Problem 1. Phase-space and its characteristic flow

(a) If the number of particles per phase space volume (called the phase-space density)

$$f(t, q, p) = \frac{dN}{d^n q d^n p} \tag{1}$$

is conserved, then the phase-space density obeys a conservation law

$$\frac{\partial f}{\partial t} + \frac{\partial (f \dot{q}^i)}{\partial q^i} + \frac{\partial (f \dot{p}_i)}{\partial p_i} = 0\,. \tag{2}$$

This equation of motion is analogous to a compressible fluid, where the density $\rho(t, \boldsymbol{x})$ satisfies the continuity equation

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0\,, \tag{3}$$

with $\boldsymbol{v}(t, \boldsymbol{x})$ the velocity of the fluid. Eq. (2) does not require Hamilton's EOM, it just says that once a particle always a particle, regardless of the EOM.

(i) Show that if Hamilton's EOM are also satisfied *and* particle number is conserved, the Liouville equation (also called the free-streaming Boltzmann equation)

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial q^i}\dot{q}^i + \frac{\partial f}{\partial p_i}\dot{p}_i = 0\,, \tag{4}$$

is satisfied, and that this equation can be written as

$$\partial_t f + \{f, H\}_{p,q} = 0\,, \tag{5}$$

(ii) Eq. (4) is analogous to an incompressible fluid, where $\nabla \cdot \boldsymbol{v} = 0$, and thus we have from Eq. (3)

$$\partial_t \rho + \boldsymbol{v} \cdot \nabla \rho = 0\,. \tag{6}$$

What is the phase-space analog of the incompressibility constraint $\nabla \cdot \boldsymbol{v} = 0$?

(b) Eqs. (4) and (5) imply that $f(t, q, p)$ that f is constant along the flow lines. Heuristically, this means that we can find the solution to the equation Eq. (5) by tracing the trajectories backward in time to the initial time t_0 where the initial condition $f_0(q, p)$ is specified. This is known as the method of characteristics, and we will develop this method here, see also wikipedia.

(i) Show by direct substitution that for a free particle $H = P^2/2m$ the solution to

$$\frac{\partial f(t, Q, P)}{\partial t} + \{f, H\}_{P,Q} = 0 \tag{7}$$

is

$$f(t, Q, P) = f_0(Q - \frac{P}{m}t, P)\,. \tag{8}$$

where $f_0(q, p)$ is the initial condition at time $t = 0$. The somewhat confusing minus sign is just a reflection of the familiar fact that if I want to translate a function $F(x)$ forward by a distance $\Delta x = vt$, I want the new function $F(x - vt)$.

(ii) Show more generally that the characteristic solution to Eq. (7) is

$$f(t, Q, P) = f_0(q(Q, P; t, t_0),\, p(Q, P; t, t_0))\,, \tag{9}$$

where $f_0(q, p)$ is the initial condition at time $t = t_0$.
Hint: To prove Eq. (9), first show that q, p obey the EOM

$$\partial_t q(Q, P; t, t_0) = -\left(\frac{\partial q}{\partial Q}\frac{\partial H}{\partial P} - \frac{\partial q}{\partial P}\frac{\partial H}{\partial Q}\right) \equiv -\{q, H\}_{P,Q} \tag{10}$$

$$\partial_t p(Q, P; t, t_0) = -\left(\frac{\partial p}{\partial Q}\frac{\partial H}{\partial P} - \frac{\partial p}{\partial P}\frac{\partial H}{\partial Q}\right) \equiv -\{p, H\}_{P,Q} \tag{11}$$

and then prove Eq. (9).

The meaning of Eq. (9) is as follows (see Fig. 1) – start at time t_0 with coordinates $(\tilde{q}, \tilde{p})|_{t_0} = (q, p)$, and flow them forward in time to time t were the coordinates are now $(\tilde{q}, \tilde{p})|_t = (Q, P)$. This flow determines the map $(q, p) \to Q(q, p; t, t_0)$ and $(q, p) \to P(q, p; t, t_0)$. The inverse map is $q(Q, P; t, t_0)$ and $p(Q, P; t, t_0)$ which are specified in Eq. (9). Thus the characteristic solution can be loosely written

$$f(t, Q, P) = f_0(q, p)\,. \tag{12}$$

Alternatively, (q, p) in Eq. (9) are defined as follows: we start at time $t' = t$ with coordinates $(\tilde{q}, \tilde{p}) = (Q, P)$ and evolve $(\tilde{q}, \tilde{p})$ backwards in time t' with Hamilton's equation

$$\frac{d\tilde{q}(t')}{dt'} = \frac{\partial H(\tilde{q}, \tilde{p})}{\partial \tilde{p}}\,, \tag{13}$$

$$\frac{d\tilde{p}(t')}{dt'} = -\frac{\partial H(\tilde{q}, \tilde{p})}{\partial \tilde{q}}\,, \tag{14}$$

until $t' = t_0$. The traced curve for $t' < t$ is a function of Q, P, t, t'. This evolution determines the required map:

$$q(Q, P, t, t_0) = \tilde{q}(t')|_{t'=t_0} \tag{15}$$

$$p(Q, P, t, t_0) = \tilde{p}(t')|_{t'=t_0} \tag{16}$$

This “tracing backward” procedure is known the characteristic solution of the first order partial differential equation. The curves are known as characteristics. The same method can be used to solve any first order partial differential equation at least locally.

(c) The phase space density at the initial time $t = 0$ is

$$f(0, x, p) = \frac{1}{2\pi\Delta x_0 \Delta p_0} \exp\left[-\frac{x^2}{2\Delta x_0^2} - \frac{(p - P_0)^2}{2\Delta p_0^2}\right] \tag{17}$$

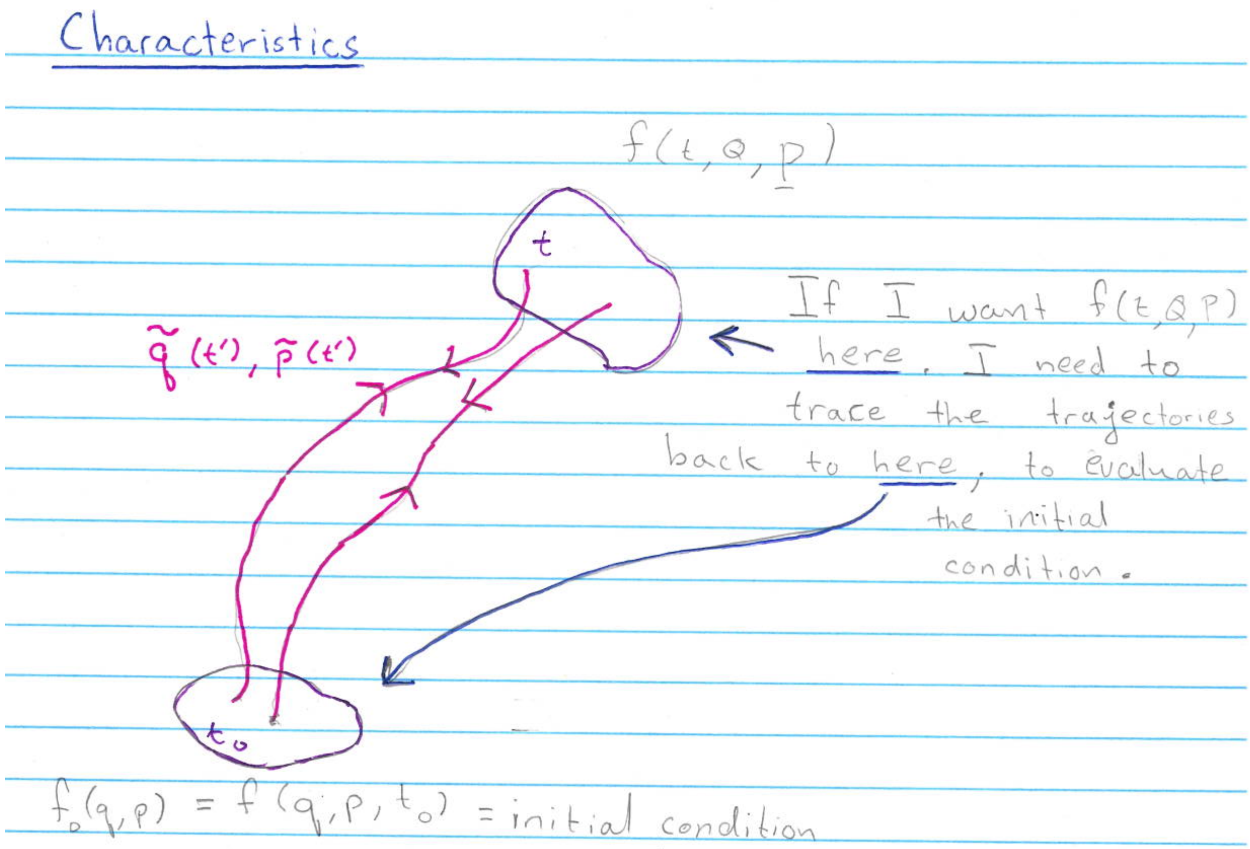


Figure 1: Characteristics of the Liouville equation .

(i) Determine the phase space distribution $f(t, x, p)$ at later time t for a group of free particles, i.e. $H(x, p) = p^2/2$.

(ii) Sketch contour in the phase-space (x, p) where $f(t, x, p)$ is $1/e$ of its maximum (with $e \simeq 2.718$), at time $t = 0$ and at a significantly later time.

For definiteness take units where $m = \Delta x_0 = \Delta p_0 = 1$ take $P_0 = 3\Delta p_0$.

(d) The phase space density at the initial time is

$$f(0, x, p) = \frac{1}{2\pi \Delta x_0 \Delta p_0} \exp\left[-\frac{(x - X_0)^2}{2\Delta x_0^2} - \frac{p^2}{2\Delta p_0^2} \right] \tag{18}$$

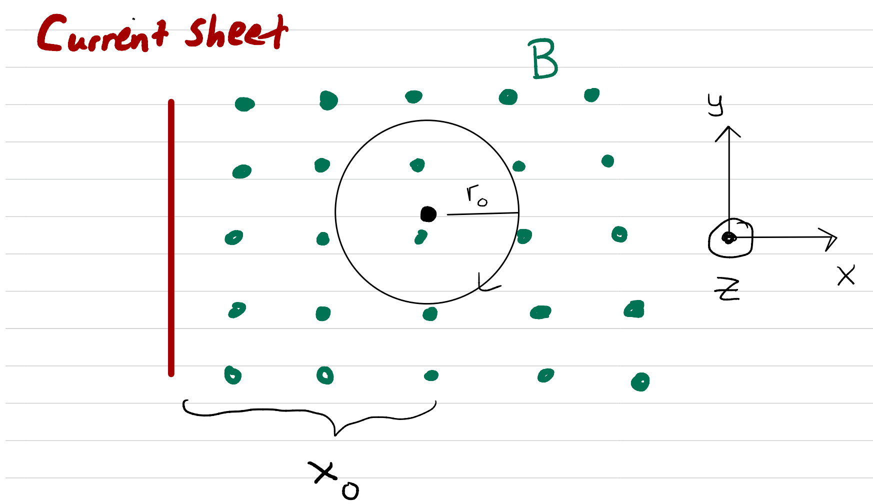
(i) Determine the phase space distribution $f(t, x, p)$ at later time t for a group of particles in a harmonic oscillator, i.e $H(x, p) = (p^2 + \omega_0^2 x^2)/2$.

(ii) Sketch contour in the phase-space (x, p) where $f(t, x, p)$ is $1/e$ of its maximum (with $e \simeq 2.718$) at time $t = 0$ and at several subsequent times.

For definiteness take units where $m = \Delta x_0 = \Delta p_0 = 1$. Take $X_0 = 3\Delta x_0$ and $m\omega_0 = 3\Delta p_0$

Problem 2. A slowly changing magnetic field

Consider the circular orbits in the xy plane with $x > 0$ of a particle mass m and charge q in a constant and uniform magnetic field B in the z direction. (This magnetic field could be created by a sheet of current in the yz plane at $x = 0$ as shown below.)



(a) Use the Hamiltonian formulation to determine the radius and angular frequency of the circular orbits. Relate the center of the circular orbit to the canonical momenta of the problem. Use the gauge

$$\boldsymbol{A} = B(0, x, 0)\,.$$

It is useful to define the cyclotron frequency[1], $\omega_B = qB/mc$.

Now imagine that starting at $t = 0$ the strength of the magnetic field is slowly increased from its initial value of $B_0 \equiv B(0)$.

(b) If the original orbit has radius r_0 and is centered at $\boldsymbol{x}_0 = (x_0, 0, 0)$ with $x_0 > 0$, determine how the radius and the center of the circular orbits change as $B(t)$ is slowly increased. Describe your results qualitatively by drawing a sketch, and give a qualitative explanation for the change in radius.

[1]We have given cyclotron frequency in Gaussian units. In SI units $\omega_B = qB/m$.

Problem 3. Short problems

Answer briefly. No more than a few lines

(a) Derive the canonical transformation rules $(q, p) \to (Q, P)$ for type $F_2(q, P, t)$

$$p = \frac{\partial F_2}{\partial q} \tag{19}$$

$$Q = \frac{\partial F_2}{\partial P} \tag{20}$$

$$H' = H + \frac{\partial F_2}{\partial t} \tag{21}$$

from the action principle. (This is essentially just reproducing what was done in lecture).

(b) It is well known that replacing the Lagrangian by

$$L'(q, \dot{q}, t) = L(q, \dot{q}, t) + \frac{df}{dt}(q, t) \tag{22}$$

does not change the equations of motion. Show that this change in the Lagrangian amounts to a canonical transformation in the corresponding Hamiltonian setup, and find the generating function of type F_2 for this transformation.

(c) Consider the Hamiltonian for a particle in a electromagnetic field

$$H = \frac{(\boldsymbol{p} - e\boldsymbol{A})^2}{2m} + e\varphi(t, \boldsymbol{r}) \tag{23}$$

Under a gauge transformation the electromagnetic potentials $\boldsymbol{A}, \varphi$ change, but the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ do not. The change in the potentials is specified a function $\Lambda(t, \boldsymbol{r})$, with new potentials

$$\boldsymbol{A} \to \boldsymbol{A}'(t, \boldsymbol{r}) = \boldsymbol{A} + \nabla\Lambda(t, \boldsymbol{r}) \tag{24}$$

$$\varphi \to \varphi'(t, \boldsymbol{r}) = \varphi - \partial_t \Lambda(t, \boldsymbol{r}) \tag{25}$$

Show that this change in the Hamiltonian can be written as a canonical transformation, and find the corresponding F_2 generating function.

(d) (Optional but recommended) Spell out the relation between parts (c) and parts (b), by examining the Lagrangian for a particle in an electromagnetic field

$$L = \frac{1}{2}m\dot{\boldsymbol{r}}^2 - e\varphi(t, \boldsymbol{r}) + \frac{e}{c}\dot{\boldsymbol{r}} \cdot \boldsymbol{A}(t, \boldsymbol{r}) \tag{26}$$

(e) What is the transformation $(\boldsymbol{r}, \boldsymbol{p}) \to (\boldsymbol{R}, \boldsymbol{P})$ generated by $F_2(\boldsymbol{r}, \boldsymbol{P}) = a\boldsymbol{r} \cdot \boldsymbol{P}$. Describe this transformation qualitatively.

(f) The Hamiltonian of a charged particle of charge q in the electrostatic potential of an electric dipole with dipole moment d_0 directed along the z axis is

$$H = \frac{\boldsymbol{p}^2}{2m} + \kappa \frac{\hat{\boldsymbol{z}} \cdot \hat{\boldsymbol{r}}}{r^2} \tag{27}$$

where $\kappa = q d_0/(4\pi\epsilon_0)$ in SI units.

Use the previous item with $a = (1 + \epsilon)$ to show that said particle has

$$\boldsymbol{p} \cdot \boldsymbol{r} - 2Et = \text{const} \tag{28}$$

Problem 4. Symplectic Integrators

Optional: This problem is optional. But (a) and (b) are so nice, and the solutions to (a) and (b) are online in the course notes. If you have time, I urge you to look at those.

Many physical systems are described by Hamiltonians which give rise to equations of motion that cannot be solved analytically, but must be discretized and solved numerically. Discretizations which preserve the symmetries of the continuum theory are especially effective when numerically integrating the equations of motion for long times. In this problem, we will explore some of the techniques available to describe such systems.

Consider a one-dimensional classical system whose *finite* time evolution over time t is described by a canonical transformation. Specifically, let

$$x_0 \equiv x(0) \quad , \quad x \equiv x(t) \quad , \quad p_0 \equiv p(0) \quad , \quad p \equiv p(t)$$

and consider a generating function $F_2(x_0, p, t)$. Then the update rule from (x_0, p_0) to (x, p) is obtained by solving the canonical transformation equations

$$p_0 = \frac{\partial F_2(x_0, p, t)}{\partial x_0} \quad , \quad x = \frac{\partial F_2(x_0, p, t)}{\partial p} \tag{29}$$

We are thinking of t as being small but finite.

(a) (i) Show that this transformation (or update rule) preserves volume in phase space regardless of the size of t (that is, prove Liouville's theorem for this case).

(ii) Next show that for

$$F_2(x_0, p, t) = x_0 p + t\, H(x_0, p)$$

as $t \to 0$, the evolution (or update) equations reduce to Hamilton's equations of motion. For $H = p^2/2m + U(x)$, determine x and p in terms of x_0, p_0, and t, with t finite. This is known as a first order symplectic integrator, and preserves the phase space area, regardless of the step size t.

(b) For a Hamiltonian of the form $\frac{p^2}{2m} + U(x)$, show that the naive discretization of Newton's equations of motion (for t small but finite)

$$p = p_0 - \frac{\partial U(x_0)}{\partial x_0} t \quad , \quad x = x_0 + \frac{p_0}{m} t \tag{30}$$

does NOT preserve volume in phase space. For a harmonic oscillator, will the volume shrink or grow? What does this say about the long time behavior of this approximation? Estimate the number of iterations of this map before the error is of order one, in terms of the mass m of the particle, the spring constant k, and the finite interval t.

All this is really optional: Recall that under a time dependent canonical map from $(q_1, p_1) \to (Q, P)$ generator $F_2(q_1, P, t)$ we have

$$p_1 = \frac{\partial F_2}{\partial q} \tag{31}$$

$$Q = \frac{\partial F_2}{\partial P} \tag{32}$$

$$H'(Q, P) = H(q_1, p_1) + \frac{\partial F_2(q_1, P, t)}{\partial t} \,. \tag{33}$$

This last part studies the implications of the last equation relating H' and H for discretization, and its meaning more generally.

We are describing a canonical map from $(x_0, p_0) \to (x, p)$. The Hamiltonian for (x, p) is $p^2/2m + U(x)$ so that the exact time evolution of the coordinates at time t is the differential equation we are trying to solve

$$\dot{x} = \frac{p}{m} \tag{34}$$

$$\dot{p} = -\frac{\partial U(x)}{\partial x} \tag{35}$$

These equations determine $x_+ = x(t+\delta t)$ and $p_+ = p(t+\delta t)$ for some *infinitessimal* δt. x_+, p_+ are not the same as taking (x_0, p_0) and applying the map generated by $F_2(x_0, p_+, t + \delta t)$. However, if we evolve x_0, p_0 with a new Hamiltonian H_0

$$\dot{x}_0 = \frac{\partial H_0(x_0, p_0)}{\partial p_0} \tag{36}$$

$$\dot{p}_0 = -\frac{\partial H_0(x_0, p_0)}{\partial x_0} \tag{37}$$

by infinitessimal δt to $x_{0+} = x_0(\delta t) = x_0 + \delta x_0$ and $p_{0+} = p_0(\delta t) = p_0 + \delta p_0$, and then apply the map generated by $F_2(x_{0+}, p_+, t + \delta t)$ to x_{0+}, p_{0+} we will exactly obtain (x_+, p_+). This is the meaning of a time dependent canonical transform, we can view the evolution either with x_0, p_0 or x, p. Ideally the time evolutions of x_0, p_0 will be approximately zero if the map $F_2(x_0, P, t)$ is a good approximation for the onshell action (principal function), $\underline{S}_2(t, q, t_0, P)$.

(c) (Optional but highly receommended) Compute H_0 using by two methods: (i) by using an appropriate version of Eq. (31), and (ii) by determining what H_0 needs to be so that the map generated by $F_2(x_{0+}, p_+, t + \delta t)$, maps (x_{0+}, p_{0+}) to (x_+, p_+)

You should find by both methods that

$$H_0(q_0, p_0) \approx t \frac{\partial U(q_0)}{\partial q} \frac{p_0}{m} + O(t^2) \tag{38}$$

Here H_0 is non-zero to first order in t, and is therefore small. For a second order symplectic integrator one would find $H_0 = 0 + O(t^2)$. See Ruth, IEEE Transactions on Nuclear Science (posted online).