## HANDOUT \#12: THE HAMILTONIAN APPROACH TO MECHANICS

These notes are intended to be read as a supplement to the handout from Gregory, Classical Mechanics, Chapter 14.

## 1 The basic set-up

I assume that you have already studied Gregory, Sections 14.1-14.4. The following is intended only as a succinct summary.

We are considering a system whose equations of motion are written in Hamiltonian form. This means that:

1. The phase space of the system is parametrized by canonical coordinates $\boldsymbol{q}=\left(q_{1}, \ldots, q_{n}\right)$ and $\boldsymbol{p}=\left(p_{1}, \ldots, p_{n}\right)$.
2. We are given a Hamiltonian function $H(\boldsymbol{q}, \boldsymbol{p}, t)$.
3. The dynamics of the system is given by Hamilton's equations of motion

$$
\begin{align*}
\dot{q}_{i} & =\frac{\partial H}{\partial p_{i}}  \tag{1a}\\
\dot{p}_{i} & =-\frac{\partial H}{\partial q_{i}} \tag{1b}
\end{align*}
$$

for $i=1, \ldots, n$.
In these notes we will consider some deeper aspects of Hamiltonian dynamics.

## 2 Poisson brackets

Let us start by considering an arbitrary function $f(\boldsymbol{q}, \boldsymbol{p}, t)$. Then its time evolution is given by

$$
\begin{align*}
\frac{d f}{d t} & =\sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_{i}} \dot{q}_{i}+\frac{\partial f}{\partial p_{i}} \dot{p}_{i}\right)+\frac{\partial f}{\partial t}  \tag{2a}\\
& =\sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_{i}} \frac{\partial H}{\partial p_{i}}-\frac{\partial f}{\partial p_{i}} \frac{\partial H}{\partial q_{i}}\right)+\frac{\partial f}{\partial t} \tag{2b}
\end{align*}
$$

where the first equality used the definition of total time derivative together with the chain rule, and the second equality used Hamilton's equations of motion.

The formula (2b) suggests that we make a more general definition. Let $f(\boldsymbol{q}, \boldsymbol{p}, t)$ and $g(\boldsymbol{q}, \boldsymbol{p}, t)$ be any two functions; we then define their Poisson bracket $\{f, g\}$ to be

$$
\begin{equation*}
\{f, g\} \stackrel{\text { def }}{=} \sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_{i}} \frac{\partial g}{\partial p_{i}}-\frac{\partial f}{\partial p_{i}} \frac{\partial g}{\partial q_{i}}\right) . \tag{3}
\end{equation*}
$$

The time-evolution equation (2) can then be rewritten in compact form as

$$
\begin{equation*}
\frac{d f}{d t}=\{f, H\}+\frac{\partial f}{\partial t} . \tag{4}
\end{equation*}
$$

In the particular case where $f=q_{i}$ or $p_{i}$, the function $f$ has no explicit time-dependence, so we have simply $\dot{q}_{i}=\left\{q_{i}, H\right\}$ and $\dot{p}_{i}=\left\{p_{i}, H\right\}$, which you should verify are precisely (1).

But the importance of the Poisson bracket in Hamiltonian mechanics goes far beyond this reformulation of the equation of motion. Rather, the Poisson bracket encodes the fundamental geometrical structure of Hamiltonian phase space.

Remark. In the definition (3), the explicit time-dependence, if any, simply goes for the ride; the important thing is how $f$ and $g$ depend on $\boldsymbol{q}$ and $\boldsymbol{p}$. So, in discussing Poisson brackets, we shall often just consider functions $f(\boldsymbol{q}, \boldsymbol{p})$ and $g(\boldsymbol{q}, \boldsymbol{p})$ and not bother to discuss explicit time-dependence.

Let us begin by recording some fundamental properties of the Poisson bracket:

1. Bilinearity. We have

$$
\begin{equation*}
\left\{\alpha_{1} f_{1}+\alpha_{2} f_{2}, g\right\}=\alpha_{1}\left\{f_{1}, g\right\}+\alpha_{2}\left\{f_{2}, g\right\} \tag{5}
\end{equation*}
$$

and likewise for $g$.
2. Anticommutativity. We have

$$
\begin{equation*}
\{f, g\}=-\{g, f\} \tag{6}
\end{equation*}
$$

In particular it follows that $\{f, f\}=0$ (why?).
3. Jacobi identity. For any three functions $f, g, h$ we have

$$
\begin{equation*}
\{f,\{g, h\}\}+\{g,\{h, f\}\}+\{h,\{f, g\}\}=0 \tag{7}
\end{equation*}
$$

or equivalently (using anticommutativity)

$$
\begin{equation*}
\{\{f, g\}, h\}+\{\{g, h\}, f\}+\{\{h, f\}, g\}=0 \tag{8}
\end{equation*}
$$

We will prove the Jacobi identity in the next section.
4. Product identity. For any three functions $f, g, h$ we have

$$
\begin{equation*}
\{f g, h\}=f\{g, h\}+g\{f, h\} \tag{9}
\end{equation*}
$$

This is an easy consequence of the product law for partial differentation; you will be asked to prove it in the next problem set. It basically expresses the fact that the Poisson bracket $\{f, g\}$ involves first derivatives of $f$ and of $g$.
5. Fundamental Poisson brackets. The Poisson brackets among the canonical coordinates $\boldsymbol{q}=\left(q_{1}, \ldots, q_{n}\right)$ and $\boldsymbol{p}=\left(p_{1}, \ldots, p_{n}\right)$ are

$$
\begin{align*}
\left\{q_{i}, q_{j}\right\} & =0  \tag{10a}\\
\left\{p_{i}, p_{j}\right\} & =0  \tag{10b}\\
\left\{q_{i}, p_{j}\right\} & =\delta_{i j} \tag{10c}
\end{align*}
$$

where $\delta_{i j}$ is the Kronecker delta, i.e.

$$
\delta_{i j}= \begin{cases}1 & \text { if } i=j  \tag{11}\\ 0 & \text { if } i \neq j\end{cases}
$$

The three properties of bilinearity, anticommutativity and the Jacobi identity play such a fundamental role in many areas of mathematics that they have been given a name: an algebraic structure involving a "product" that is bilinear, anticommutative and satisfies the Jacobi identity is called a Lie algebra. ${ }^{1}$ You already know two other examples of Lie algebras:

- Vectors in $\mathbb{R}^{3}$, equipped with the cross product $\mathbf{a} \times \mathbf{b}$.
- $n \times n$ matrices, equipped with the commutator $[A, B]=A B-B A$.

In both cases the bilinearity and anticommutativity are obvious; I leave it to you to check the Jacobi identity.

We can now prove an important result in Hamiltonian dynamics:

Total time derivative of a Poisson bracket. For any two functions $f(\boldsymbol{q}, \boldsymbol{p}, t)$ and $g(\boldsymbol{q}, \boldsymbol{p}, t)$, we have

$$
\begin{equation*}
\frac{d}{d t}\{f, g\}=\left\{\frac{d f}{d t}, g\right\}+\left\{f, \frac{d g}{d t}\right\} \tag{12}
\end{equation*}
$$

[^0]Despite its fairly obvious-looking form, this formula is not obvious; it requires a bit of calculation.

Proof of (12). From the fundamental time-evolution equation (4) applied to $\{f, g\}$, we have

$$
\begin{equation*}
\frac{d}{d t}\{f, g\}=\{\{f, g\}, H\}+\frac{\partial}{\partial t}\{f, g\} \tag{13}
\end{equation*}
$$

The first term on the right-hand side can be transformed using the Jacobi identity and anticommutativity:

$$
\begin{align*}
\{\{f, g\}, H\} & =-\{\{g, H\}, f\}-\{\{H, f\}, g\}  \tag{14a}\\
& =\{f,\{g, H\}\}+\{\{f, H\}, g\} \tag{14b}
\end{align*}
$$

And for the second term on the right-hand side, we use the fact that $\partial / \partial t$ commutes with the partial derivatives $\partial / \partial q_{j}$ and $\partial / \partial p_{j}$ occurring in the definition of the Poisson bracket; it therefore follows that

$$
\begin{equation*}
\frac{\partial}{\partial t}\{f, g\}=\left\{\frac{\partial f}{\partial t}, g\right\}+\left\{f, \frac{\partial g}{\partial t}\right\} \tag{15}
\end{equation*}
$$

(you should check the details!). Adding (14) and (15) and using the fundamental timeevolution equation (4) for $f$ and for $g$, we obtain (12).

In particular, if $f$ and $g$ are constants of motion, then so is $\{f, g\}$. So this provides a method for obtaining new constants of motion, given old ones! Of course, these new constants of motion are not guaranteed to be nontrivial. (For instance, we might have $\{f, g\}=0$.) But here is one nontrivial example:

Example: Angular momentum. Consider a single particle in Cartesian coordinates, so that $\boldsymbol{q}=\left(q_{1}, q_{2}, q_{3}\right)$ is the position and that $\boldsymbol{p}=\left(p_{1}, p_{2}, p_{3}\right)$ is the ordinary linear momentum. In the next problem set I will ask you to show that three components of the angular momentum $\mathbf{L}=\boldsymbol{q} \times \boldsymbol{p}$ have the Poisson brackets

$$
\begin{align*}
\left\{L_{1}, L_{2}\right\} & =L_{3}  \tag{16a}\\
\left\{L_{2}, L_{3}\right\} & =L_{1}  \tag{16b}\\
\left\{L_{3}, L_{1}\right\} & =L_{2} \tag{16c}
\end{align*}
$$

It follows that if two components of the angular momentum happen to be constants of motion, then the third component of the angular momentum must also be a constant of motion.

Note, by contrast, that nothing of the kind follows if only one component of the angular momentum is a constant of motion. Indeed, we have seen lots of examples of systems where one component of angular momentum (e.g. the $z$ component) is conserved but the other two are not.

## 3 A unified notation for phase space

The key idea of the Hamiltonian formulation of mechanics is the extremely symmetric role played by the coordinates $\boldsymbol{q}$ and the conjugate momenta $\boldsymbol{p}$ - in contrast to the Lagrangian formulation, where the coordinates $\boldsymbol{q}$ and the velocities $\dot{\boldsymbol{q}}$ play very different roles. So it would be nice to introduce a notation that makes this symmetry between the $\boldsymbol{q}$ and $\boldsymbol{p}$ more explicit.

This unified notation is defined by the obvious approach of assembling the coordinates $\boldsymbol{q}=\left(q_{1}, \ldots, q_{n}\right)$ and the conjugate momenta $\boldsymbol{p}=\left(p_{1}, \ldots, p_{n}\right)$ into a single vector $\boldsymbol{X}=$ $\left(q_{1}, \ldots, q_{n}, p_{1}, \ldots, p_{n}\right)$ of length $2 n$. That is, we define phase-space coordinates $\boldsymbol{X}=$ $\left(X_{1}, \ldots, X_{2 n}\right)$ by

$$
X_{i}= \begin{cases}q_{i} & \text { for } 1 \leq i \leq n  \tag{17}\\ p_{i-n} & \text { for } n+1 \leq i \leq 2 n\end{cases}
$$

We then introduce a $2 n \times 2 n$ matrix $\Omega$ whose $n \times n$ blocks look like

$$
\Omega=\left(\begin{array}{cc}
0_{n} & I_{n}  \tag{18}\\
-I_{n} & 0_{n}
\end{array}\right)
$$

where $I_{n}$ denotes the $n \times n$ identity matrix and $0_{n}$ denotes the $n \times n$ zero matrix; or in more detail,

$$
\Omega_{i j}= \begin{cases}1 & \text { if } j=i+n  \tag{19}\\ -1 & \text { if } i=j+n \\ 0 & \text { otherwise }\end{cases}
$$

Note that the matrix $\Omega$ is antisymmetric, and that $\Omega^{2}=-I$ (why?). This matrix is just the trick we need to get the appropriate minus sign into Hamilton's equations: namely, Hamilton's equations

$$
\begin{align*}
\dot{q}_{i} & =\frac{\partial H}{\partial p_{i}}  \tag{20a}\\
\dot{p}_{i} & =-\frac{\partial H}{\partial q_{i}} \tag{20b}
\end{align*}
$$

for $i=1, \ldots, n$ can trivially be rewritten as

$$
\begin{equation*}
\dot{X}_{i}=\sum_{j=1}^{2 n} \Omega_{i j} \frac{\partial H}{\partial X_{j}} \tag{21}
\end{equation*}
$$

for $i=1, \ldots, 2 n$. (I leave it to you to check that this works: you will simply need to check separately the cases $1 \leq i \leq n$ and $n+1 \leq i \leq 2 n$.)

Likewise, in this notation the Poisson bracket of two functions $f(\boldsymbol{X}, t)$ and $g(\boldsymbol{X}, t)$ takes the very simple form

$$
\begin{equation*}
\{f, g\}=\sum_{i, j=1}^{2 n} \frac{\partial f}{\partial X_{i}} \Omega_{i j} \frac{\partial g}{\partial X_{j}} \tag{22}
\end{equation*}
$$

(Again, you should check this!) And the fundamental Poisson brackets among the canonical coordinates are simply

$$
\begin{equation*}
\left\{X_{i}, X_{j}\right\}=\Omega_{i j} \tag{23}
\end{equation*}
$$

(You should check this too!)
We see here the fundamental role played by the matrix $\Omega$ in defining the "geometry" of Hamiltonian phase space; it is analogous to the fundamental role played by the identity matrix $I$ in defining the geometry of Euclidean space.

In what follows it will also be extremely convenient to use Einstein's summation convention: namely, whenever an index appears exactly twice in a product - as does the index $j$ on the right-hand side of (21), and as do both of the indices $i$ and $j$ on the righthand side of (22) - then it is automatically considered to be summed from 1 to $2 n$ unless explicitly stated otherwise. So, for example, we abbreviate (21) by

$$
\begin{equation*}
\dot{X}_{i}=\Omega_{i j} \frac{\partial H}{\partial X_{j}}, \tag{24}
\end{equation*}
$$

and we abbreviate (22) by

$$
\begin{equation*}
\{f, g\}=\frac{\partial f}{\partial X_{i}} \Omega_{i j} \frac{\partial g}{\partial X_{j}} . \tag{25}
\end{equation*}
$$

This convention saves a lot of writing of summation signs, because in practice repeated indices are nearly always intended to be summed. (The prototype for this is matrix multiplication.)

Let me now use this unified notation to give the promised proof of the Jacobi identity for Poisson brackets. Gregory says (p. 416) that Jacobi's identity
is quite important, but there seems to be no way of proving it apart from crashing it out, which is very tedious. Unless you can invent a smart method, leave this one alone.

I would like to show you that with the unified notation this proof is a fairly straightforward calculation. So let us consider three functions $f, g, h$ of the phase-space coordinate $\boldsymbol{X}$; and let us prove the Jacobi identity in the form

$$
\begin{equation*}
\{f,\{g, h\}\}+\{g,\{h, f\}\}+\{h,\{f, g\}\}=0 \tag{26}
\end{equation*}
$$

By (22) [and using the summation convention] we have

$$
\begin{align*}
\{f,\{g, h\}\} & =\frac{\partial f}{\partial X_{i}} \Omega_{i j} \frac{\partial\{g, h\}}{\partial X_{j}}  \tag{27a}\\
& =\frac{\partial f}{\partial X_{i}} \Omega_{i j} \frac{\partial}{\partial X_{j}}\left(\frac{\partial g}{\partial X_{k}} \Omega_{k l} \frac{\partial h}{\partial X_{l}}\right)  \tag{27b}\\
& =\Omega_{i j} \Omega_{k l}[\underbrace{\frac{\partial f}{\partial X_{i}} \frac{\partial^{2} g}{\partial X_{j} \partial X_{k}} \frac{\partial h}{\partial X_{l}}}_{\text {"term 1" }}+\underbrace{\frac{\partial f}{\partial X_{i}} \frac{\partial^{2} h}{\partial X_{j} \partial X_{l}} \frac{\partial g}{\partial X_{k}}}_{\text {"term 2" }}] . \tag{27c}
\end{align*}
$$

Similarly, the other two triple brackets $\{g,\{h, f\}\}$ and $\{h,\{f, g\}\}$ will contains "terms 3-6" obtained by replacing $(f, g, h)$ by the cyclic permutation $(g, h, f)$ for terms $3-4$ and by $(h, f, g)$ for terms 5-6. Now I claim that term 1 will cancel term 6 , term 3 will cancel term 2 , and term 5 will cancel term 4. Let me show the proof in detail for $1 \leftrightarrow 6$; the other cases will obviously follow by cyclic permutation of $(f, g, h)$. We have

$$
\begin{equation*}
\text { term } 1+\operatorname{term} 6=\Omega_{i j} \Omega_{k l}\left[\frac{\partial f}{\partial X_{i}} \frac{\partial^{2} g}{\partial X_{j} \partial X_{k}} \frac{\partial h}{\partial X_{l}}+\frac{\partial h}{\partial X_{i}} \frac{\partial^{2} g}{\partial X_{j} \partial X_{l}} \frac{\partial f}{\partial X_{k}}\right] \tag{28}
\end{equation*}
$$

In the "term 6 " part of this equation, let us interchange the summation indices $k$ and $l$ (both of them are being summed from 1 to $2 n$, so we have a right to interchange their names): since $\Omega_{l k}=-\Omega_{k l}$, we have

$$
\begin{align*}
\text { term } 1+\text { term } 6 & =\Omega_{i j} \Omega_{k l}\left[\frac{\partial f}{\partial X_{i}} \frac{\partial^{2} g}{\partial X_{j} \partial X_{k}} \frac{\partial h}{\partial X_{l}}-\frac{\partial h}{\partial X_{i}} \frac{\partial^{2} g}{\partial X_{j} \partial X_{k}} \frac{\partial f}{\partial X_{l}}\right]  \tag{29a}\\
& =\Omega_{i j} \Omega_{k l}\left(\frac{\partial f}{\partial X_{i}} \frac{\partial h}{\partial X_{l}}-\frac{\partial h}{\partial X_{i}} \frac{\partial f}{\partial X_{l}}\right) \frac{\partial^{2} g}{\partial X_{j} \partial X_{k}}  \tag{29b}\\
& \stackrel{\text { def }}{=} \Omega_{i j} \Omega_{k l} F_{i j k l} \tag{29c}
\end{align*}
$$

where $F_{i j k l}$ is symmetric in $j, k$ and antisymmetric in $i, l$. But we then have

$$
\begin{align*}
\Omega_{i j} \Omega_{k l} F_{i j k l} & =\Omega_{l k} \Omega_{j i} F_{l k j i} & & \text { by renaming dummy indices }  \tag{30a}\\
& =\Omega_{k l} \Omega_{i j} F_{l k j i} & & \text { by antisymmetry of } \Omega \text { (used twice) }  \tag{30b}\\
& =-\Omega_{k l} \Omega_{i j} F_{i j k l} & & \text { since } F_{i j k l} \text { is symmetric in } j, k \text { and antisymmetric in } i, l \tag{30c}
\end{align*}
$$

But a quantity equal to its own negative must be zero: that is, $\Omega_{i j} \Omega_{k l} F_{i j k l}=0$ as claimed.

## 4 Canonical transformations

When we were studying Lagrangian mechanics, we saw that one of its advantages over the Newtonian formulation is that it is covariant under arbitrary changes of coordinates: that is, instead of the original coordinates $\boldsymbol{q}=\left(q_{1}, \ldots, q_{n}\right)$ we could use some new coordinates $\boldsymbol{q}^{\prime}=\left(q_{1}^{\prime}, \ldots, q_{n}^{\prime}\right)$, defined in an arbitrary way as a function of the old coordinates:

$$
\begin{align*}
q_{1}^{\prime} & =q_{1}^{\prime}\left(q_{1}, \ldots, q_{n}, t\right) \\
& \vdots  \tag{31}\\
q_{n}^{\prime} & =q_{n}^{\prime}\left(q_{1}, \ldots, q_{n}, t\right)
\end{align*}
$$

If we then define the Lagrangian $L^{\prime}\left(\boldsymbol{q}^{\prime}, \dot{\boldsymbol{q}}^{\prime}, t\right)$ to have the same values as $L$, i.e.

$$
\begin{equation*}
L^{\prime}\left(\boldsymbol{q}^{\prime}, \dot{\boldsymbol{q}}^{\prime}, t\right)=L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) \tag{32}
\end{equation*}
$$

it turns out that the Lagrange equations of motion for $L^{\prime}$ are equivalent to those for $L$. (To prove this directly from the differential equations is a nontrivial calculation; but as pointed out by Gregory, Chapter 13, pp. 387-388, this is an immediate consequence of the variational principle.)

One of the outstanding features of the Hamiltonian formalism is that it possesses an even wider flexibility: not only can we reparametrize coordinate space $\boldsymbol{q}$ to $\boldsymbol{q}^{\prime}$ as in the Lagrangian formalism (with a corresponding "dual" change from $\boldsymbol{p}$ to $\boldsymbol{p}^{\prime}$ ); we can even choose new coordinates that mix $\boldsymbol{q}$ and $\boldsymbol{p}$ ! These transformations turn out to be of immense importance, both theoretical and practical. Here we will only have time to scratch the surface of the theory of canonical transformations.

Let us consider, as usual, a $2 n$-dimensional Hamiltonian phase space parametrized by canonical coordinates $\boldsymbol{q}=\left(q_{1}, \ldots, q_{n}\right)$ and $\boldsymbol{p}=\left(p_{1}, \ldots, p_{n}\right)$. These canonical coordinates have the fundamental Poisson brackets

$$
\begin{align*}
\left\{q_{i}, q_{j}\right\} & =0  \tag{33a}\\
\left\{p_{i}, p_{j}\right\} & =0  \tag{33b}\\
\left\{q_{i}, p_{j}\right\} & =\delta_{i j} \tag{33c}
\end{align*}
$$

Now let $Q_{1}, \ldots, Q_{n}$ and $P_{1}, \ldots, P_{n}$ be arbitrary functions of $\boldsymbol{q}$ and $\boldsymbol{p}$ (and also $t$ if we wish). We say that $\boldsymbol{Q}=\left(Q_{1}, \ldots, Q_{n}\right)$ and $\boldsymbol{P}=\left(P_{1}, \ldots, P_{n}\right)$ form new canonical coordinates for phase space if they have the correct Poisson brackets, i.e.

$$
\begin{align*}
\left\{Q_{i}, Q_{j}\right\} & =0  \tag{34a}\\
\left\{P_{i}, P_{j}\right\} & =0  \tag{34b}\\
\left\{Q_{i}, P_{j}\right\} & =\delta_{i j} \tag{34c}
\end{align*}
$$

Such a transformation $(\boldsymbol{q}, \boldsymbol{p}) \mapsto(\boldsymbol{Q}, \boldsymbol{P})$ is called a canonical transformation.
In terms of the unified notation this can be stated even more simply. We start from canonical coordinates $\boldsymbol{X}=\left(X_{1}, \ldots, X_{2 n}\right)$ satisfying the fundamental Poisson brackets

$$
\begin{equation*}
\left\{X_{i}, X_{j}\right\}=\Omega_{i j} \tag{35}
\end{equation*}
$$

We then consider new coordinates $\boldsymbol{Y}=\left(Y_{1}, \ldots, Y_{2 n}\right)$ that depend in a completely arbitrary way on $\boldsymbol{X}$ (and on $t$ if we wish). The coordinates $\boldsymbol{Y}$ form new canonical coordinates if their Poisson brackets are

$$
\begin{equation*}
\left\{Y_{i}, Y_{j}\right\}=\Omega_{i j} \tag{36}
\end{equation*}
$$

In this case the transformation $\boldsymbol{X} \mapsto \boldsymbol{Y}$ is called a canonical transformation.
But we can easily work out what this means concretely, by using the definition (22) of Poisson brackets in the unified notation. We have

$$
\begin{align*}
\left\{Y_{i}, Y_{j}\right\} & =\sum_{k, l=1}^{2 n} \frac{\partial Y_{i}}{\partial X_{k}} \Omega_{k l} \frac{\partial Y_{j}}{\partial X_{l}}  \tag{37a}\\
& =\left(J \Omega J^{\mathrm{T}}\right)_{i j} \tag{37b}
\end{align*}
$$

if we define the Jacobian matrix of the transformation from $\boldsymbol{X}$ to $\boldsymbol{Y}$,

$$
\begin{equation*}
J_{i j} \stackrel{\text { def }}{=} \frac{\partial Y_{i}}{\partial X_{j}} . \tag{38}
\end{equation*}
$$

So the transformation $\boldsymbol{X} \mapsto \boldsymbol{Y}$ is a canonical transformation if and only if

$$
\begin{equation*}
J \Omega J^{\mathrm{T}}=\Omega \tag{39}
\end{equation*}
$$

Note that $J$ is actually a function of $\boldsymbol{X}$; so what we mean by (39) is that this equation should hold for all $\boldsymbol{X}$, i.e. everywhere in phase space.

A $2 n \times 2 n$ matrix $J$ satisfying (39) is called a symplectic matrix. So a transformation $\boldsymbol{X} \mapsto \boldsymbol{Y}$ is a canonical transformation if and only if its Jacobian at every point of phase space is a symplectic matrix.

Example 1: Linear transformations. A linear transformation $\boldsymbol{Y}=J \boldsymbol{X}$ is a canonical transformation if and only if the matrix $J$ (which is indeed the Jacobian matrix of the transformation, everywhere in phase space) is a symplectic matrix.

One example is the transformation

$$
\begin{align*}
Q_{i} & =p_{i}  \tag{40a}\\
P_{i} & =-q_{i} \tag{40b}
\end{align*}
$$

that interchanges the $\boldsymbol{q}$ and $\boldsymbol{p}$ (and makes one compensating sign change). You should figure out what the matrix $J$ is in this case, and convince yourself that it is indeed symplectic. (Hint: Use $\Omega^{\mathrm{T}}=-\Omega$ and $\Omega^{2}=-I$.)

Here is an opposite example: Make linear transformations of the $\boldsymbol{q}$ and $\boldsymbol{p}$ separately,

$$
\begin{align*}
& \boldsymbol{Q}=A \boldsymbol{q}  \tag{41a}\\
& \boldsymbol{P}=B \boldsymbol{p} \tag{41b}
\end{align*}
$$

where $A$ and $B$ are invertible $n \times n$ matrices. Then

$$
J=\left(\begin{array}{cc}
A & 0  \tag{42}\\
0 & B
\end{array}\right)
$$

Let us now impose the fundamental equation $J \Omega J^{\mathrm{T}}=\Omega$ [cf. (39)]:

$$
\left(\begin{array}{cc}
A & 0  \tag{43}\\
0 & B
\end{array}\right)\left(\begin{array}{cc}
0 & I \\
-I & 0
\end{array}\right)\left(\begin{array}{cc}
A^{\mathrm{T}} & 0 \\
0 & B^{\mathrm{T}}
\end{array}\right)=\left(\begin{array}{cc}
0 & I \\
-I & 0
\end{array}\right)
$$

Carrying out the matrix multiplications on the left-hand side (you should do it!), we get

$$
\left(\begin{array}{cc}
0 & A B^{\mathrm{T}}  \tag{44}\\
-B A^{\mathrm{T}} & 0
\end{array}\right)
$$

Note now that the two required equations $A B^{\mathrm{T}}=I$ and $B A^{\mathrm{T}}=I$ are in fact equivalent (they are transposes of each other). So we can take $A$ to be any invertible $n \times n$ matrix, provided that we then take $B$ to be its inverse transpose:

$$
\begin{equation*}
B=\left(A^{-1}\right)^{\mathrm{T}}=\left(A^{\mathrm{T}}\right)^{-1} \tag{45}
\end{equation*}
$$

(note that inverse and transpose commute). All such matrices (42) are symplectic matrices, and hence all such transformations (41) are canonical transformations.
(Of course, there are also many symplectic matrices that are not block-diagonal, as our example (40) showed.)

Example 2: General transformations of the coordinates $\boldsymbol{q}$. As mentioned at the beginning of this section, in the Lagrangian formalism we are free to reparametrize coordinate space any way we like, i.e. use new generalised coordinates $\boldsymbol{Q}=f(\boldsymbol{q})$ where $f$ is an arbitrary (bijective) function. In the Hamiltonian formalism we also have this freedom, but we need to make also a corresponding "dual" change from $\boldsymbol{p}$ to $\boldsymbol{P}$ :

$$
\begin{align*}
\boldsymbol{Q} & =f(\boldsymbol{q})  \tag{46a}\\
\boldsymbol{P} & =G(\boldsymbol{q}) \boldsymbol{p} \tag{46b}
\end{align*}
$$

where $G(\boldsymbol{q})$ is an $n \times n$ matrix that we will need to determine.
Let $\mathcal{J}=\mathcal{J}(\boldsymbol{q})$ be the Jacobian matrix of the transformation from $\boldsymbol{q}$ to $\boldsymbol{Q}$ :

$$
\begin{equation*}
\mathcal{J}_{i j} \stackrel{\text { def }}{=} \frac{\partial Q_{i}}{\partial q_{j}} . \tag{47}
\end{equation*}
$$

And let us write $\mathcal{K}=\mathcal{K}(\boldsymbol{q}, \boldsymbol{p})$ for the Jacobian matrix $\partial P / \partial q$ :

$$
\begin{equation*}
\mathcal{K}_{i j} \stackrel{\text { def }}{=} \frac{\partial P_{i}}{\partial q_{j}}=\sum_{k=1}^{n} \frac{\partial G_{i k}(\boldsymbol{q})}{\partial q_{j}} p_{k} . \tag{48}
\end{equation*}
$$

Then the $2 n \times 2 n$ Jacobian matrix $J=\partial Y / \partial X=\partial(Q, P) / \partial(q, p)$ is

$$
J=\left(\begin{array}{cc}
\mathcal{J} & 0  \tag{49}\\
\mathcal{K} & G
\end{array}\right)
$$

when written in terms of its $n \times n$ blocks; here the rows are $(Q, P)$ and the columns are ( $q, p$ ). 13 MAR 2024: Previously I had accidentally interchanged the rows and columns; a student pointed out my error. Let us now impose again the fundamental equation $J \Omega J^{\mathrm{T}}=\Omega$ :

$$
\left(\begin{array}{cc}
\mathcal{J} & 0  \tag{50}\\
\mathcal{K} & G
\end{array}\right)\left(\begin{array}{cc}
0 & I \\
-I & 0
\end{array}\right)\left(\begin{array}{cc}
\mathcal{J}^{\mathrm{T}} & \mathcal{K}^{\mathrm{T}} \\
0 & G^{\mathrm{T}}
\end{array}\right)=\left(\begin{array}{cc}
0 & I \\
-I & 0
\end{array}\right) .
$$

Carrying out the matrix multiplications on the left-hand side (you should again do it!), we get

$$
\left(\begin{array}{cc}
0 & \mathcal{J} G^{\mathrm{T}}  \tag{51}\\
-G \mathcal{J}^{\mathrm{T}} & -G \mathcal{K}^{\mathrm{T}}+\mathcal{K} G^{\mathrm{T}}
\end{array}\right)
$$

If we choose

$$
\begin{equation*}
G(\boldsymbol{q})=\left(\mathcal{J}(\boldsymbol{q})^{-1}\right)^{\mathrm{T}}=\left(\mathcal{J}(\boldsymbol{q})^{\mathrm{T}}\right)^{-1} \tag{52}
\end{equation*}
$$

then the upper-right and lower-left entries of (51) equal the desired entries of $\Omega$ (namely, $I$ and $-I$, respectively). HELP!!!! How to prove that $-G \mathcal{K}^{\mathrm{T}}+\mathcal{K} G^{\mathrm{T}}=0$, (i.e., that $\mathcal{K} G^{\mathrm{T}}$ is symmetric) when $G$ is defined by (52)??? It ought to follow from the identity $\partial \mathcal{J}_{i j} / \partial q_{k}=\partial \mathcal{J}_{i k} / \partial q_{j}$, which is a consequence of (47), but I haven't been able to do it. Can anyone help me???

So the transformation from the old to new momenta is "dual" to the transformation from old to new coordinates in the sense that the matrix $G=\partial P / \partial p$ has to be the inverse matrix to $\mathcal{J}=\partial Q / \partial q$.

Example 3: Time evolution. Consider a system started at time zero at a phase-space point $\boldsymbol{X}_{0}=\left(\boldsymbol{q}_{0}, \boldsymbol{p}_{0}\right)$, and let it evolve for a time $t$. Let us write $\boldsymbol{X}(t)$ for the phase-space point where the system arrives at time $t$ : this is a function of the initial condition $\boldsymbol{X}_{0}$ and $t$. So, for each value of $t$, we can consider $\boldsymbol{X}(t)$ as a function of $\boldsymbol{X}_{0}$. Let us show that, for each $t$, the transformation $\boldsymbol{X}_{0} \mapsto \boldsymbol{X}(t)$ is a canonical transformation.

By hypothesis, the function $\boldsymbol{X}\left(\boldsymbol{X}_{0}, t\right)$ satisfies the partial differential equation ${ }^{2}$

$$
\begin{equation*}
\frac{\partial X_{i}(t)}{\partial t}=\left\{X_{i}(t), H\right\} \tag{53}
\end{equation*}
$$

(where Poisson brackets are taken with respect to the canonical coordinates $\boldsymbol{X}_{0}$ ) together with the initial conditions

$$
\begin{equation*}
\boldsymbol{X}(0)=\boldsymbol{X}_{0} . \tag{54}
\end{equation*}
$$

So let us now compute how the Poisson bracket $\left\{X_{i}(t), X_{j}(t)\right\}$ varies with time:

$$
\begin{align*}
\frac{\partial}{\partial t}\left\{X_{i}(t), X_{j}(t)\right\} & =\left\{\frac{\partial X_{i}}{\partial t}, X_{j}\right\}+\left\{X_{i}, \frac{\partial X_{j}}{\partial t}\right\}  \tag{55a}\\
& =\left\{\left\{X_{i}, H\right\}, X_{j}\right\}+\left\{X_{i},\left\{X_{j}, H\right\}\right\} \quad \text { by the PDE (53) }  \tag{55b}\\
& =-\left\{X_{j},\left\{X_{i}, H\right\}\right\}+\left\{X_{i},\left\{X_{j}, H\right\}\right\} \quad \text { by antisymmetry }  \tag{55c}\\
& =\left\{X_{j},\left\{H, X_{i}\right\}\right\}+\left\{X_{i},\left\{X_{j}, H\right\}\right\} \quad \text { again by antisymmetry }  \tag{55d}\\
& =-\left\{H,\left\{X_{i}, X_{j}\right\}\right\} \quad \text { by the Jacobi identity }  \tag{55e}\\
& =\left\{\left\{X_{i}, X_{j}\right\}, H\right\} \quad \text { again by antisymmetry } \tag{55f}
\end{align*}
$$

[^1]So $F_{i j}(t) \stackrel{\text { def }}{=}\left\{X_{i}(t), X_{j}(t)\right\}$ is a function of $\boldsymbol{X}_{0}$ and $t$ that satisfies the partial differential equation

$$
\begin{equation*}
\frac{\partial F_{i j}(t)}{\partial t}=\left\{F_{i j}(t), H\right\} \tag{56}
\end{equation*}
$$

with initial condition

$$
\begin{equation*}
F_{i j}(t)=\left\{\left(\boldsymbol{X}_{0}\right)_{i},\left(\boldsymbol{X}_{0}\right)_{j}\right\}=\Omega_{i j} . \tag{57}
\end{equation*}
$$

But the solution of this partial differential equation is simply the constant function $\Omega_{i j}$ !
More precisely, the constant function $\Omega_{i j}$ does solve this partial differential equation, since $\left\{\Omega_{i j}, H\right\}=0$ [the Poisson bracket of a constant function with any other function is zero]. And I am taking for granted that, by general theory, we can prove that the solution is unique. Therefore, the solution can only be the constant function $\Omega_{i j}$.

One property of canonical transformations is that they preserve phase-space volume, i.e. $|\operatorname{det} J|=1$. This is, in fact, an immediate consequence of (39): taking determinants of both sides, we get

$$
\begin{equation*}
(\operatorname{det} J)^{2}(\operatorname{det} \Omega)=\operatorname{det} \Omega \tag{58}
\end{equation*}
$$

and hence (since $\operatorname{det} \Omega \neq 0$ ) $\operatorname{det} J=+1$ or -1 . (In fact, with more work one can prove that $\operatorname{det} J=+1 .{ }^{3}$ )

Applying this in particular to the canonical transformation associated with time evolution (Example 3 above), we obtain Liouville's theorem: the time evolution under Hamilton's equations preserves phase-space volumes. This will be discussed further in the next section.

Let us now look more closely at infinitesimal canonical transformations. That is, we consider a transformation $\boldsymbol{X} \mapsto \boldsymbol{Y}$ that is very close to the identity map, i.e.

$$
\begin{equation*}
\boldsymbol{Y}=\boldsymbol{X}+\epsilon \boldsymbol{\Psi}(\boldsymbol{X}) \tag{59}
\end{equation*}
$$

for some vector function $\boldsymbol{\Psi}(\boldsymbol{X})$ - or writing it in components,

$$
\begin{equation*}
Y_{i}=X_{i}+\epsilon \psi_{i}(\boldsymbol{X}) \tag{60}
\end{equation*}
$$

for some functions $\psi_{i}(\boldsymbol{X})(1 \leq i \leq 2 n)$. We now attempt to determine conditions on the $\left\{\psi_{i}\right\}$ such that this transformation is canonical through first order in $\epsilon$; we do this by testing the conditions (39) on the Jacobian matrix

$$
\begin{equation*}
J_{i j} \stackrel{\text { def }}{=} \frac{\partial Y_{i}}{\partial X_{j}} \tag{61}
\end{equation*}
$$

[^2]of the transformation $\boldsymbol{X} \mapsto \boldsymbol{Y}$. We see from (60) that the Jacobian matrix $J$ is
\[

$$
\begin{equation*}
J=I+\epsilon K \tag{62}
\end{equation*}
$$

\]

where

$$
\begin{equation*}
K_{i j} \stackrel{\text { def }}{=} \frac{\partial \psi_{i}}{\partial X_{j}} \tag{63}
\end{equation*}
$$

is the Jacobian matrix of the transformation $\boldsymbol{X} \mapsto \boldsymbol{\Psi}$. Substituting (62) into (39) and keeping only terms through first order in $\epsilon$, we see that the infinitesimal transformation (59) is canonical if and only if

$$
\begin{equation*}
K \Omega+\Omega K^{\mathrm{T}}=0 \tag{64}
\end{equation*}
$$

Since $\Omega$ is antisymmetric, we can also write this as

$$
\begin{equation*}
K \Omega-\Omega^{\mathrm{T}} K^{\mathrm{T}}=0 \tag{65}
\end{equation*}
$$

or in other words

$$
\begin{equation*}
K \Omega-(K \Omega)^{\mathrm{T}}=0 \tag{66}
\end{equation*}
$$

So this says that the matrix $K \Omega$ is symmetric, or equivalently that the matrix

$$
\begin{equation*}
\Omega(K \Omega) \Omega^{\mathrm{T}}=\Omega K \tag{67}
\end{equation*}
$$

is symmetric. This suggests that we should define a new vector function $\boldsymbol{\Phi}(\boldsymbol{X})$ by

$$
\begin{equation*}
\boldsymbol{\Phi}(\boldsymbol{X})=\Omega \Psi(\boldsymbol{X}) \tag{68}
\end{equation*}
$$

- or in components,

$$
\begin{equation*}
\varphi_{i}(\boldsymbol{X})=\sum_{j=1}^{2 n} \Omega_{i j} \psi_{j}(\boldsymbol{X}) \tag{69}
\end{equation*}
$$

- so that its Jacobian matrix will be $\Omega K$, i.e.

$$
\begin{equation*}
\frac{\partial \varphi_{i}}{\partial X_{j}}=(\Omega K)_{i j} \tag{70}
\end{equation*}
$$

Then the symmetry of the matrix $\Omega K$ says that

$$
\begin{equation*}
\frac{\partial \varphi_{i}}{\partial X_{j}}=\frac{\partial \varphi_{j}}{\partial X_{i}} \tag{71}
\end{equation*}
$$

for all pairs $i, j$. But this is precisely the necessary and sufficient condition for the vector function $\boldsymbol{\Phi}(\boldsymbol{X})$ to be (locally at least) the gradient of a scalar function $F(\boldsymbol{X})$. [You know this in 3 dimensions: a vector field is (locally at least) the gradient of a scalar field if and only if its curl is zero. But the principle holds true in any number of dimensions.] Thus, the infinitesimal transformation (59) is canonical if and only if there exists a scalar function $F(\boldsymbol{X})$ such that

$$
\begin{equation*}
\varphi_{i}(\boldsymbol{X})=\frac{\partial F}{\partial X_{i}} \tag{72}
\end{equation*}
$$

Left-multiplying this by $\Omega$ and using the fact that $\boldsymbol{\Psi}(\boldsymbol{X})=-\Omega \boldsymbol{\Phi}(X)$ since $\Omega^{2}=-I$, we get

$$
\begin{equation*}
\psi_{i}(\boldsymbol{X})=-\sum_{j=1}^{2 n} \Omega_{i j} \frac{\partial F}{\partial X_{j}} \tag{73}
\end{equation*}
$$

This is the necessary and sufficient condition for the infinitesimal transformation (59) to be canonical. It is convenient to get rid of the minus sign by defining $G=-F$; we thus conclude that the infinitesimal transformation (59) is canonical if and only if there exists a scalar function $G(\boldsymbol{X})$ such that

$$
\begin{equation*}
\psi_{i}(\boldsymbol{X})=\Omega_{i j} \frac{\partial G}{\partial X_{j}} \tag{74}
\end{equation*}
$$

(where we are now using the summation convention to lighten the notation). That is, every infinitesimal canonical transformation is of the form

$$
\begin{equation*}
Y_{i}=X_{i}+\epsilon \Omega_{i j} \frac{\partial G}{\partial X_{j}}, \tag{75}
\end{equation*}
$$

and conversely every infinitesimal transformation of this form is canonical. We call $G$ the generator of this infinitesimal canonical transformation. We also write (75) in the shorthand form

$$
\begin{equation*}
\delta X_{i}=\epsilon \Omega_{i j} \frac{\partial G}{\partial X_{j}} . \tag{76}
\end{equation*}
$$

But by (22) this also has an elegant expression in terms of Poisson brackets, namely

$$
\begin{equation*}
\delta X_{i}=\epsilon\left\{X_{i}, G\right\} . \tag{77}
\end{equation*}
$$

So this is one reason why Poisson brackets play such a central role in Hamiltonian mechanics: they show how to generate infinitesimal canonical transformations.

One important special case of (77) is when the generator $G$ is simply the Hamiltonian $H$ : then [by (4)] the transformation (77) is simply time evolution (forward by a time $\epsilon$ ). And we have already seen in Example 3 above that time evolution is a canonical transformation. But this second proof, using infinitesimal transformations, is arguably simpler than the first proof I gave you.

Another important special case is when the generator $G$ is one of the components of angular momentum $\mathbf{L}$, say $L_{z}$. You will show in the next problem set that the (infinitesimal) canonical transformation generated by $L_{z}$ is a (infinitesimal) rotation around the $z$ axis.

## 5 Liouville's theorem and the Poincaré recurrence theorem

This section is an elaboration on Gregory, Section 14.5.
In the previous section we saw that the time evolution $\boldsymbol{X}_{0} \mapsto \boldsymbol{X}(t)$ is a canonical transformation: that is, the Jacobian matrix

$$
\begin{equation*}
J(t) \stackrel{\text { def }}{=} \frac{\partial \boldsymbol{X}(t)}{\partial \boldsymbol{X}_{0}} \tag{78}
\end{equation*}
$$

is a symplectic matrix for all $t$. And since every symplectic matrix has determinant +1 , we can conclude that

$$
\begin{equation*}
\operatorname{det} J(t)=+1 \quad \text { for all } t \tag{79}
\end{equation*}
$$

That is:
Liouville's theorem. The time evolution under Hamilton's equations for any Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p}, t)$ preserves phase-space volumes (and preserves orientation).

As mentioned earlier, it is easy to see, by taking determinants, that every symplectic matrix has determinant $\pm 1$; and though in fact every symplectic matrix has determinant +1 , this takes more work to prove. But we can show that $\operatorname{det} J(t)=+1$ without using this deeper fact. The reasoning is simple: $J(t)$ is a continuous function of $t$, and $J(0)$ is the identity matrix. So $\operatorname{det} J(t)$ is a continuous function of $t$, and $\operatorname{det} J(0)=+1$. Since a continuous function cannot jump from +1 to -1 , it follows that $\operatorname{det} J(t)=+1$ for all $t$.

A similar argument applies to rigid-body motion, where the orientation of a rigid body at time $t$, relative to its orientation at time 0 , is given by an orthogonal matrix $R(t)$ [that is, a $3 \times 3$ real matrix satisfying $R^{\mathrm{T}} R=I$ ]. Taking determinants of the identity $R^{\mathrm{T}} R=I$, we deduce that $\operatorname{det} R= \pm 1$, and here both signs can occur: the orthogonal group consists of both rotations ( $\operatorname{det} R=+1$ ) and reflections ( $\operatorname{det} R=$ $-1)$. But we can still reason as before: $R(t)$ is a continuous function of $t$, and $R(0)$ is the identity matrix. So $\operatorname{det} R(t)$ is a continuous function of $t$, and $\operatorname{det} R(0)=+1$. Since a continuous function cannot jump from +1 to -1 , it follows that $\operatorname{det} R(t)=+1$ for all $t$. So the motion of a rigid body involves only rotations, not reflections. (This is, of course, physically obvious.)

Of course, the statement that time evolution preserves phase-space volumes is vastly weaker than the statement that time evolution is a canonical transformation. But it is, nevertheless, an important corollary.

Indeed, if all we want is Liouville's theorem and not the stronger result about time evolution being a canonical transformation, then there is a much simpler proof. Recall that a fluid flow in $\mathbb{R}^{3}$ is incompressible (i.e. preserves spatial volumes) if and only if the velocity vector field $\mathbf{v}(x, y, z, t)$ has zero divergence:

$$
\begin{equation*}
\nabla \cdot \mathbf{v}=0 \tag{80}
\end{equation*}
$$

The same holds, in fact, for the flow of a "fluid" in $\mathbb{R}^{N}$ for any dimension $N$. So let us apply this to the Hamiltonian flow in $2 n$-dimensional phase space generated by a Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p}, t)$. The velocity vector field is

$$
\begin{equation*}
\mathbf{v}=(\dot{\boldsymbol{q}}, \dot{\boldsymbol{p}})=\left(\frac{\partial H}{\partial p_{1}}, \ldots, \frac{\partial H}{\partial p_{n}},-\frac{\partial H}{\partial q_{1}}, \ldots,-\frac{\partial H}{\partial q_{n}}\right), \tag{81}
\end{equation*}
$$

and its divergence is

$$
\begin{equation*}
\nabla \cdot \mathbf{v}=\sum_{i=1}^{n} \frac{\partial}{\partial q_{i}}\left(\frac{\partial H}{\partial p_{i}}\right)+\sum_{i=1}^{n} \frac{\partial}{\partial p_{i}}\left(-\frac{\partial H}{\partial q_{i}}\right)=0 \tag{82}
\end{equation*}
$$

Now consider an autonomous Hamiltonian system, i.e. one in which the Hamiltonian $H=H(\boldsymbol{q}, \boldsymbol{p})$ does not depend on $t$. Then the time-evolution map $\mathcal{R}_{t}: \boldsymbol{X}_{0} \mapsto \boldsymbol{X}(t)$ also maps $\mathcal{R}_{t}: \boldsymbol{X}(s) \mapsto \boldsymbol{X}(s+t)$. Therefore, the time evolution defines a one-parameter group:

$$
\begin{equation*}
\mathcal{R}_{t} \circ \mathcal{R}_{s}=\mathcal{R}_{s} \circ \mathcal{R}_{t}=\mathcal{R}_{s+t} . \tag{83}
\end{equation*}
$$

Let us now apply this to a system of particles in a box, as follows. We consider $N$ particles with Euclidean coordinates $\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}$ and momenta $\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}$, with Hamiltonian

$$
\begin{equation*}
H(\boldsymbol{q}, \boldsymbol{p})=\sum_{i=1}^{N} \frac{\mathbf{p}_{i}^{2}}{2 m_{i}}+U\left(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}\right) \tag{84}
\end{equation*}
$$

We shall assume that:

1. The particles are confined to a bounded set $V \subset \mathbb{R}^{3}$. (This can be done, for instance, by taking $U\left(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}\right)$ to be $+\infty$ when one or more of the particles $\mathbf{r}_{i}$ is outside $V$, and letting $U\left(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}\right)$ smoothly approach $+\infty$ when one or more of the particles $\mathbf{r}_{i}$ approaches the boundary of $V$.)
2. The potential energy is bounded below:

$$
\begin{equation*}
U\left(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}\right) \geq-C \tag{85}
\end{equation*}
$$

for some number $C<\infty$. (This excludes things like point-particles with attractive electric or gravitational forces, since for such particles the potential energy would approach $-\infty$ as the distance between the particles approaches zero. But no real-life application of classical mechanics would involve particles whose radius is strictly zero. Indeed, the force between atoms or molecules is strongly repulsive at short distances, due to the electrical repulsion between nuclei.)

Now consider, for any value $E$, the region of the $6 N$-dimensional phase space where the Hamiltonian is $\leq E$ :

$$
\begin{equation*}
\mathcal{V}_{\leq E} \stackrel{\text { def }}{=}\left\{\left(\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}, \mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\right) \in \mathbb{R}^{6 N}: H(\boldsymbol{q}, \boldsymbol{p}) \leq E\right\} \tag{86}
\end{equation*}
$$

This region has finite volume: the particle positions $\mathbf{r}_{1}, \ldots, \mathbf{r}_{N}$ are confined to the bounded region $V$, and the particle momenta $\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}$ are confined to the ellipsoid

$$
\begin{equation*}
\sum_{i=1}^{N} \frac{\mathbf{p}_{i}^{2}}{2 m_{i}} \leq E+C \tag{87}
\end{equation*}
$$

We also observe that since the Hamiltonian is a conserved quantity, the time evolution $\mathcal{R}_{t}$ maps $\mathcal{V}_{\leq E}$ to itself.

Now fix some number $T>0$ : we will consider the time evolution at integer multiples of $T$, i.e. $\mathcal{R}_{T}, \mathcal{R}_{2 T}, \mathcal{R}_{3 T}, \ldots$. And let $U$ be any nonempty open set lying in $\mathcal{V}_{\leq E}$ (for instance, an $\epsilon$-ball around some point in the interior of $\mathcal{V}_{\leq E}$ ). We can now state:

Poincaré recurrence theorem (weak form). There exists $n>0$ such that $U \cap \mathcal{R}_{n T} U \neq \varnothing$.

In other words, there exists a time $n T$ at which at least one of the points in $U$ has returned to $U$. If $U$ is an $\epsilon$-ball, this implies:

There exists a time $n T$ at which at least one of the points in $U$ has returned to within $2 \epsilon$ of its starting position.

Please remember that "position" here means position in the 6 N -dimensional phase space. So it means that

There exists a time $n T$ at which, for at least one of the points in $U$, all of the particles have returned to within $2 \epsilon$ of their initial positions and their initial momenta.

Imagine this for a system of $N=10^{23}$ molecules of a gas, bouncing around in the box $V$. If we wait long enough, we will come to a time when every single one of the molecules has returned simultaneously to within $2 \epsilon$ of its initial position and its initial momentum! And this, no matter how small $\epsilon>0$ is!

Proof of the Poincaré recurrence theorem. By Liouville's theorem, the map $\mathcal{R}_{T}$ is volume-preserving. Therefore $\operatorname{vol}\left(\mathcal{R}_{n T} U\right)=\operatorname{vol}(U)$ for all $n$. And of course $\operatorname{vol}(U)>0$ because $U$ is a nonempty open set. Moreover, all the sets $\mathcal{R}_{T} U, \mathcal{R}_{2 T} U, \mathcal{R}_{3 T} U, \ldots$ are contained in $\mathcal{V}_{\leq E}$, since $U \subset \mathcal{V}_{\leq E}$ and the time evolution maps $\mathcal{V}_{\leq E}$ to itself.

If the sets $\mathcal{R}_{T} U, \mathcal{R}_{2 T} U, \mathcal{R}_{3 T} U, \ldots$ were disjoint, then we would have

$$
\begin{equation*}
\operatorname{vol}\left(\mathcal{V}_{\leq E}\right) \geq \sum_{n=1}^{\infty} \operatorname{vol}\left(\mathcal{R}_{n T} U\right)=\infty \tag{88}
\end{equation*}
$$

contrary to the fact that $\operatorname{vol}\left(\mathcal{V}_{\leq E}\right)<\infty$. So there must exist positive integers $m<n$ such that $\mathcal{R}_{m T} U \cap \mathcal{R}_{n T} U \neq \varnothing$. But applying $\left(\mathcal{R}_{m T}\right)^{-1}=\mathcal{R}_{-m T}$ to this identity, we conclude that

$$
\begin{equation*}
U \cap \mathcal{R}_{(n-m) T} U \neq \varnothing, \tag{89}
\end{equation*}
$$

which proves the claim.
With a bit more work, one can prove:
Poincaré recurrence theorem (strong form). For almost every point $\boldsymbol{x} \in U$, there exists $n>0$ such that $\mathcal{R}_{n T} \boldsymbol{x} \in U$.

Here "almost every" means in the sense of measure theory, i.e. "except for a set of measure zero". Indeed, one can prove:

Poincaré recurrence theorem (very strong form). For almost every point $\boldsymbol{x} \in U$, we have $\mathcal{R}_{n T} \boldsymbol{x} \in U$ for infinitely many values of $n$.

It is important that we here say "almost every"; it is not in general true that every trajectory comes back to near its initial position. Consider, for instance, a pendulum formed by a mass $m$ attached to a rigid rod. There are some initial conditions for which, as $t \rightarrow+\infty$, the pendulum approaches the point of unstable equilibrium $\left(\theta=\pi, p_{\theta}=0\right)$, without ever reaching it. These trajectories obviously do not have the recurrence property. But these trajectories occur only for one special value of the energy; and the points with that energy form a lower-dimensional submanifold in phase space, and hence have zero volume.

Of course, Poincaré's recurrence theorem doesn't tell us anything about how long we have to wait until $U \cap \mathcal{R}_{n T} U \neq \varnothing$. But from the proof we can get a crude estimate of this recurrence time. For a system of $N$ particles, the phase space is $6 N$-dimensional, so the volume of an $\epsilon$-ball is of order $\epsilon^{6 N}$. On the other hand, the volume of the set $\mathcal{V}_{\leq E}$ is very crudely

$$
\begin{equation*}
\operatorname{vol}\left(\mathcal{V}_{\leq E}\right) \sim \operatorname{vol}(V)^{N}(E+C)^{3 N / 2} \tag{90}
\end{equation*}
$$

where the first factor gives the allowed volume in position space and the second factor gives the allowed volume in momentum space. Then the recurrence time - or at least, the upper bound on the recurrence time given by our proof - is the ratio of these volumes:

$$
\begin{equation*}
\frac{\operatorname{vol}\left(\mathcal{V}_{\leq E}\right)}{\operatorname{vol}(U)} \sim\left(\frac{\operatorname{vol}(V)(E+C)^{3 / 2}}{\epsilon^{6}}\right)^{N} \tag{91}
\end{equation*}
$$

Here the quantity in parentheses on the right-hand side is basically what the ratio of the volumes of $\mathcal{V}_{\leq E}$ to $U$ would be for a system consisting of a single particle. So imagine that this ratio is merely 10 , and imagine that the number of particles is merely $N=100$; then the recurrence time is almost certainly longer than the age of the universe!

The practical relevance of Poincaré's recurrence theorem for statistical physics is thus far from clear. But it is an important result in the mathematical field known as ergodic theory.


[^0]:    ${ }^{1}$ After the Norwegian mathematician Sophus Lie (1842-1899), who created the theory of continuous symmetry - what is now known as the theory of Lie groups and Lie algebras - and applied it to differential geometry and differential equations. These theories now play a central role in many areas of mathematics and theoretical physics.

[^1]:    ${ }^{2}$ The meaning of $\partial / \partial t$ in equation (53) may be a bit confusing, since it is not the same as the meaning of $\partial / \partial t$ in equation (4). So let me try to explain.
    In equation (4), $f$ is a function of $\boldsymbol{q}, \boldsymbol{p}$ and $t: \partial f / \partial t$ denotes the explicit time-dependence (if any) in $f$, while $\{f, H\}$ captures the time-dependence of $f$ that comes through its dependence on $\boldsymbol{q}$ and $\boldsymbol{p}$, which themselves evolve in time according to Hamilton's equations (1).
    In the present situation, by contrast, there is no explicit time-dependence in $f$, because $f$ is just a coordinate $X_{i}$ (that is, either a $q_{i}$ or a $p_{i}$ ). So $\boldsymbol{X}(t)$ evolves in time only by the Poisson bracket $\{\boldsymbol{X}, H\}[\mathrm{cf}$. (1)]. So the left-hand side of (53) would normally be written with $d$, not $\partial$. The reason I write it here with $\partial$ is that we are now considering $\boldsymbol{X}$ to be a function not only of $t$ but also of the initial conditions $\boldsymbol{X}_{0}$; so I write $\partial / \partial t$ to mean the derivative with respect to $t$ when the initial conditions $\boldsymbol{X}_{0}$ are held fixed. (Usually we just consider the initial conditions to be fixed, so we don't make the dependence on $\boldsymbol{X}_{0}$ explicit; but here the whole point is to consider simultaneously all possible initial conditions $\boldsymbol{X}_{0}$, in order to study the properties of the map $\boldsymbol{X}_{0} \mapsto \boldsymbol{X}(t)$.)

[^2]:    ${ }^{3}$ The standard proof that det $J=+1$ uses the pfaffian, which is a kind of "square root of the determinant" for antisymmetric matrices. See https://en.wikipedia.org/wiki/Pfaffian and https://en.wikipedia. org/wiki/Symplectic_matrix\#Determinantal_properties

