphi(\widetilde{\mathbf{X}}(t), t)$$

for a smooth function $\varphi(\mathbf{x}, t)$. Use the *chain rule* for the Stratonovich differential

$$d\widetilde{Y}(t) = \partial_t\varphi(\widetilde{\mathbf{X}}(t), t)dt + \partial_i\varphi(\widetilde{\mathbf{X}}(t), t) \circ d\widetilde{X}_i(t)$$

together with part (a) to derive the *Ito formula*

$$d\widetilde{Y}(t) = \partial_t\varphi(\widetilde{\mathbf{X}}, t)dt + \partial_i\varphi(\widetilde{\mathbf{X}}, t)d\widetilde{X}_i(t) + \frac{1}{2} D_{ij}(\widetilde{\mathbf{X}}, t)\partial_i\partial_j\varphi(\widetilde{\mathbf{X}}, t)dt,$$

where

$$D_{ij}(\mathbf{x}, t) = g_i^a(\mathbf{x}, t)g_j^a(\mathbf{x}, t)$$

is the diffusion tensor.

Hint: Rewrite the chain rule for the Stratonovich equation as

$$d\widetilde{Y}(t) = \left[\partial_t\varphi(\widetilde{\mathbf{X}}(t), t) + \partial_i\varphi(\widetilde{\mathbf{X}}(t), t)\mathring{f}_i(\widetilde{\mathbf{X}}, t)\right] dt + \partial_i\varphi(\widetilde{\mathbf{X}}(t), t)g_i^a(\widetilde{X}, t) \circ dW_a(t)$$

and then derive the equivalent Ito equation.

3. This problem discusses the backward evolution operator for the stochastically-forced Navier-Stokes dynamics:

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} = -\boldsymbol{\nabla} p + \nu \triangle \mathbf{u} + \mathbf{f}_B,$$

where $\mathbf{f}_B$ is a Gaussian random field with mean zero and covariance

$$\langle f_{B\,i}(\mathbf{x},t) f_{B\,j}(\mathbf{x}',t')\rangle = B_{ij}(\mathbf{x},\mathbf{x}')\delta(t-t').$$

Then, for any smooth functional $A[\mathbf{u}]$ of the velocity field, the backward operator is

$$(\mathcal{L}^* A)[\mathbf{u}] = \int d^d x\, F_i[\mathbf{u};\mathbf{x}] \frac{\delta A}{\delta u_i(\mathbf{x})}[\mathbf{u}] + \frac{1}{2}\int d^d x \int d^d x'\, B_{ij}(\mathbf{x},\mathbf{x}') \frac{\delta^2 A}{\delta u_i(\mathbf{x})\delta u_j(\mathbf{x}')}[\mathbf{u}],$$

where $\mathbf{F}[\mathbf{u}] = -(\mathbf{u} \cdot \boldsymbol{\nabla})\mathbf{u} - \boldsymbol{\nabla} p + \nu \triangle \mathbf{u}$.

(a) For the kinetic energy

$$E[\mathbf{u}] = \frac{1}{2}\int d^d x\, |\mathbf{u}(\mathbf{x})|^2,$$

show that

$$(\mathcal{L}^* E)[\mathbf{u}] = -\nu \int d^d x\, |\boldsymbol{\nabla} \mathbf{u}(\mathbf{x})|^2 + \frac{1}{2}\sum_i \int d^d x\, B_{ii}(\mathbf{x},\mathbf{x}).$$

Assume either a periodic domain or “stick” ($\mathbf{u} = \mathbf{0}$) boundary conditions at the surface in a wall-bounded domain.

Hint: Show that $(\delta/\delta u_i(\mathbf{x}))E[\mathbf{u}] = u_i(\mathbf{x})$.

(b) Use the result in (a) to derive the following *energy balance equation*

$$\nu \int d^d x\, \langle |\boldsymbol{\nabla} \mathbf{u}(\mathbf{x})|^2 \rangle_* = \frac{1}{2}\sum_i \int d^d x\, B_{ii}(\mathbf{x},\mathbf{x}), \qquad \text{(B)}$$

where the average $\langle \cdot \rangle_*$ is with respect to the stationary density $\rho_*[\mathbf{u}]$ that satisfies

$$\mathcal{L}\rho_*[\mathbf{u}] = 0.$$

Explain the physical meaning of the lefthand and righthand sides of equation (B).