PHASE SPACE

TERENCE TAO

1. Phase space

In physics, phase space is a concept which unifies classical (Hamiltonian) mechanics and quantum mechanics; in mathematics, phase space is a concept which unifies symplectic geometry with harmonic analysis and PDE.

In classical mechanics, the phase space is the space of all possible states of a physical system; by "state" we do not simply mean the positions q of all the objects in the system (which would occupy *physical space* or *configuration space*), but also their velocities or *momenta* p (which would occupy *momentum space*). One needs both the position and momentum of system in order to determine the future behavior of that system. Mathematically, the configuration space might be defined by a manifold M (either finite[1] or infinite dimensional), and for each position $q \in M$ in that space, the momentum p of the system would take values in the cotangent[2] space $T_q^* M$ of that space. Thus phase space is naturally represented here by the *cotangent bundle* $T^*M := \{(q,p) : q \in M, p \in T_q^* M\}$, which comes with a canonical *symplectic form* $\omega := dp \wedge dq$.

Hamilton's equation of motion describe the motion $t \mapsto (q(t), p(t))$ of a system in phase space as a function of time in terms of a *Hamiltonian* $H : M \to \mathbf{R}$, by *Hamilton's equations of motion*

$$\frac{d}{dt} q(t) = \frac{\partial H}{\partial p}(q(t), p(t)); \quad \frac{d}{dt} p(t) = -\frac{\partial H}{\partial q}(q(t), p(t)),$$

or equivalently in terms of the symplectic form ω as

$$\dot{x}(t) = \nabla_\omega H(x(t)),$$

where $x(t) := (q(t), p(t))$ is the trajectory of the system in phase space, and ∇_ω is the symplectic gradient, thus $\omega(\cdot, \nabla_\omega H) = dH$. Thus Hamilton's equation of motion are the analogue of gradient flow for H on the manifold T^*M, but with respect to a symplectic form ω rather than a Riemannian metric.

[1] To simplify the discussion we shall completely ignore any issues such as differentiability, smoothness, etc. and work instead on a purely formal level.

[2] This may seem surprising; since velocity $\dot{q}$ naturally lives in the tangent space $T_q M$, one would expect momentum to also. However, from Lagrangian mechanics, in which the system evolves by finding formal critical points of a Lagrangian $\int L(q(t), \dot{q}(t))\ dt$, the momentum is defined as $p := \frac{\partial L}{\partial \dot{q}}$, which lives most naturally in the cotangent space. Dually, the Hamiltonian links momentum to velocity by Hamilton's equation $\dot{q} = \frac{\partial H}{\partial p}$.

An alternative description of Hamiltonian's equations is in terms of *observables*, which in classical mechanics is simply a function $A : T^*M \to \mathbf{R}$ in phase space (thus the Hamiltonian is itself an observable, known as the *energy*). Hamilton's equation of motion then become

$$\frac{d}{dt}A(x(t)) = \{A, H\}(x(t))$$

where $\{A, H\} := \omega(\nabla_\omega A, \nabla_\omega H)$ is the *Poisson bracket* of A and H.

Now we turn to quantum mechanics. As is well known, a quantum mechanical state does not necessarily have a well-defined position or a well-defined momentum (and certainly cannot have both). Nevertheless, the notion of phase space T^*M, and of a Hamiltonian $H : T^*M \to \mathbf{R}$ survives, and indeed can be viewed as a crucial link between what otherwise looks like two very different theories. A state is now not a point in phase space, but is instead a *wave function*, which is a complex-valued function $\psi : M \to \mathbf{C}$ (usually normalized to have total probability one). The classical Hamiltonian $H : T^*M \to \mathbf{R}$ is then *quantized* to a self-adjoint operator $\mathbf{Op}(H) : M \to M$. The precise prescription of this quantization is technical (and not even unique), but can be described informally as follows. Certain classes of wave function are strongly localized in both position and momentum; for instance a function which is a "wave packet", which roughly speaking is a function which looks (in local co-ordinates) like

$$\psi(q) \approx e^{\frac{i}{\hbar}(q-q_0)\cdot p_0}\varphi(q - q_0), \tag{1}$$

where $\varphi(q - q_0)$ is a bump function localized to near q_0, and $\hbar > 0$ is a small parameter (Planck's constant), can be viewed as having position roughly q_0 and frequency roughly $\frac{p_0}{\hbar}$, and hence momentum roughly p_0 (by Planck's law $p = \hbar\xi$). The operator $\mathbf{Op}(H)$ should behave like the classical Hamiltonian in the sense that

$$\mathbf{Op}(H)\psi \approx H(q_0, p_0)\psi$$

whenever ψ is localized to have position near q_0 and momentum near p_0. Hamilton's equations of motion can then be replaced by *Schrödinger's equation of motion*

$$\frac{d\psi}{dt} = -\frac{i}{\hbar}\mathbf{Op}(H)\psi.$$

This equation may not initially resemble Hamilton's equation, but they become much more similar when tested against observables. Indeed, for any observable $A : T^*M \to \mathbf{R}$, with its corresponding quantization $\mathbf{Op}(A)$, we have (formally, at least) the *Heisenberg equation*

$$\frac{d}{dt}\langle \mathbf{Op}(A)\psi(t), \psi(t)\rangle = \langle \frac{i}{\hbar}[\mathbf{Op}(H), \mathbf{Op}(A)]\psi(t), \psi(t)\rangle$$

where $[\mathbf{Op}(H), \mathbf{Op}(A)] = \mathbf{Op}(H)\mathbf{Op}(A) - \mathbf{Op}(A)\mathbf{Op}(H)$ is the *Lie bracket* or *commutator* of $\mathbf{Op}(H)$ and $\mathbf{Op}(A)$.

The analogy between quantum mechanics and classical mechanics provides a fertile heuristic platform for analyzing functions $\psi : M \to \mathbf{C}$ in general (not necessarily wave functions associated to a quantum system) by viewing them as distributions in phase space, though the famous *Heisenberg uncertainty principle* prevents this analogy from being formalized perfectly (unless one introduces correction terms which are lower order in $\hbar$). From such tools as localized Fourier transforms one can write an arbitrary function ψ as a linear combination of wave packets such as (1), and the coefficients of such combination thus should describe how ψ is distributed in phase space, just as how the decomposition of a musical sound wave into individual notes descibes how a musical piece is distributed in both time and frequency. The precise way to describe this distribution is not unique (and perhaps surprisingly, the exact choice of distribution is not always particularly important!); one choice is to introduce the *Wigner distribution* $W_\psi(q,p)$, defined in the Euclidean setting $M = \mathbf{R}^n$ by the formula

$$W_\psi(q,p) := \int_{\mathbf{R}^n} e^{-2\pi i v \cdot p} \psi(q+v/2)\overline{\psi(q-v/2)}\ dv.$$

We caution that while this distribution is a quantum analogue of the probability distribution in phase space in classical statistical mechanics, it is not non-negative everywhere (although it is positive in various averaged senses).

The phase space distribution (also known as the *phase space portrait*, or the *score* of a function, in analogy to the musical example mentioned earlier) is a useful guide for understanding the singularities of a function, and how that function will behave with respect to various operators (such as the observables $\mathbf{Op}(H)$ mentioned above) and under evolution by various PDE; the rigorous formalization of these heuristics is known as *microlocal analysis*, *time-frequency analysis*, or *semi-classical analysis*.

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