Statistical mechanics

Problem sheet 0.

1. A number of particles with positions $\mathbf{r}_i$ are subjected to internal forces $\mathbf{F}_{ij}$, where $\mathbf{F}_{ij}$ is the force exerted by particle j on particle i.

   What is meant by a virtual displacement? And what does it mean to say that a virtual displacement does no virtual work?

   Show that if the forces have the form

$$\mathbf{F}_{ij} = f(r_{ij})\mathbf{r}_{ij},$$

   where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and if the particles are connected as a rigid body, the virtual work is zero.

2. Use the chain rule to show that for a change of variable $\mathbf{r} = \mathbf{r}(\mathbf{q}, t)$,

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial \mathbf{r}_i}{\partial q_j}\right) &= \frac{\partial \mathbf{v}_i}{\partial q_j}, \\ \frac{\partial \mathbf{v}_i}{\partial \dot{q}_j} &= \frac{\partial \mathbf{r}_i}{\partial q_j}, \end{aligned}$$

   where $\mathbf{v}_i = \dot{\mathbf{r}}_i$, and deduce that Newton's equations can be written in the form

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} = Q_j,$$

   where you should define the generalised forces Q_j and the kinetic energy T.

   Hence deduce the form of Lagrange's and Hamilton's equations.

   Show that Lagrange's equations also follow from a variational principle for the *action*

$$I = \int_{t_1}^{t_2} L\, dt,$$

   where t_1 and t_2 are fixed, as are the values of q_i at these times. Why do $\dot{q}_i$ not have to be specified at the endpoints of the interval?

3. Find the characteristic functions $\phi(t)$ for the following distributions:

   Normal, $f(x) = \dfrac{1}{\sigma\sqrt{2\pi}} \exp\left[-\dfrac{(x-\mu)^2}{2\sigma^2}\right]$;

   Gamma, $f(x) = \dfrac{\lambda^s x^{s-1} e^{-\lambda x}}{\Gamma(s)}$ on $(0, \infty)$;

Cauchy, $f(x) = \dfrac{1}{\pi(1+x^2)}$.

What are the mean and variance of each distribution?

4. Let $\{X_i\}$ be a series of independent trials from a distribution of mean μ and variance σ^2, and let $S_n = \sum_1^n X_i$. By consideration of appropriate characteristic functions, show that

$$S_n \sim N(\mu n, \sigma^2 n) \quad \text{as} \quad n \to \infty,$$

and deduce the law of large numbers,

$$\frac{S_n}{n} \xrightarrow{D} \delta(x-\mu) \quad \text{as} \quad n \to \infty.$$

Explain how this result can be used to provide a practical tool for the estimation of probability of an event $a \in E$.

5. Show from first principles that if $dV = dx_1\, dx_2\, dx_3$ is a material volume element, then

$$\frac{d(dV)}{dt} = (\boldsymbol{\nabla}.\,\mathbf{u})\, dV,$$

where $\mathbf{u}$ is the velocity field. Show this in two ways: using Eulerian coordinates, and using Lagrangian coordinates.

By consideration of Newton's second law applied to an infinitesimal tetrahedron, explain why Newton's third law applies, and deduce that the surface force on a volume element can be written in the form $\boldsymbol{\sigma}.\mathbf{n}$.

Hence derive the Navier-Stokes equation in the form

$$\rho\frac{d\mathbf{u}}{dt} = \boldsymbol{\nabla}.\,\boldsymbol{\sigma}.$$

6. In cartesian coordinates, and using the summation convention, the term $\nabla^2\mathbf{u}$ is defined by

$$\nabla^2\mathbf{u} \equiv \mathbf{e}_i\frac{\partial^2 u_i}{\partial x_j \partial x_j},$$

where $\mathbf{e}_i$ is an orthonormal basis for $\mathbf{R}^3$. Use the definitions of

$$\boldsymbol{\nabla}\phi = \mathbf{e}_i\frac{\partial \phi}{\partial x_i},$$

$$\boldsymbol{\nabla}.\,\mathbf{a} = \frac{\partial a_k}{\partial x_k},$$

$$\nabla \times \mathbf{v} = \varepsilon_{ijk} \mathbf{e}_i \frac{\partial v_j}{\partial x_k},$$

where ε_{ijk} is the alternating tensor:

$$\varepsilon_{ijk} = \begin{cases} +1, & \{ijk\} = \{123\}, \{231\}, \{312\}, \\ -1, & \{ijk\} = \{132\}, \{213\}, \{321\}, \\ 0 & \text{otherwise}, \end{cases}$$

to show that

$$\nabla^2 \mathbf{u} \equiv \nabla(\nabla . \mathbf{u}) - \nabla \times \nabla \times \mathbf{u},$$

which thus provides a coordinate-free definition of this term.

Hint: the alternating tensor satisfies the relation

$$\varepsilon_{ijk}\varepsilon_{ipq} = \delta_{jp}\delta_{kq} - \delta_{jq}\delta_{kp}.$$

7. Suppose that a map $x \to f(x, \mu)$ has a fixed point x^*, and that the derivative $f'(x, 0) = -1$, so that the map has a period-doubling bifurcation at $\mu = 0$. By expanding in Taylor series in the vicinity of the bifurcation point, show in detail that a period-doubling bifurcation generates a single periodic orbit, and give a criterion for its stability in terms of the Schwarzian derivative at the fixed point,

$$Sf = \frac{f'''}{f'} - \frac{3}{2}\left(\frac{f''}{f'}\right)^2.$$

8. Draw a graph of $F(x) = 4x^3 - 3x$ on the interval $[-1, 1]$. Show that the map $x \to F(x)$ has three fixed points, and examine their stability. By using a suitable trigonometric transformation, show that the map is chaotic, and construct a suitable symbolic representation for orbits of F. [*Hint: write x as a ternary fraction*]. Use the symbolic representation of x to find how many fixed points and period two cycles there are, and verify your answer using the map.