Statistical Physics: Tutorial 4

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Dynamics & Time's Arrow

A: Core problems

1. **Classical reversibility**

   Consider Newtonian dynamics of a particle in the form

   $$\frac{d^2\underline{x}}{dt^2} = \frac{1}{m}\,\underline{F}$$

   and apply time reversal: $t' = -t$. Firstly assume that the applied force derives from the gradient of a potential: $\underline{F} = -\underline{\nabla}\,\phi$: show that the time-reversed equation of motion is identical in form to the initial equation. Then assume that the force is the electromagnetic Lorentz force:

   $$\underline{F} = q(\underline{E} + \underline{v}\wedge\underline{B});$$

   how is the force and the resulting equation of motion affected by time reversal in this case?

2. **Quantum reversibility**

   Consider Schrödinger's equation in the form

   $$\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}.$$

   If a solution of this equation is $\psi = \phi(\mathbf{x}, t)$, show that the time-reversed solution $\psi_1 = \phi(\mathbf{x}, -t)$ does not solve the equation, but that $\psi_2 = \phi^*(\mathbf{x}, -t)$ does give a solution. The momentum operator is $\mathbf{p} = (\hbar/i)\nabla$; show that the time-reversed solution ψ_2 reverses all momentum eigenvalues.

3. **Concavity of entropy** Show that the function $s(x) = -kx\ln x$ is concave i.e.

   $$\frac{\mathrm{d}^2 s}{\mathrm{d}x^2} \leq 0.$$

   Show by a sketch that this implies

   $$s(\alpha x_1 + (1-\alpha)x_2) \geq \alpha s(x_1) + (1-\alpha)s(x_2),$$

   where $0 \leq \alpha \leq 1$. Hence show that $s(\overline{x}) \geq \overline{s(x)}$.

4. **Density matrix**

   (a) The density matrix is defined as $\rho = \sum_i p_i|i\rangle\langle i|$, where p_i is the probability of the system being found in eigenstate $|i\rangle$. Prove that the expectation value of an operator A is given by a trace:

   $$\langle A\rangle = \sum_i p_i\langle i|A|i\rangle = \mathrm{Tr}[A\rho] = \mathrm{Tr}[\rho A]\,.$$

(b) Consider a particle of spin 1/2, with eigenstates of z spin $|\uparrow\rangle$ and $|\downarrow\rangle$. The particle is placed in an eigenstate of spin along a direction specified by polar coordinates θ and ϕ, which is $|\psi\rangle = \cos(\theta/2)\exp(-i\phi/2)|\uparrow\rangle + \sin(\theta/2)\exp(i\phi/2)|\downarrow\rangle$: show that the density matrix is

$$\rho = \begin{pmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2)\exp(-i\phi) \\ \cos(\theta/2)\sin(\theta/2)\exp(i\phi) & \sin^2(\theta/2) \end{pmatrix} .$$

The particle now interacts with the walls of a box so that it has no definite polarization. Show that averaging ρ over solid angle yields the mixed state $\rho = \mathrm{diag}(1/2, 1/2)$.

(c) The probability of measuring z spin up is $\mathrm{Tr}(\,|\uparrow\rangle\langle\uparrow|\,\rho)$. Show that this is 1/2 both for the unpolarized mixed state and for a pure state of x spin up.

B: Further problems

1. **Liouville's theorem and Gibbs entropy**

   (a) ρ is the probability density for a system in its $6N$-dimensional space and

   $$\underline{V} = (\dot{q}_1, \ldots, \dot{q}_{3N}, \dot{p}_1, \ldots, \dot{p}_{3N})$$

   is the phase-space velocity. Explain why probability conservation requires the general relation

   $$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot (\rho \underline{V}) = 0.$$

   (b) Use Hamilton's equations, $\dot{q} = \partial H/\partial p$, $\dot{p} = -\partial H/\partial q$, to prove that $\underline{\nabla} \cdot \underline{V}$ vanishes, so that

   $$\frac{\partial \rho}{\partial t} + \underline{V} \cdot \underline{\nabla} \rho = 0.$$

   Explain why this allows us to state that the phase-space probability fluid is incompressible.

   (c) Hence show by using the divergence theorem that the Gibbs entropy is a constant of the motion:

   $$\frac{\partial S}{\partial t} = -k \frac{\partial}{\partial t} \int \rho \ln \rho \; d\Gamma = 0.$$

2. **Liouville's equation for a Hamiltonian system**

   (a) If $u(q_i, p_i, t)$ is a function of the canonical variables of a Hamiltonian system, show that its total time derivative,

   $$\frac{du}{dt} = \frac{\partial u}{\partial t} + \sum_i \left(\frac{\partial q_i}{\partial t} \frac{\partial u}{\partial q_i} + \frac{\partial p_i}{\partial t} \frac{\partial u}{\partial p_i} \right),$$

   is

   $$\frac{du}{dt} = \frac{\partial u}{\partial t} + [u, H],$$

   where the Poisson bracket is defined by

   $$[F, G] = \sum_i \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} \right).$$

   What is the total time derivative of the Hamiltonian H ?

   (b) Show that Liouville's equation for the phase space density, ρ, may be written as

   $$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + [\rho, H] = 0.$$

   Show that two ways to have a stationary ensemble, i.e.

   $$\frac{\partial \rho}{\partial t} = 0 ,$$

   are $\rho =$ constant or $\rho = \rho(H)$. Can you relate these cases to familiar ensembles?