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

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

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

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

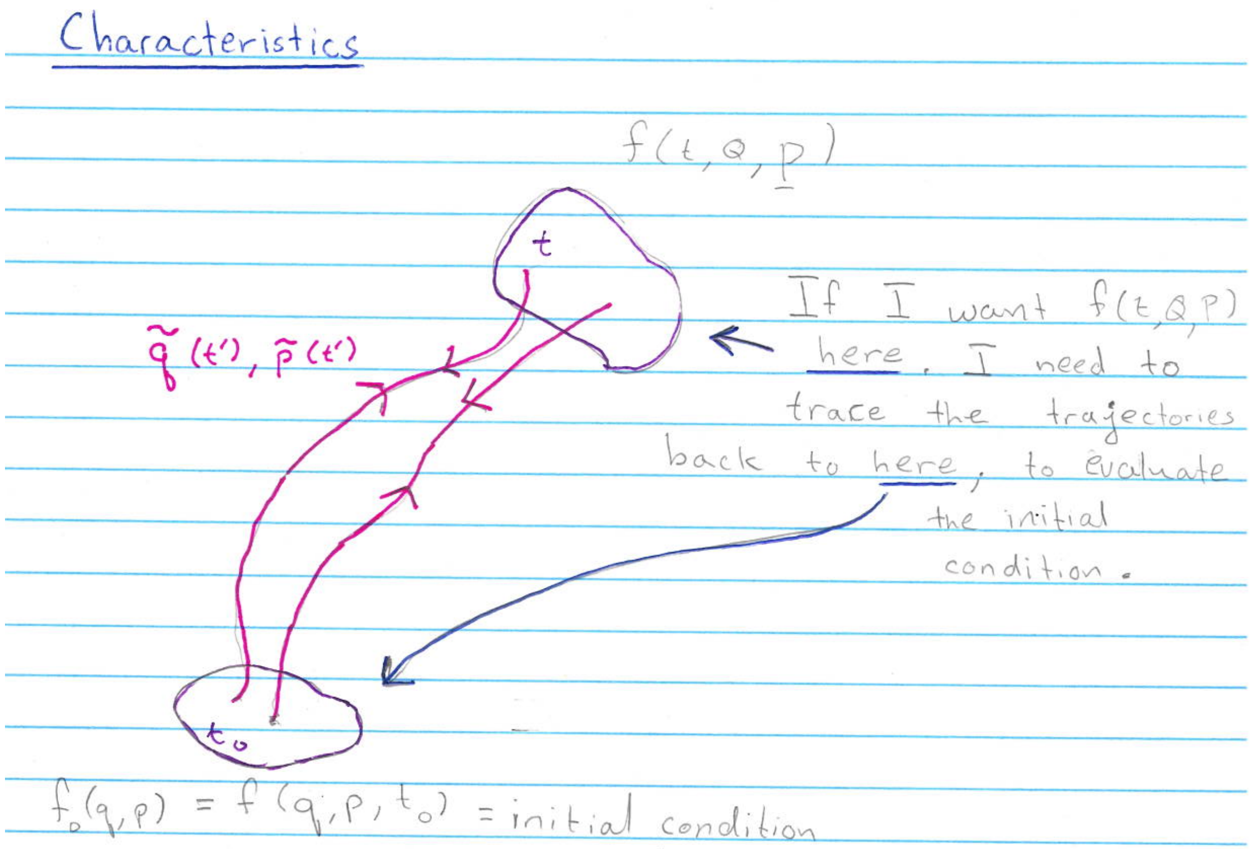


Figure 1: Characteristics of the Liouville equation .

(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 $m\omega_0 = 3\Delta p_0$

Solution

(a) We just differentiate through

$$\frac{\partial f}{\partial t} + \dot{q}^i \frac{\partial f}{\partial q^i} + \dot{p}^i \frac{\partial f}{\partial p_i} + f \left(\frac{\partial \dot{q}^i}{\partial q^i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = 0 \,. \tag{19}$$

The last terms vanish by the Hamilton's EOM :

$$\left(\frac{\partial \dot{q}^i}{\partial q^i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = \left(\frac{\partial^2 H}{\partial q^i \partial p_i} - \frac{\partial^2 H}{\partial p_i \partial q^i} \right) = 0, \tag{20}$$

leading to the required result. The incompressibility constraint is the lhs of Eq. (20), and is a consequence of Hamilton's EOM. It appeared prominently in our study of Lioville's theorem.

(b.i) Just differentiate

$$\partial_t f = - \left(\partial_Q f_0 \right) \left(\frac{P}{m} \right) , \tag{21}$$

$$\partial_Q f = (\partial_Q f_0) \,. \tag{22}$$

This leads to the result:

$$\partial_t f + \dot{Q} \partial_Q f + \dot{P} \partial_P f = 0 \,, \tag{23}$$

after using the EOM of the free theory, $\dot{Q} = P/m$ and $\dot{P} = 0$.

(b.ii) Then the solution is supposed to take the form:

$$f(t, Q, P) = f_0(q(Q, P, t), p(Q, P, t)) \,. \tag{24}$$

To verify this we first note that

$$\partial_t f = \left(\frac{\partial f_0}{\partial q} \partial_t q + \frac{\partial f_0}{\partial p} \partial_t p \right) , \tag{25}$$

while

$$\partial_Q f = \frac{\partial f_0}{\partial q} \frac{\partial q}{\partial Q} + \frac{\partial f_0}{\partial p} \frac{\partial p}{\partial Q} \,, \tag{26}$$

$$\partial_P f = \frac{\partial f_0}{\partial q} \frac{\partial q}{\partial P} + \frac{\partial f_0}{\partial p} \frac{\partial p}{\partial P} \,. \tag{27}$$

So with no thought we find

$$\begin{aligned} \partial_t f + \partial_Q f \partial_P H - \partial_P f \partial_Q H = & \frac{\partial f_0}{\partial q} \left(\dot{q} + \frac{\partial q}{\partial Q} \frac{\partial H}{\partial P} - \frac{\partial q}{\partial P} \frac{\partial H}{\partial Q} \right) \\ & + \frac{\partial f_0}{\partial q} \left(\dot{p} + \frac{\partial p}{\partial Q} \frac{\partial H}{\partial P} - \frac{\partial p}{\partial P} \frac{\partial H}{\partial Q} \right) \,. \end{aligned} \tag{28}$$

Then, thinking now, we recognize that if we advance Q and P by δt, we will have the same initial condition at time t_0. This means that

$$q(Q + \dot{Q}\delta t, P + \dot{P}\delta t, t + \delta t) = q(Q, P, t)\,, \tag{29}$$

and similarly for the momentum

$$p(Q + \dot{Q}\delta t, P + \dot{P}\delta t, t + \delta t) = p(Q, P, t)\,. \tag{30}$$

These constraints lead to

$$\partial_t q(Q, P, t) + \frac{\partial q}{\partial Q}\frac{\partial H}{\partial P} - \frac{\partial q}{\partial P}\frac{\partial H}{\partial Q} = 0\,, \tag{31a}$$

$$\partial_t p(Q, P, t) + \frac{\partial p}{\partial Q}\frac{\partial H}{\partial P} - \frac{\partial p}{\partial P}\frac{\partial H}{\partial Q} = 0\,. \tag{31b}$$

This says that p and q evolve backwards in time:

$$\partial_t p(q, P, t) = -\left\{q, H\right\}_{P,Q}\,, \tag{32}$$

$$\partial_t p(Q, P, t) = -\left\{p, H\right\}_{P,Q}\,. \tag{33}$$

With these relations, Eq. (31), and Eq. (28) the result follows.

(b.iii) As we increment t_0 at fixed Q, P we must remain on the same curve (see picture). This means

$$\partial_{t_0} q = \frac{\partial H(q, p, t_0)}{\partial p} \tag{34}$$

$$\partial_{t_0} p = -\frac{\partial H(q, p, t_0)}{\partial q} \tag{35}$$

This gives a different strategy to find q, p: Start with $t_0 = t$ where $q = Q$ and $p = P$, and evolve (q, p) in t_0. Since t_0 is before t, this means evolving backward in time, to the time where you know the initial conditions for $f(t, x, p)$.

(c) According to (b.i) we have

$$f(t, X, P) = f_0(X - Pt) \tag{36}$$

where we have set $m = 1$. This means

$$f(t, X, P) = \frac{1}{2\pi\Delta x_0 \Delta p_0} \exp\left[-\frac{(X - Pt)^2}{2\Delta x_0^2} - \frac{(P - P_0)^2}{2\Delta p_0^2}\right] \tag{37}$$

A contour plot of $f(t, X, P)$ is plotted for several times for $\Delta x_0 = \Delta p_0 = 1$ and $P_0 = 3$ in Fig. 2. We see a characteristic "shearing" of the phase space under free motion.

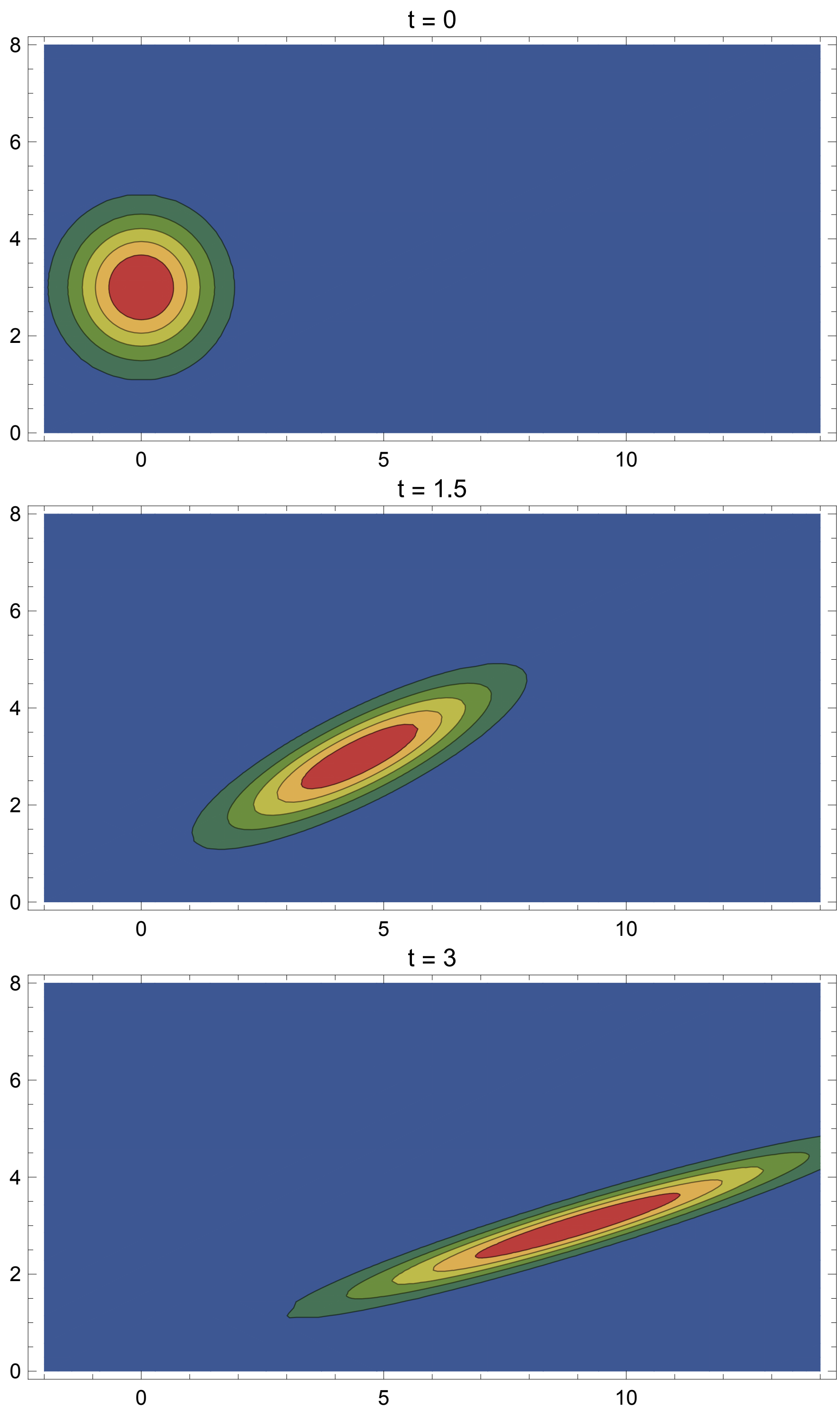


Figure 2: A Gaussian blob under free evolution. The contours show the constant values for $f(t, X, P)$ in the (X, P) plane. These contours are shown at $t = 0, 1.5, 3.0$. The center of the blob moves with $x = P_0 t$ with $P_0 = 3$. The area of each shaded region remains constant in time.

(d) The Harmonic oscillator works similarly, although the character of the solution is very different. The solution to the harmonic oscillator is

$$Q = q\cos(\omega_0 t) + \frac{p}{\omega_0}\sin(\omega_0 t)\,, \tag{38}$$

$$\frac{P}{\omega_0} = -\,q\sin(\omega_0 t) + \frac{p}{\omega_0}\cos(\omega_0 t)\,. \tag{39}$$

This is just a rotation of $(q, p/\omega_0)$ to $(Q, P/\omega_0)$. The inverse relation/rotation is

$$q = Q\cos(\omega_0 t) - \frac{P}{\omega_0}\sin(\omega_0 t)\,, \tag{40}$$

$$\frac{p}{\omega_0} = +\,Q\sin(\omega_0 t) + \frac{P}{\omega_0}\cos(\omega_0 t)\,. \tag{41}$$

Then substituting this into the expression for f_0 we find

$$f(t,X,P) = \frac{1}{2\pi\Delta x_0\Delta p_0}\exp\left[-\frac{(X\cos(\omega_0 t) - \frac{P}{\omega_0}\sin(\omega_0 t) - X_0)^2}{2\Delta x_0^2} - \frac{(-Q\omega_0\sin(\omega_0 t) + P\cos(\omega_0 t))^2}{2\Delta p_0^2}\right]\,. \tag{42}$$

A plot this for $m = \Delta x_0 = \Delta p_0 = 1$ and $X_0 = 3$ and $\omega_0 = 2$ at various times is shown in the figure below in Fig. 3. If we start at $t = 0$ with $q = 3$ and $P = 0$ (the center of the gaussian blob),

$$X = 3\cos(t/\tau)\,, \tag{43}$$

$$P = 3\omega_0\cos(t/\tau)\,, \tag{44}$$

where $\tau = 2\pi/\omega_0$. This trajectory is also shown in the figure. At $t = 0$ the contour where $f(t, X, P)$ is $1/e$ of its maxium is a circle

$$\frac{1}{2}(X - X_0)^2 + \frac{1}{2}P^2 = 1 \tag{45}$$

At time $t = \tau/4$ this contour is an ellipse with the same area

$$\frac{1}{2\omega_0^2}(P - \omega_0 X_0)^2 + \frac{\omega_0^2}{2}Q^2 = 1 \tag{46}$$

If one were to rescale the P axis by a factor of ω_0 then one would see circular motion corresponding to the sho motion in the $X, P/\omega_0$ plane. The trajectory of the center of the Gaussian blob is

$$X = 3\cos(t/\tau) \tag{47}$$

$$P/\omega_0 = 3\cos(t/\tau) \tag{48}$$

The contours are shown in Fig. 4

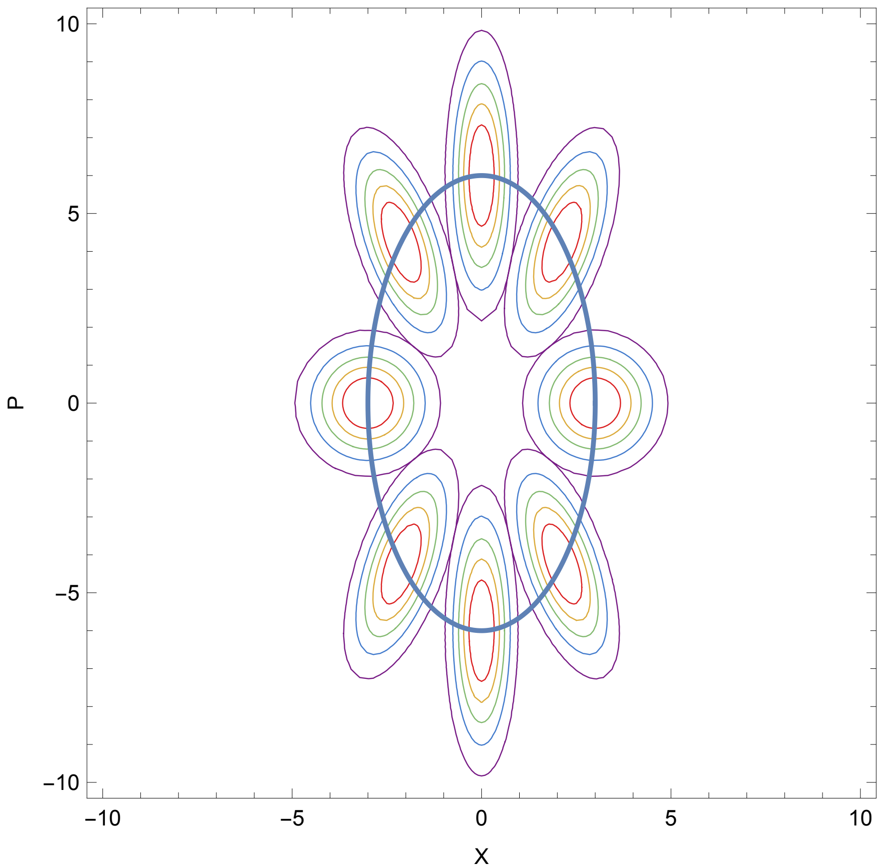


Figure 3: A Gaussian blob under the evolution of the SHO. The contours show the constant values for $f(t, X, P)$ in the (X, P) plane. Going *clockwise* around the ellipse (the blue line) we show the contours at $t = 0, \tau/8, 2\tau/8, \ldots$ where the period of the motion is $\tau \equiv 2\pi/\omega_0$ with $\omega_0 = 2$. The center of the Gaussian blob follows and ellipse for a simple harmonic oscillator (see text). We have set $\Delta x = \Delta p = m = 1$ and have $X_0 = 3$ and $\omega_0 = 2$

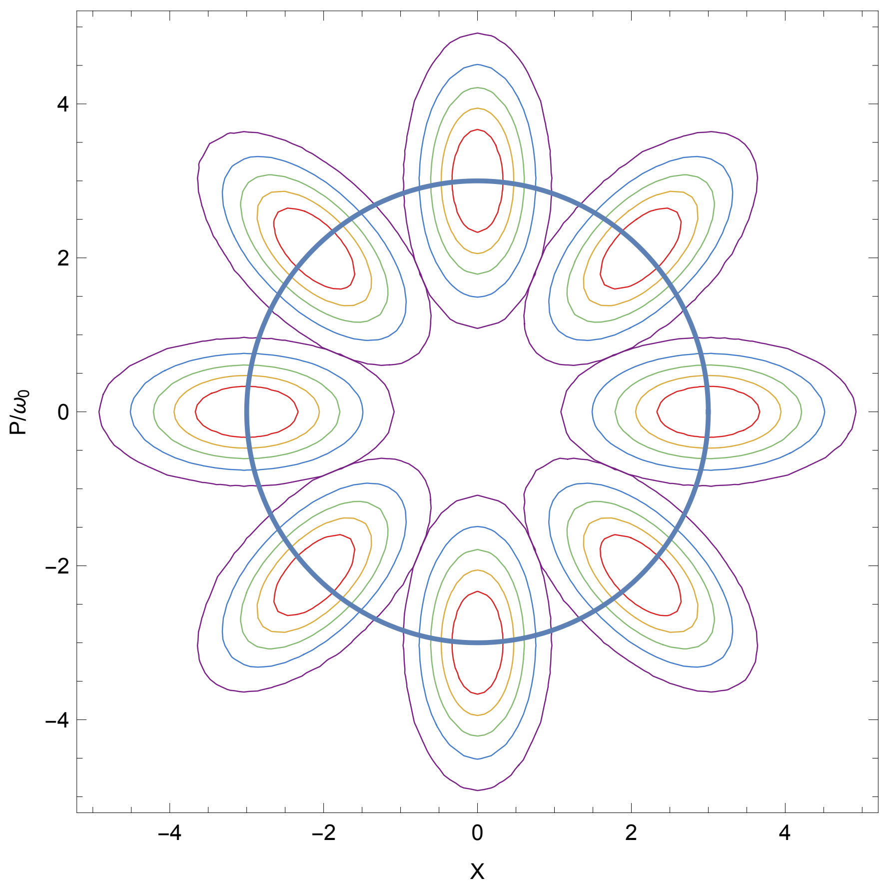
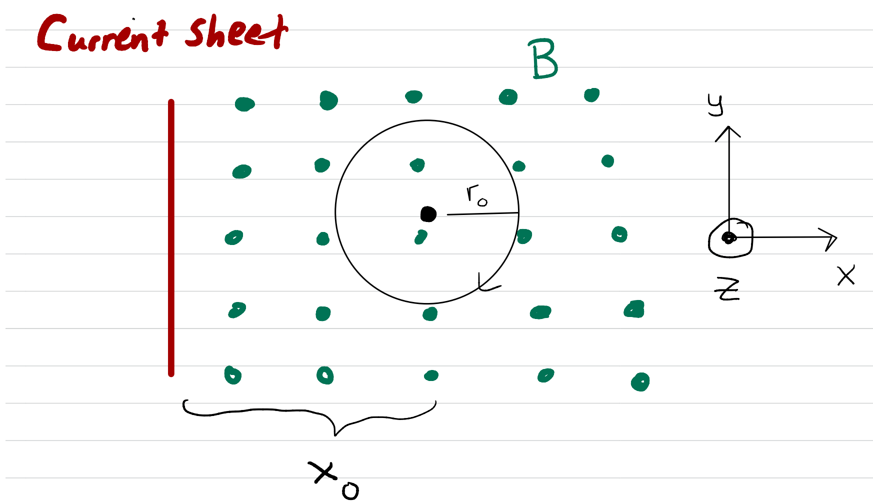


Figure 4: The same as Fig. 3 but we have rescaled the momentum axis by ω_0.

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 $\omega_B = qB/m$.

Solution

(a) The Lagrangian is

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{q}{c}\left(A_x\dot{x} + A_y\dot{y}\right), \tag{49}$$

Or

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + m\omega_B(t)x\dot{y}\,. \tag{50}$$

We construct the Hamiltonian which matches onto the general form discussed in class:

$$H = \frac{1}{2m}\left(p_x^2 + (p_y - m\omega_B x)^2\right)\,. \tag{51}$$

The equation of motion for p_y is cyclic in character

$$p_y = \text{const}, \tag{52}$$

Thus the effective Hamiltonian for the motion in x is then

$$H_{\text{eff}} = \frac{p_x^2}{2m} + \frac{1}{2}m\omega_B^2\left(x - \frac{p_y}{m\omega_B}\right)^2, \tag{53}$$

which is a shifted harmonic oscillator in x. The harmonic motion is around

$$\frac{p_y}{m\omega_B}\,. \tag{54}$$

which determines the center of the circle.

The radius of the circle is determined by the energy of the $1D$ problem We have that the turning points of the x motion for the equivalent $1d$ problem determines the radius

$$\epsilon = \frac{1}{2}m\omega_B^2 r_0^2\,, \tag{55}$$

or

$$r_0 = \sqrt{\frac{2\epsilon}{m\omega_B^2}}\,. \tag{56}$$

(b) Then using the theory of adiabatic invariants we have

$$I = \oint p_x dx\,, \tag{57}$$

is constant. We have from lecture that the adiabatic invariant for the SHO is

$$I = \frac{\epsilon}{\omega_B}\,. \tag{58}$$

So we can express the radius and center as

$$r(t) = \sqrt{\frac{2I}{m\omega_B}}\,, \qquad x_0 = \frac{p_y}{m\omega_B}\,, \tag{59}$$

Since I and p_y are adiabatically constant and constant respectively we find:

$$r(t) = r(0)\sqrt{\frac{B(0)}{B(t)}}\,, \qquad x_0(t) = x_0(0)\frac{B(0)}{B(t)}\,. \tag{60}$$

Discussion: Interpreting the result, the radius shrinks keeping the flux fixed:

$$\pi r(t)^2 B(t) = \text{const}\,, \tag{61}$$

and the circular orbits move closer to $x = 0$.

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 $F_2(q, P, t)$

$$p = \frac{\partial F_2}{\partial q} \tag{62}$$

$$Q = \frac{\partial F_2}{\partial P} \tag{63}$$

$$H' = H + \frac{\partial F_2}{\partial t} \tag{64}$$

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

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

$$L'(q, \dot{q}, t) = L(q, \dot{q}, t) + \frac{df}{dt}(q, t) \tag{65}$$

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

$$H = \frac{(\boldsymbol{p} - e\boldsymbol{A})^2}{2m} + e\varphi(t, \boldsymbol{r}) \tag{66}$$

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

$$\boldsymbol{A} \to \boldsymbol{A}'(t, \boldsymbol{r}) = \boldsymbol{A} + \nabla\Lambda(t, \boldsymbol{r}) \tag{67}$$

$$\varphi \to \varphi'(t, \boldsymbol{r}) = \varphi - \partial_t\Lambda(t, \boldsymbol{r}) \tag{68}$$

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

$$L = \frac{1}{2}m\dot{\boldsymbol{r}}^2 - e\varphi(t, \boldsymbol{r}) + \frac{e}{c}\dot{\boldsymbol{r}} \cdot \boldsymbol{A}(t, \boldsymbol{r}) \tag{69}$$

(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

$$H = \frac{\boldsymbol{p}^2}{2m} + \kappa \frac{\hat{\boldsymbol{z}} \cdot \hat{\boldsymbol{r}}}{r^2} \tag{70}$$

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

$$\boldsymbol{p} \cdot \boldsymbol{r} - 2Et = \text{const} \tag{71}$$

Solution

(a) The action of the two system is (respectively)

$$S_1 = \int dt\,(p\dot{q} - H(p,q))\ , \tag{72}$$

$$S_2 = \int dt\left(P\dot{Q} - H'(P,Q)\right)\ . \tag{73}$$

Instead of using S_2 we will can

$$S_2' = \int dt\left(-Q\dot{P} - H(P,Q)\right) \tag{74}$$

which differs from S_2 only by a total derivative, $d(PQ)/dt$, which does not affect the equation of motion for the (P,Q) system. There is a map between (q,p) and (Q,P), i.e. $Q(q,p)$ and $P(q,p)$. With this map we could use S_2' as an action for (p,q) instead of S_1. The difference in the two actions must then be a total derivative if the q,p EOM derived from these actions is to be the same. The difference is

$$S_1 - S_2' = \int dt\left(p\dot{q} + Q\dot{P} - (H - H')dt\right) \tag{75}$$

and is required to take the form of a total derivative

$$S_1 - S_2' = \int dt \frac{dF_2(q,P,t)}{dt} = \int dt\left(\frac{\partial F_2}{\partial q}\dot{q} + \frac{\partial F_2}{\partial P}\dot{P} + \frac{\partial F_2}{\partial t}\right) \tag{76}$$

Comaring these two forms gives the transformation rule

$$p = \frac{\partial F_2}{\partial q} \tag{77}$$

$$Q = \frac{\partial F_2}{\partial P} \tag{78}$$

$$H' - H = \frac{\partial F_2}{\partial P} \tag{79}$$

(b) If we repalce

$$L' = L + \frac{df(q,t)}{dt} \tag{80}$$

$$L' = L + \frac{\partial f}{\partial q}\dot{q} + \frac{\partial f}{\partial t} \tag{81}$$

Then the canonical momentum changed, and the coordinate is not:

$$Q = q \tag{82}$$

$$P = \frac{\partial L'}{\partial \dot{q}} = p + \frac{\partial f}{\partial q} \tag{83}$$

This is generated by

$$F_2 = qP - f(q,t) \tag{84}$$

(c) We take the original Hamiltonian $H(q,p)$ and construct the new $H'(Q,P)$. We take as our generating function:

$$F_2 = \boldsymbol{r}\cdot\boldsymbol{P} - \frac{e}{c}\Lambda(\boldsymbol{r},t) \tag{85}$$

Then using the rules:

$$\boldsymbol{p} = \boldsymbol{P} - \frac{e}{c}\nabla\Lambda \tag{86}$$

$$\boldsymbol{R} = \boldsymbol{r} \tag{87}$$

Putting together the ingrediants

$$H'(\boldsymbol{P},\boldsymbol{R}) = H(\boldsymbol{p},\boldsymbol{r}) - e\frac{\partial\Lambda}{\partial t} \tag{88}$$

Or more explicitly

$$H'(\boldsymbol{P},\boldsymbol{R}) = \frac{(\boldsymbol{P} - (e/c)\boldsymbol{A}')^2}{2m} + e\varphi' \tag{89}$$

where $\boldsymbol{A}'$ and φ' are given in Eq. (**??**).

(d) Under a gauge transformation

$$L \to L' = L + \frac{e}{c}\frac{d\Lambda(t,\boldsymbol{r})}{dt} \tag{90}$$

(e) It is a scale transformation

$$\boldsymbol{P} = \frac{\boldsymbol{p}}{a} \tag{91}$$

$$\boldsymbol{R} = a\boldsymbol{r} \tag{92}$$

Note the transformation preserves the form: $\boldsymbol{p}\cdot d\boldsymbol{r} = \boldsymbol{P}\cdot d\boldsymbol{R}$.

(f) For infinitessimal transform $G = \boldsymbol{r}\cdot\boldsymbol{p}$ the transformation Generated by G on observable O gives the Poisson bracket:

$$\epsilon\{O,G\}\,. \tag{93}$$

Here the transformation rule is

$$\boldsymbol{r} \to (1+\epsilon)\boldsymbol{r} = \boldsymbol{r} + \epsilon\boldsymbol{r}\,, \tag{94}$$

$$\boldsymbol{p} \to \frac{\boldsymbol{p}}{(1+\epsilon)} = \boldsymbol{p} - \epsilon\boldsymbol{p}\,, \tag{95}$$

which matches the Poisson Brackets

$$\{\boldsymbol{r}, G\} = \boldsymbol{r}\,, \tag{96}$$

$$\{\boldsymbol{p}, G\} = -\,\boldsymbol{p}\,. \tag{97}$$

Under the transformation of Eq. (94) we find

$$H \to \frac{1}{(1+\epsilon)^2} H \simeq H - 2\epsilon H\,, \tag{98}$$

and this implies the Poisson bracket

$$\{H, \boldsymbol{r} \cdot \boldsymbol{p}\} = -2H\,. \tag{99}$$

Thus since $\dot{O} = \{O, H\}$ we have

$$\frac{d(\boldsymbol{r} \cdot \boldsymbol{p})}{dt} = +2H\,. \tag{100}$$

Since $H(q, p) = E$ is constant we have

$$\boldsymbol{r} \cdot p - 2Et = \text{constant} \tag{101}$$

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

$$p_0 = \frac{\partial F_2(x_0, p, t)}{\partial x_0} \quad , \quad x = \frac{\partial F_2(x_0, p, t)}{\partial p} \tag{102}$$

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)

$$p = p_0 - \frac{\partial U(x_0)}{\partial x_0} t \quad , \quad x = x_0 + \frac{p_0}{m} t \tag{103}$$

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

$$p_1 = \frac{\partial F_2}{\partial q} \tag{104}$$

$$Q = \frac{\partial F_2}{\partial P} \tag{105}$$

$$H'(Q, P) = H(q_1, p_1) + \frac{\partial F_2(q_1, P, t)}{\partial t}. \tag{106}$$

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

$$\dot{x} = \frac{p}{m} \tag{107}$$

$$\dot{p} = -\frac{\partial U(x)}{\partial x} \tag{108}$$

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

$$\dot{x}_0 = \frac{\partial H_0(x_0, p_0)}{\partial p_0} \tag{109}$$

$$\dot{p}_0 = -\frac{\partial H_0(x_0, p_0)}{\partial x_0} \tag{110}$$

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. (104), 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

$$H_0(q_0, p_0) \approx t \frac{\partial U(q_0)}{\partial q} \frac{p_0}{m} + O(t^2) \tag{111}$$

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).

Solution

The solution uses a slightly different notation from the problem statement:

	problem statement	solution
new coords at time t	(x, p)	(x', p')
old coords at time zero	(x_0, p_0)	(x, p)

(a) (i) Show that this evolution preserves volume in phase space (that is, prove Liouville's theorem for this case).

We need to compute the Jacobian determinant of the transformation:

$$\det(\text{Jac}) = \begin{vmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{vmatrix} = \begin{vmatrix} \frac{\partial^2 F_2}{\partial p' \partial x} + \frac{\partial^2 F_2}{\partial p' \partial p'} \frac{\partial p'}{\partial x} & \frac{\partial^2 F_2}{\partial p' \partial p'} \frac{\partial p'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{vmatrix} = \frac{\partial^2 F_2}{\partial p' \partial x} \frac{\partial p'}{\partial p} \ .$$

But differentiating $p = \frac{\partial F_2}{\partial x}$ with respect to p gives

$$1 = \frac{\partial^2 F_2}{\partial p' \partial x} \frac{\partial p'}{\partial p} \ ,$$

and hence the Jacobian determinant is 1.

A solution with the volume form:

$$dp \wedge dx = \frac{\partial^2 F_2}{\partial x \partial p'} dp' \wedge dx = dp' \wedge \frac{\partial^2 F_2}{\partial p' \partial x} dx = dp' \wedge dx'$$

is also acceptable.

(ii) Next show that for

$$F_2 = xp' + \delta t \, H$$

as $\delta t \equiv t' - t \to 0$, the evolution equations reduce to Hamilton's equations of motion.

Equation (1) becomes:

$$p = p' + \delta t \frac{\partial H}{\partial x} \quad , \quad x' = x + \delta t \frac{\partial H}{\partial p'} \quad \Rightarrow \quad p' - p = -\delta t \frac{\partial H}{\partial x} \quad , \quad x' - x = \delta t \frac{\partial H}{\partial p'}$$

which, in the limit $\delta t \to 0$, $p' \to p$, $x' \to x$ reduces to

$$\dot{p} = -\frac{\partial H}{\partial x} \quad , \quad \dot{x} = \frac{\partial H}{\partial p}$$

(b) (5 points) For a Hamiltonian of the form $\frac{p^2}{2m} + U(x)$, show that the naive discretization of Newton's equations of motion (for δt small but finite)

$$p' = p - \frac{\partial U(x)}{\partial x} \delta t \quad , \quad x' = x + \frac{p}{m} \delta t \tag{2}$$

does NOT preserve volume in phase space.

The Jacobian determinant is

$$\det(\text{Jac}) = \begin{vmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{vmatrix} = \begin{vmatrix} 1 & \frac{\delta t}{m} \\ -\delta t \frac{\partial^2 U}{\partial x \partial x} & 1 \end{vmatrix} = 1 + \frac{(\delta t)^2}{m} \frac{\partial^2 U}{\partial x \partial x}$$

For a harmonic oscillator, $U = \frac{1}{2} k x^2$ with $k > 0$, and hence the Jacobian is $1 + \frac{k}{m}(\delta t)^2 > 1$, which means the volume grows. The approximation is unstable and after approximately

$$N \approx \left(\frac{k}{m} (\delta t)^2 \right)^{-1}$$

iterations will deviate from the exact solution by order one.

(c) What is the analogous discretization using canonical transformations? Find the right $F_2(x, p')$, and work out the equations corresponding to the discretization in part (b).

The right $F_2(x, p')$ follows from part ii) of a):

$$F_2(x, p') = x p' + \delta t \left(\frac{(p')^2}{2m} + U(x) \right) .$$

The evolution equations are (1) from above; here they become:

$$p = p' + \delta t \frac{\partial U}{\partial x} \quad , \quad x' = x + \delta t \frac{p'}{m} ,$$

which we rewrite as:

$$p' = p - \delta t \frac{\partial U}{\partial x} \quad , \quad x' = x + \delta t \frac{p'}{m} .$$

Notice in the second equation, p' appears on the right hand side, rather than p as in part (b). We proved that *all* canonical transformations preserve volume in phase space. We do not expect the errors from the discretization procedure to grow with time (of course, numerical errors can accumulate, though these are typically much smaller than discretization errors).