

Lecture 20: March 17

Instructor: Veit Elser

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20.1 Origins and consequences of Liouville's theorem

20.1.1 Quantum incompressibility

If phase space volumes were *not* constant under time evolution, there would be a problem reconciling classical and quantum mechanics. In classical mechanics we may specify both the position and momentum of a particle to arbitrary precision. This is not the case in quantum mechanics. Before we discuss how this fundamental constraint impacts even classical mechanics, let's review some facts from elementary quantum mechanics.

A *wavepacket state* of a particle moving in one dimension has a wavefunction with three parameters:

$$\Psi(x) = A \exp \left(i p_0 (x - x_0) / \hbar - \frac{(x - x_0)^2}{4 \Delta x^2} \right). \quad (20.1)$$

The parameter p_0 corresponds to the particle's momentum, x_0 its position, and Δx is the spatial extent of the wavepacket — the uncertainty in the particle's position. The factor A is not a parameter because it is determined by normalization. A simple calculation shows that

$$\langle (x - x_0)^2 \rangle = \frac{\int \Psi^* (x - x_0)^2 \Psi dx}{\int \Psi^* \Psi dx} = (\Delta x)^2. \quad (20.2)$$

The particle momentum of the wavepacket state is also not precisely defined. The best way to see that is to check that the wavefunction can be expressed as the following integral over all momenta p :

$$\Psi(x) = A' \int \exp \left(i p (x - x_0) / \hbar - \frac{\Delta x^2}{\hbar^2} (p - p_0)^2 \right) dp. \quad (20.3)$$

The wavepacket is therefore a superposition of “plane-wave” states of definite momentum p , with p distributed as a Gaussian function about the mean momentum p_0 . The width of this Gaussian determines the value of the momentum uncertainty¹:

$$(\Delta p)^2 = \langle (p - p_0)^2 \rangle = \frac{\int \Psi^* \left(-i \hbar \frac{d}{dx} - p_0 \right)^2 \Psi dx}{\int \Psi^* \Psi dx} = \left(\frac{\hbar}{2 \Delta x} \right)^2. \quad (20.4)$$

The more precisely we specify the position of the particle ($\Delta x \rightarrow 0$), the more imprecise is the particle's momentum — and vice versa. Wavepacket states can be summed up by a statement that resembles Heisenberg's uncertainty principle:

$$\Delta x \Delta p = \hbar/2. \quad (20.5)$$

¹The most expeditious method of calculation uses the integral expression (20.3) and the identity $\int \exp(i(p - p')x/\hbar) dx = 2\pi\hbar \delta(p - p')$.

This is an *equality*, rather than the more familiar inequality, because we have specialized to wavepacket states. Wavepackets provide a bridge between classical mechanics and quantum mechanics — a method of approximating the latter by the former. In a sense, wavepacket states just have two parameters: the mean position x_0 and the mean momentum p_0 . The width parameter Δx only serves to specify the dimensions $(\Delta x, \Delta p)$ of the rectangular phase space region, centered on (x_0, p_0) , that we associate with the wavepacket. By (20.5), the phase space “assigned” to a state always has area $\hbar/2$.

Two wavepacket states can be considered to be distinct when their respective phase space regions — rectangles of area $\hbar/2$ — are disjoint. From this we can estimate the number of quantum states associated with the phase space regions $A(t)$ we study in Hamiltonian mechanics:

$$\text{number of states} = \frac{\text{area}(A(t))}{\hbar/2}. \quad (20.6)$$

It is a good thing, thanks to Liouville’s theorem, that the area of $A(t)$ does not change with time: otherwise quantum states (wavepackets with parameters in the interior of $A(t)$) would have to be created or destroyed! The perfect incompressibility of the substance of phase space — *hamiltonium* — must have seemed mysterious to Liouville. Quantum mechanics resolves this mystery by conferring phase space with a particular microscopic structure.

The wavepacket description generalizes to systems with arbitrary numbers of degrees of freedom N . A particle wavepacket in three dimensions occupies a region of area $\hbar/2$ in each of three planes of phase space, $(\Delta x, \Delta p_x)$, $(\Delta y, \Delta p_y)$ and $(\Delta z, \Delta p_z)$, for a $6D$ -volume of $(\hbar/2)^3$. Wavepacket states can be constructed for any system described classically by generalized coordinates and conjugate momenta. The number of such states associated with a $2N$ dimensional phase space region $A(t)$ equals $\text{vol}(A(t))/(\hbar/2)^N$. By Liouville’s theorem, this number remains constant in time as $A(t)$ evolves. In quantum mechanics this is explained by the principle that quantum states are neither created nor destroyed in the course of time evolution.

20.1.2 Poincaré recurrence

The constancy in time of the volumes of phase space regions gives us the machinery to prove general properties of dynamical systems that appear paradoxical in light of everyday experience. In particular, the recurrence property of Poincaré asserts — given some technical assumptions — that a system “will eventually return arbitrarily close to its initial conditions given enough time”. This seems outrageous when we imagine applying it to a gas that is prepared in a state where all the molecules start in one half of a box.

We will prove the theorem of Poincaré as an exercise in phase space reasoning. Upon close examination, the statement of the theorem is weaker than the popular version quoted above. This removes part of the paradox. The theorem also says nothing about the time required for the initial conditions to be approximately restored. A diverging time scale for recurrence, say as a function of the number of degrees of freedom, would also bring the theorem in line with everyday experience.

The technical condition we need is that the volume of phase space accessible to the system is bounded. Many systems naturally satisfy this condition. Consider a system of molecules with repulsive interactions confined to a box. The box bounds the available range of the q ’s (particle positions) while the fixed energy of the system and the positive (repulsive) potential energy bounds the kinetic energy and therefore the range of the p ’s (particle momenta).

Let $A(0)$ be a region of phase space representing the possible initial conditions of the system. As $A(0)$ is made progressively smaller, the initial conditions are more precisely defined. After time t the initial conditions in $A(0)$ will have evolved to region $A(t)$. We will assume that there exists a time t_0 such that $A(0)$ and $A(t_0)$ are disjoint. If such a time did not exist, as might happen when $A(0)$ is the neighborhood of a stable equilibrium point, then it would not be necessary to prove “recurrence”.

The statement of recurrence takes the following form:

Poincaré recurrence theorem: There exists a phase space point $z(0) \in A(0)$ and a finite time t such that $z(0)$ flows to $z(t) \in A(0)$ in time t .

The proof goes as follows. Consider regions $A(t_0)$, $A(2t_0)$, $A(3t_0)$, etc. that $A(0)$ flows to after times t_0 , $2t_0$, $3t_0$ etc. All of these regions have exactly the same volume by Liouville's theorem. Moreover, this infinite sequence of regions cannot all be disjoint, otherwise the accessible volume of phase space would not be bounded. Therefore, there must exist regions $A(mt_0)$ and $A(nt_0)$, for $m < n$, that intersect. Let $z(nt_0)$ be a point in the intersection of these regions.

Now run time backwards (reversed-time evolution) by $-nt_0$ on region $A(nt_0)$ and $-mt_0$ on region $A(mt_0)$. This reverse time evolution also sends $z(nt_0)$ to $z(0)$, when $z(nt_0)$ is treated as a point in $A(nt_0)$, and to $z((n-m)t_0)$ when $z(nt_0)$ is treated as a point in $A(mt_0)$. The result of these time-reversed evolutions is a single region $A(0)$ that contains the two points $z(0)$ and $z((n-m)t_0)$. We have therefore constructed a point $z(0)$ that flows to $z(t)$ in time $t = (n-m)t_0$, and both points are in the same region $A(0)$. That concludes the proof.

In addition to the “recurrence time” being possibly very long, the statement of the recurrence theorem alerts us to the possibility that one might have to work very hard to find a “recurring initial condition” in the region $A(0)$, no matter how small we make this region. A useful way to think about this challenge is addressed in the next lecture.