# Homework #6 – Solutions

**Problem 1**. (a) We shall give two independent solutions of Part (a).

**SOLUTION I**. The first solution uses the formula from the classnotes:

$$\rho(\omega,t) = \rho_0(\Omega(0;\omega,t))\left|\frac{\partial\Omega}{\partial\omega}(0;\omega,t)\right|$$

where $\omega(t) = \Omega(t;\omega,t_0)$ is the solution of the MD equations of motion starting at $\omega$ at time $t_0$. We shall apply this formula twice.

We first use the formula for the initial measure $\rho_0(\omega) \equiv 1$. It was proved in class that this measure is invariant in time, as a consequence of the Liouville theorem

$$\hat{\mathcal{L}}\rho_0 \equiv 0 \implies \rho(\omega,t) \equiv 1 \quad \forall t$$

Hence, the above formula implies that the determinant is unity:

$$1 = 1\cdot\left|\frac{\partial\Omega}{\partial\omega}(0;\omega,t)\right| \quad \text{or} \quad \left|\frac{\partial\Omega}{\partial\omega}(0;\omega,t)\right| = 1$$

We next use the formula for the initial measure

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

in the problem statement. Thus,

$$\rho(\boldsymbol{\omega},t) = \rho_0\left(\boldsymbol{\Omega}(0;\boldsymbol{\omega},t)\right)\cdot 1 = \rho_0\left(\boldsymbol{\Omega}(0;\boldsymbol{\omega},t)\right).$$

We next note that the dynamics is autonomous, so that there is no absolute origin of time. Thus,

$$\boldsymbol{\Omega}(0;\boldsymbol{\omega},t) = \boldsymbol{\Omega}(-t;\boldsymbol{\omega},0) = \boldsymbol{\omega}(-t).$$

We therefore obtain the stated result:

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

<u>Remark:</u> It is also possible to give a direct proof of the result for the determinant

$$\det\left(\frac{\partial\boldsymbol{\Omega}}{\partial\boldsymbol{\omega}}(t;\boldsymbol{\omega},0)\right) = 1.$$

The starting point is the equation of motion

$$\frac{d}{dt}\boldsymbol{\Omega}(t) = \mathbf{f}(\boldsymbol{\Omega}(t))$$

which implies by the chain rule

$$\frac{d}{dt}\frac{\partial\boldsymbol{\Omega}(t)}{\partial\boldsymbol{\omega}} = \frac{\partial\mathbf{f}}{\partial\boldsymbol{\Omega}}(\boldsymbol{\Omega}(t))\,\frac{\partial\boldsymbol{\Omega}(t)}{\partial\boldsymbol{\omega}}.$$

We then use the well-known identity

$$\ln\det\left(\frac{\partial\boldsymbol{\Omega}(t)}{\partial\boldsymbol{\omega}}\right) = \mathrm{tr}\ln\left(\frac{\partial\boldsymbol{\Omega}(t)}{\partial\boldsymbol{\omega}}\right)$$

to obtain

$$\frac{d}{dt} \ln \det \left( \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right) = \frac{d}{dt} \operatorname{tr} \ln \left( \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right)$$

$$= \operatorname{tr} \left( \left( \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right)^{-1} \frac{\partial \dot{\boldsymbol{\Omega}}(t)}{\partial \boldsymbol{\omega}} \right)$$

$$= \operatorname{tr} \left( \left( \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right)^{-1} \cdot \frac{\partial \mathbf{f}}{\partial \boldsymbol{\Omega}} (\boldsymbol{\Omega}(t)) \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right)$$

$$= \operatorname{tr} \left( \frac{\partial \mathbf{f}}{\partial \boldsymbol{\Omega}} (\boldsymbol{\Omega}(t)) \right)$$ by cyclicity of the trace

$$= (\nabla_{\boldsymbol{\Omega}} \cdot \mathbf{f})(\boldsymbol{\Omega}(t))$$

$$= 0,$$

since $(\nabla_{\boldsymbol{\omega}} \cdot \mathbf{f})(\boldsymbol{\omega}) = 0$ for a Hamiltonian vector field $\mathbf{f}$.

On the other hand, since

$$\boldsymbol{\Omega}(0; \boldsymbol{\omega}, 0) = \boldsymbol{\omega},$$

$$\frac{\partial \boldsymbol{\Omega}(0)}{\partial \boldsymbol{\omega}} = I \implies \ln \det \left( \frac{\partial \boldsymbol{\Omega}(0)}{\partial \boldsymbol{\omega}} \right) = 0.$$

Because this quantity is time-independent

$$\ln \det \left( \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right) = 0 \quad \forall t$$

$$\implies \det \left( \frac{\partial \boldsymbol{\Omega}(t)}{\partial \boldsymbol{\omega}} \right) = 1 \quad \forall t.$$

SOLUTION II. For any dynamical system

$$\frac{d}{dt}\tilde{n}_m(\mathbf{x},t) = \hat{\mathcal{L}}^* \tilde{n}_m(\mathbf{x},t).$$

For a system that satisfies the Liouville theorem, such as the Hamiltonian MD system

$$\hat{\mathcal{L}}^* = -\hat{\mathcal{L}}.$$

Thus,

$$\frac{d}{dt}\tilde{n}_m(\mathbf{x},t) = -\hat{\mathcal{L}}\,\tilde{n}_m(\mathbf{x},t)$$

and, by the chain rule,

$$\frac{d}{dt}\tilde{n}_m(\mathbf{x},-t) = \hat{\mathcal{L}}\,\tilde{n}_m(\mathbf{x},-t),$$

which thus satisfies the forward (Liouville) equation. Integrating over $\mathbf{x}$ and summing over $m$ gives another solution

$$\frac{d}{dt}\tilde{\mathcal{E}}(t) = \hat{\mathcal{L}}\,\tilde{\mathcal{E}}(t) \qquad (*)$$

with

$$\tilde{\mathcal{E}}(t) = \sum_{m=1}^{N}\int d^dx\,\lambda_m(\mathbf{x})\,\tilde{n}_m(\mathbf{x},-t).$$

Since $\frac{d}{dt}$ and $\hat{\mathcal{L}} = \mathbf{f}(\boldsymbol{\omega})\cdot\nabla_{\boldsymbol{\omega}}$ are both 1st-order linear differential operators, we can multiply both sides of $(*)$ by $\varphi'(\tilde{\mathcal{E}}(t))$ for an arbitrary smooth function $\varphi$ to obtain

$$\varphi'(\tilde{\Sigma}(t))\,\frac{d\tilde{\Sigma}(t)}{dt} = \varphi'(\tilde{\Sigma}(t))\,\hat{\mathcal{L}}\tilde{\Sigma}(t)$$

or

$$\frac{d}{dt}\varphi(\tilde{\Sigma}(t)) = \hat{\mathcal{L}}\varphi(\tilde{\Sigma}(t)).$$

Thus, any nonlinear function $\varphi$ of a solution of the Liouville equation is another solution! If we use $\varphi(\Sigma) = \exp\Sigma$, we obtain that

$$\frac{1}{Z}\exp(\tilde{\Sigma}(t)) = \frac{1}{Z}\exp\left(-\sum_{m=1}^{M}\int d^dx\,\lambda_m(\mathbf{x})\,\tilde{n}_m(\mathbf{x},-t)\right)$$

is a solution of the Liouville equation. Since it obviously coincides with $\rho_0(\omega)$ in the problem statement at $t=0$, we obtain that

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

(b) By the fundamental theorem of calculus

$$\int_{-t}^{0} ds\,\frac{d}{ds}\left(\sum_m\int d^dx\,\lambda_m(\mathbf{x},t+s)\,\tilde{n}_m(\mathbf{x},s)\right)$$

$$= \sum_m\int d^dx\,\lambda_m(\mathbf{x},t)\,\tilde{n}_m(\mathbf{x}) - \sum_m\int d^dx\,\lambda_m(\mathbf{x})\,\tilde{n}_m(\mathbf{x},-t),$$

for any smooth fields that satisfy $\lambda_m(\mathbf{x},0) = \lambda_m(\mathbf{x})$, $m=1,\ldots,M$, By the product rule,

$$\frac{d}{ds}\left( \sum_m \int d^d x \; \lambda_m(x, t+s)\, \tilde{n}_m(x,s) \right)$$

$$= \sum_m \int d^d x \left( \dot{\lambda}_m(x, t+s)\, \tilde{n}_m(x,s) + \lambda_m(x,t+s)\, \dot{\tilde{n}}_m(x,s) \right).$$

Employing the conservation law

$$\dot{\tilde{n}}_m(x,s) = -\nabla\cdot \tilde{J}_m(x,s)$$

and integrating by parts in $x$ gives

$$\frac{d}{ds}\left( \sum_m \int d^d x \; \lambda_m(x, t+s)\, \tilde{n}_m(x,s) \right)$$

$$= \sum_m \int d^d x \left( \dot{\lambda}_m(x, t+s)\, \tilde{n}_m(x,s) + \nabla\lambda_m(x,t+s)\cdot \tilde{J}_m(x,s) \right).$$

Finally, we obtain

$$-\sum_m \int d^d x \; \lambda_m(x)\, \tilde{n}_m(x,-t)$$

$$= -\sum_m \int d^d x \; \lambda_m(x,t)\, \tilde{n}_m(x)$$

$$+ \sum_m \int_{-t}^{0} ds \int d^d x \left( \dot{\lambda}_m(x,t+s)\, \tilde{n}_m(x,s) + \nabla\lambda_m(x,t+s)\cdot \tilde{J}_m(x,s) \right)$$

from which the problem statement immediately follows.

Remarks: The formula derived in this problem is very useful, since it represents the exact solution of the Liouville equation for an initial local equilibrium distribution

$$\rho_0(\omega) = \frac{1}{Z} \exp\left( -\sum_m \int d^dx \, \lambda_m(\mathbf{x}) \, \hat{n}_m(\mathbf{x}) \right)$$

as another local equilibrium

$$\rho_t(\omega) = \frac{1}{Z} \exp\left( -\sum_m \int d^dx \, \lambda_m(\mathbf{x},t) \, \hat{n}_m(\mathbf{x}) \right)$$

plus a correction term from the time-integral. This correct may be shown to be small when $\lambda_m(\mathbf{x},t)$ is chosen to satisfy the ideal Euler equations (or a suitable generalization). This approach allows one to derive the Navier-Stokes correction to ideal hydrodynamics and the Green-Kubo formulas for the transport coefficients. See

D. N. Zubarev, Dokl. Akad. Nauk. SSSR 140 92 (1961);
J. A. McLennan, Jr. Phys. Fluids 4 1319 (1961)

and the excellent textbook

J. A. McLennan, Jr. Introduction to Nonequilibrium Statistical Mechanics (Prentice-Hall, 1989)

free to download at

http://www.lulu.com/content/374052

Problem 2. (a) By employing our definition of the Ito differential from class, a

$$\phi(\tilde{\mathbf{x}}(t))\, d\tilde{W}_a(t) = \phi(\tilde{\mathbf{x}}(t)) \circ d\tilde{W}_a(t) - \frac{1}{2} g_k^a(\tilde{\mathbf{x}},t)\, \partial_k \varphi(\tilde{\mathbf{x}}(t))\, dt,$$

we can write the Ito equation

$$d\tilde{x}_i = f_i(\tilde{\mathbf{x}},t)\, dt + g_i^a(\tilde{\mathbf{x}},t)\, d\tilde{W}_a(t)$$

as

$$d\tilde{x}_i = \Big[ \overbrace{f_i(\tilde{\mathbf{x}},t) - \frac{1}{2} g_k^a(\tilde{\mathbf{x}},t)\, \partial_k g_i^a(\tilde{\mathbf{x}},t)}^{\mathring{f}_i(\tilde{\mathbf{x}},t)} \Big] dt$$

$$+ g_i^a(\tilde{\mathbf{x}},t) \circ d\tilde{W}_a(t),$$

which is the equivalent Stratonovich equation.

(b) Defining

$$\tilde{\varphi}(t) = \varphi(\tilde{\mathbf{x}}(t), t),$$

we now use the standard chain rule for the Stratonovich differential

$$d\tilde{\varphi}(t) = \partial_t \varphi(\tilde{\mathbf{x}}(t), t)\, dt + \partial_i \varphi(\tilde{\mathbf{x}}(t), t) \circ d\tilde{x}_i(t)$$

to obtain

$$d\tilde{\varphi}(t) = \left( \partial_t + \mathring{f}_i(\tilde{\mathbf{x}},t)\, \partial_i \right) \varphi(\tilde{\mathbf{x}},t)\, dt$$

$$+ \partial_i \varphi(\tilde{\mathbf{x}},t)\, g_i^a(\tilde{\mathbf{x}},t) \circ d\tilde{W}_a(t).$$

The final Stratonovich differential can, in turn, be transformed to an Ito differential, as

$$
\begin{aligned}
&\partial_i \varphi(\hat{\mathbf{x}},t)\, g_i^a(\hat{\mathbf{x}},t) \circ d\tilde{W}_a(t) \\
&\quad = \partial_i \varphi(\tilde{\mathbf{x}},t)\, g_i^a(\tilde{\mathbf{x}},t)\, d\tilde{W}_a(t) \\
&\qquad + \frac{1}{2} \partial_k \Big[ \partial_i \varphi(\mathbf{x},t)\, g_i^a(\mathbf{x},t) \Big]_{\mathbf{x}=\tilde{\mathbf{x}}(t)} g_k^a(\tilde{\mathbf{x}},t)\, dt \\
&\quad = \partial_i \varphi(\tilde{\mathbf{x}},t)\, g_i^a(\tilde{\mathbf{x}},t)\, d\tilde{W}_a(t) \\
&\qquad + \frac{1}{2} \partial_i \partial_k \varphi(\tilde{\mathbf{x}},t) \underbrace{g_i^a(\tilde{\mathbf{x}},t)\, g_k^a(\tilde{\mathbf{x}},t)}_{D_{ik}(\tilde{\mathbf{x}},t)}\, dt \\
&\qquad + \frac{1}{2} \partial_i \varphi(\tilde{\mathbf{x}},t)\, g_k^a(\tilde{\mathbf{x}},t)\, \partial_k g_i^a(\tilde{\mathbf{x}},t)\, dt .
\end{aligned}
$$

Substituting into the previous result for $d\tilde{\varphi}(t)$ gives, by cancellation of the last term above with the opposite term in $\mathring{f}(\hat{\mathbf{x}},t)$,

$$
\begin{aligned}
d\tilde{\varphi}(t) &= \partial_t \varphi(\tilde{\mathbf{x}},t)\, dt \\
&\quad + \Big[ f_i(\tilde{\mathbf{x}},t)\, dt + g_i^a(\tilde{\mathbf{x}},t)\, d\tilde{W}_a(t) \Big] \partial_i \varphi(\tilde{\mathbf{x}},t) \quad \Big\}\ d\tilde{X}_i(t)\, \partial_i \varphi(\tilde{\mathbf{X}}(t)) \\
&\quad + \frac{1}{2} D_{ij}(\tilde{\mathbf{x}},t)\, \partial_i \partial_j \varphi(\tilde{\mathbf{x}},t)\, dt .
\end{aligned}
$$

Problem 3. (a) Using the usual rules of functional differentiation, we obtain for

$$E = \frac{1}{2}\int d^d z\, |\mathbf{u}(\mathbf{z})|^2 = \frac{1}{2}\sum_k \int d^d z\, |u_k(\mathbf{z})|^2$$

that

$$\frac{\delta E}{\delta u_i(\mathbf{x})} = \int d^d z\, u_k(\mathbf{z})\, \delta_{ik}\, \delta^d(\mathbf{x}-\mathbf{z}) = u_i(\mathbf{x})$$

and

$$\frac{\delta^2 E}{\delta u_i(\mathbf{x})\delta u_j(\mathbf{y})} = \frac{\delta u_i(\mathbf{x})}{\delta u_j(\mathbf{y})} = \delta_{ij}\, \delta^d(\mathbf{x}-\mathbf{y}).$$

Thus,

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

$$= \int d^d x\, u_i(\mathbf{x})\, F_i[\mathbf{u};\mathbf{x}] + \frac{1}{2}\int d^d x\int d^d y\, \delta_{ij}\,\delta^d(\mathbf{x}-\mathbf{y})\, B_{ij}(\mathbf{x},\mathbf{y})$$

$$= \int d^d x\, u_i(\mathbf{x})\, F_i[\mathbf{u};\mathbf{x}] + \frac{1}{2}\int d^d x\, B_{ii}(\mathbf{x},\mathbf{x}).$$

We now use incompressibility $\nabla \cdot \mathbf{u} = 0$ and

$$F_i[\mathbf{u};\mathbf{x}] = -(\mathbf{u}\cdot\nabla)\mathbf{u} - \nabla p + \nu \Delta \mathbf{u}$$

to write

$$u_i(\mathbf{x}) F_i[\mathbf{u};\mathbf{x}] = -\nabla \cdot \left[ \frac{1}{2}|\mathbf{u}|^2 \mathbf{u} + p\mathbf{u} - \nu \nabla\left(\frac{1}{2}|\mathbf{u}|^2\right)\right] - \nu |\nabla \mathbf{u}|^2 .$$

The gradient term vanishes in the integral over space, to give

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

(b) Since $\langle \hat{\mathcal{L}}^* E \rangle_* = 0$, we obtain

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

The LHS represents the energy dissipation by viscosity, while the RHS represents the energy input by the stochastic stirring force.