Crash course on Quantum Mechanics

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Jan 22, 2003

One of the main applications of Functional Analysis is the solid mathematical foundation of quantum mechanics. Here I outline a few key ideas.

In classical mechanics of point particles, the physical state of a particle is given by two vectors, $\mathbf{x}$ and $\mathbf{v}$ in $\mathbf{R}^d$ (typically $d = 3$ is the dimension of our physical space), where $\mathbf{x}$ represents the position and $\mathbf{v}$ the velocity of the particle. Several (say N) particles can be described by a single position and velocity vectors $\mathbf{x}, \mathbf{v} \in \mathbf{R}^{Nd}$ in a high dimensional space.

If we know the forces acting on these particles, by Newton's equation we can predict its dynamics. Newton's equation is a second order ordinary differential equation for the (time-dependent) position $\mathbf{x}(t)$ of the particles

$$\frac{d^2}{dt^2}\mathbf{x}(t) = F(\mathbf{x}(t))$$

where F is the force field. Here we assumed that the force depends only on the position, but for example the magnetic forces depend also on the velocity, so $F(\mathbf{x}, \dot{\mathbf{x}})$ is also possible.

By the basic existence and uniqueness theory of ordinary differential equations, the Newton's equation has a unique solition for all times if the initial conditions $x(0) = x$, $\dot{x}(0) = v$ at $t = 0$ are given. We need two initial conditions because the equation is of second order and for the same reason the position and velocity determines the complete state of the particle.

If the system is conservative, i.e it preserves energy, then the force field is a gradient field and it is given by a real valued potential function U

$$F(\mathbf{x}) = -\nabla U(x).$$

The total energy of the system

$$E = \frac{1}{2}\mathbf{v}^2 + U(\mathbf{x})$$

is preserved under the evolution (CHECK!) (Here mass and other physical quantities and units are neglected)

In quantum mechanics, the state of a particle is described by a **wavefunction** ψ, that is a complex valued L^2-function defined on the configuration space $\mathbf{R}^3$ (in case of 1 particle). We also assume that ψ is normalized, $\|\psi\|_{L^2(\mathbf{R}^3)} = 1$. The space $L^2(\mathbf{R}^3)$ is the Hilbert space of physical states; and although most physical states are normalized, it is convenient to extend the discussion to non-normalized states as well to be able to work in a linear structure.

The interpretation is that the normalized measure given by the density $|\psi(x)|^2 dx$ determines the probability of the location of the particle. A basic postulate of quantum mechanics is that one cannot locate the position of the particle deterministically, but one can answer to questions of probabilistic nature: "What is the probability to find a particle in a certain domain of the configuration space?". This is answered by this density function as

$$\text{Prob}\Big(\text{the particle is in A}\Big) = \int_A |\psi(x)|^2 dx$$

where A is a measurable subset of $\mathbf{R}^3$.

Similarly, the Fourier transform, $\widehat{\psi}(v)$ of the wavefunction ψ gives the distribution of the velocity (more precisely, momentum) of the particle:

$$\text{Prob}\Big(\text{the velocity of the particle is in A}\Big) = \int_A |\widehat{\psi}(v)|^2 dv$$

The state of the particle evolves with time, hence it is described by a time-dependent wavefunction, $\psi_t(x)$ that is a normalized L^2 function at any time t. The evolution is described by the Schrödinger equation

$$i\partial_t\psi_t(x) = H\psi_t(x)$$

where H is an operator (the so called Hamilton-operator or energy operator of the system) that acts on the Hilbert space of states.

The Hamiltonian is the basic object in quantum physics, it contains the physical description of the model. It encodes the energy of the system, namely the energy of a state ψ in a system described by H is

$$E = (\psi, H\psi)$$

where $(\cdot,\cdot)$ is the usual scalar product in L^2. For example, the simplest quantum system, a freely moving quantum particle in a potential field U is given by

$$H = -\frac{1}{2}\Delta_{\mathbf{x}} + U(\mathbf{x}) \qquad (1)$$

where

$$\Delta_{\mathbf{x}} := \sum_{j=1}^{3} \frac{\partial^2}{\partial x_j^2}$$

is the Laplace operator.

For example, the quantum system of an electron subject to the Coulumb potential of a nucleus of charge Z sitting at the origin is described by (1) with $U(\mathbf{x}) = -Z/|\mathbf{x}|$. Note that the form and the role of the potential is exactly the same as in classical mechanics, but instead of the velocity-square for the kinetic energy we have the (minus) Laplacian. The analogy is easy to see if we accept that the velocity (more precisely, the momentum) in quantum mechanics is given by $-i\nabla_{\mathbf{x}}$, i.e. it is given by the *operator of differentiation* on the physical states ψ, and note that $(-i\nabla_{\mathbf{x}})^2 = -\Delta_{\mathbf{x}}$.

It is also one of the basic postulate of QM that the wavefunction cannot be measured ("observed") directly. Only quantities of the form

$$(\psi, O\psi)$$

can be results of experiments, where O is an operator on the Hilbert space. In particular, an overall phase factor, $\psi \mapsto \psi e^{ic}$, $c \in \mathbf{R}$, does not change the result of the physical measurements. In other words the physical states are normalized L^2 functions modulo an overall phase multiple. Again, it is better to work on the original Hilbert space and not on the factorized one in order to keep the linear structure and simply keep in mind that the representation of the physical state by a normalized wavefunction is not unique.

At this level we have to accept these strangely looking postulates as axioms. There are many discussions and research on the axiomatic foundation of quantum mechanics and some schools debate that this should be the starting point. However, it is a fact of the Nature and verified by enormous number of experiments, that this model, whatever strange it looks, predicts all quantum phenomenon with enormous precision. Its most important justification is quite pragmatic: it works, i.e. its predictions coincide with the experiments.

The evolution of the system (i.e. the solution to the Schrödinger equation (1)) can be formally given as

$$\psi_t(\mathbf{x}) = e^{-itH}\psi_0(\mathbf{x}) \qquad (2)$$

analogously to the solution to the system of first order differential equations; if

$$\dot{\mathbf{u}}(t) = A\mathbf{u}(t)$$

then

$$\mathbf{u}(t) = e^{tA}\mathbf{u}(0)$$

However, there is a seemingly technical but important problem: how to exponentiate the operator H?? For finite matrices, we simply defined

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}$$

and the series converged in any matrix norm, because $\|A^n\| \le \|A\|^n$ and $\|A\| < \infty$.

In case of quantum mechanics, even the simplest system, a freely moving electron with no potential ($U = 0$, $H = -\frac{1}{2}\Delta$) gives rise to exponentiating the Laplacian that is an unbounded operator. We know that there is no such constant K that

$$\|\Delta f\|_{L^2} \le K\|f\|_{L^2}.$$

Actually the situation is even worse; Δ is defined on C^2 functions, and we know we can extend the definition to the Sobolev space H^2, but there is no way to extend $\Delta : L^2 \mapsto L^2$. Since Δ is a symmetric but unbounded operator, this would contradict to the Hellinger-Toeplitz theorem.

Therefore the naive definition

$$e^{-it\Delta} = \sum_{n=0}^{\infty} \frac{(-it\Delta)^n}{n!} \qquad (3)$$

does not work, at least it does not work on all L^2 functions (it works on C^∞ functions whose derivatives are sufficiently decaying). This is the main consequence of Hellinger-Toeplitz (which was a corollary of the Closed Graph Theorem, that was a corollary of the Open Mapping Theorem).

The solution to this problem is more complicated than one naively thinks. The main point is that i in the exponent helps. While $e^{-t\Delta}$ cannot be defined from L^2 to L^2, $e^{-it\Delta}$ can. The main reason being that $-\Delta$ behaves like a nonnegative real number (due to the fact that $(\psi, (-\Delta)\psi) = \int |\nabla\psi|^2 \ge 0$), so $e^{-t\Delta}$ blows up exponentially, while the norm of $e^{-it\Delta}$ remains 1 for any t, like $|e^{-ict}| = 1$ for any $c \in \mathbf{R}$. This boundedness will enable us to extend the definition of $e^{-it\Delta}$ from the set of nice, smooth, decaying functions (that are dense in L^2) to all L^2 functions. Recall that if $f_n \to f$ and A is bounded, then Af_n converges, hence $\lim Af_n$ *can be used to extend* A from a dense subset to the whole Hilbert space L^2.

However, showing that $e^{-it\Delta}$ is an operator with norm 1 on nice, smooth, decaying functions is not easy. Even if the formula (3) makes sense (converges) for such nice functions, it is not clear why it should remain bounded independently of t. Think of the power series expansion of e^{-ict}:

$$e^{-ict} = \sum_{n=0}^{\infty} \frac{(-ict)^n}{n!} \qquad (4)$$

While the absolute value of the sum is 1, it is hard to see this fact if you do not know the left hand side. The terms around $n \sim ct$ in the sum are exponentially big:

$$\left| \frac{(-ict)^{ct}}{(ct)!} \right| \sim e^{ct}$$

nevertheless, due to the i factor, these big terms miraculously cancel each other so that the result is 1. The same cancellation must be understood for the series (3) with powers of the Laplacian. Similarly to the proof of the fact that the right hand side of (4) is of order one, we will not attack this problem directly from the power series point of view, but we will try to give an independent meaning of $e^{-it\Delta}$. This is a long story and will be left to Functional Analysis II.