

Re: 10 questions on QM postulates

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> I am an undergrad physics student who just completed a course in
> modern physics (mostly an introduction to QM). I have several
> questions related to the postulates of Quantum mechanics which I find
> intriguing and which my textbook imo did not address adequately. I
> have listed my questions below. I know there are a lot of questions;
> answering just one at a time would be great.

I'd be interested to know which book you used in your course.

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> 1) How can the mathematical concept of hermitian operators be
> translated into physical terms? What are all the conditions which
> ultimately restrict operators such that they can be only hermitian as
> opposed to any other type?

That's a very deep question, and I also asked it to my professor when he introduced the concept. His answer was: "The operators, describing observables, must have only real eigenvalues, and Hermitean operators have only real eigenvalues."

In my opinion, that's a short but not really satisfactory answer. After thinking about the foundations of quantum theory from time to time (I apply quantum theory every day, but one does not think about its foundations too often in this kind of work, so it's more a hobby of mine to think about it from time to time, especially when I hear something about modern quantum-optics experiments, which help a lot to understand the foundations of quantum theory), I think the real mathematical reason that the observables can be described without any inconsistencies by Hermitean (or to be more precise by essentially self-adjoint) operators is the spectral theorem, i.e., each quantum state can be described by a superposition of a complete set of generalized eigenvectors of a self-adjoint operator.

I do not claim that an operator must be necessarily self-adjoint to meet this property. I'm not sure whether it is or not, it might be sufficient that an operator commutes with its adjoint, which is usually called a "normal operator". Perhaps somebody more familiar with the mathematical details may answer this question.

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Anyway, the point of the spectral theorem is that you can interpret the (generalized) components of any Hilbert-space vector $|\psi\rangle$ with respect to the (generalized) eigenvectors $|a\rangle$ of an self-adjoint operator A as probability (distribution) amplitudes. In more physical terms, this means that, provided the system in question is prepared in the state, described by the Hilbert-space vector $|\psi\rangle$, the probability (distribution) to find the value a when measuring the observable A is given by

$$P(a|\psi) = \langle a|\psi\rangle^2 \quad (|\psi\rangle \text{ normalized, i.e. } \langle\psi|\psi\rangle = 1).$$

Here I simplify the argument a little bit by assuming that each measurement of A is complete, i.e., for each (generalized) eigenvalue a there is only one linearly independent (generalized) eigenvector.

Now the $|a\rangle$ fulfil two important properties:

(1) they are mutually orthogonal to each other (in the generalized sense, if there are continuous parts in the spectrum of A), i.e.,

$$\langle a|a'\rangle = \delta(a-a'),$$

where a and a' run over the set of (real) generalized eigenvalues of the operator A . δ is a Dirac-Delta distribution if a is in the continuous part of the operator's spectrum or a Kronecker delta if it is in the discrete part.

Note that all thinkable cases appear to be common in quantum theory: An self-adjoint operator can have only a continuous spectrum (e.g., positions and momenta of a particle), only a discrete spectrum (e.g. the modulus of angular momentum can have the eigen values $j(j+1)\hbar^2$, where $j \in \{0, 1/2, 1, \dots\}$), and the component in one direction of the angular momentum then is also discrete with the eigenvalues $\sigma\hbar$ with $\sigma \in \{-j, -j+1, \dots, j-1, j\}$) or both (e.g. the spectrum of the Hamilton operator of the hydrogen atom as a discrete part, describing energy levels of the bound proton and electron, and a continuous part, describing scattering between a proton and an electron).

That means, if a system is prepared in the eigenstate $|a\rangle$, one can never find another value than a , when measuring the observable A . This makes the whole thing consistent: If by preparation of a system, the observable A is assigned a definite value a , you must always measure this value a , otherwise it would not make sense to assign this value. Thus, the self-adjointness of the operator A ensures this necessary consistency condition in the interpretation of quantum states and preparation of a system in a state through measurement of the observable.

(2) The set of eigenvectors $|a\rangle$ is complete, i.e., you have

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$\sum_a \langle a | \psi \rangle \langle \psi | a \rangle = 1$, (completeness relation)

where for simplicity, I assume from now on the spectrum to be only discrete. If there are also continuous parts in the spectrum, you must just add the corresponding integral.

Also this is of profound importance for the consistency of the physical interpretation, because above we have stated that the probability to find the value a , when measuring the observable A , is given by

$$P(a|\psi) = \langle \psi | a \rangle \langle a | \psi \rangle = |\langle a | \psi \rangle|^2,$$

when the system is prepared in the state $|\psi\rangle$.

The completeness relation ensures that the probability to find some value in the spectrum when measuring A is 1, i.e., that one finds always a value for A , and it must be in the spectrum of the corresponding self-adjoint operator:

$$\sum_a P(a|\psi) = \sum_a \langle \psi | a \rangle \langle a | \psi \rangle = \langle \psi | \psi \rangle = 1.$$

Also the expectation values of A are easily calculated:

$$\langle A \rangle = \sum_a a P(a|\psi) = \sum_a \langle \psi | A | a \rangle \langle a | \psi \rangle = \langle \psi | A | \psi \rangle$$

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> 2) how is it possible (or: how come it does not contradict the
> principles of QM) that a continuum of eigenstates (as opposed to
> quantized eigenstates) can exist for unbound states?

Also this is a delicate question. Admittedly, what I wrote above is a mess, and most textbooks also write a mess about this point. That's just to simplify the maths a little bit for us poor physicists. The point is that continuum "states" are not true Hilbert-space states, but "generalized" states. Mathematically they belong not to Hilbert space but to a larger space, which is the dual space of a smaller subspace of the Hilbert space, namely those vectors, where the self-adjoint operator, describing the observable, is defined.

Let's take the example of the x -coordinate of a spinless particle. We can describe the Hilbert space by the complex functions whose square can be integrated over whole \mathbb{R} , i.e.,

$$\langle \psi | \psi \rangle = \int dx \psi^*(x) \psi(x) = \int dx |\psi(x)|^2 < \infty.$$

Now there are a lot of functions in this Hilbertspace, known as L^2 , where the position operator x is not defined. Take, e.g., the (unnormalized) wave function

$$\psi(x) = \sin(x)/x,$$

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which for sure is square-integrable. Here, in position representation, the x -operator is just given by the multiplication of the wave function with x , but

$$x \psi(x) = x \psi(x)$$

is not square-integrable.

The x operator is defined on a smaller sub-space Ω of L^2 , which is dense in L^2 , i.e., each wave function of L^2 can be represented as the limit of a sequence of functions in Ω (that's a mathematical theorem about self-adjoint operators in Hilbert space!).

Now the "eigenvectors" of the position operator are not functions, but distributions of generalized functions, namely

$$\phi_{x_0}(x) = \delta(x - x_0),$$

where ϕ_{x_0} denotes the generalized eigenvector of the position operator with the generalized eigenvalue x_0 .

ϕ_{x_0} is defined as a functional on the subset Ω :

$$\phi_{x_0}(\psi) = \int dx \delta(x - x_0) \psi(x) = \psi(x_0).$$

The advantage of this rather abstract formalism is that it legitimates Dirac's brilliant bra-ket calculus: we can write without much headaches:

$$\psi(x) = \int dx \langle x | \psi \rangle \delta(x - x_0),$$

where $|\psi\rangle$ is a Hilbert-space vector, providing a mapping from the abstract Hilbert space H of kets to the Hilbert space L^2 of wave functions.

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> 3) How can it be shown that the gradient (of ψ when operating) times \hbar (i.e. the momentum operator) is equivalent to \hbar/i ? Can an equivalence between the momentum operator and the classical mechanical definition of momentum (mv) be shown at all (I know, it's called the wave equation, but still)?

That's also a very good question. For me, the most satisfactory answer is provided by Noether's theorem, which you hopefully know from your classical-mechanics course: There you learn that momentum is the generator of space translations.

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> 4) How can it be shown directly (that is, without reverting to $KE = \int dx \frac{p^2}{2m}$) that the kinetic energy operator actually is a kinetic energy term?

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- > 5) How can it be shown directly (again, without reverting to $H = \frac{1}{2m} \nabla^2 + V$) that the time derivative (of ψ when used in operation) times \hbar is actually equivalent to the hamiltonian? I am asking these questions because I find it intriguing that the time derivative of ψ should be proportional to its second spatial derivative (assuming constant potentials). This does not strike me as something obvious, even though playing around with the equations suggests something like this (which I still do not conceptually understand):
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- > Assume we can set $H = -\nabla^2 - W$ (Can we really do this? Why or why not?)
- >
- > then: $-\nabla^2 \psi = \int (F \cdot dx) = \int (dp/dt) dx$
- > (here, F and dx would obviously have to point in opposite directions for the work to be negative)
- > finally, substitute the momentum operator, and we magically recover the left side of Schroedinger's equation.
- > (BTW I have never seen a "force operator". I imagine that's because it is closely linked with particles rather than waves. But is that a strong enough reason to prohibit its use? Why?)

The answer to these questions is a little bit too long to find space here in the news group. The answer is again Noether's theorem, and may be found in the very good textbook

L. Ballentine, Quantum Mechanics,

which somebody, who asks such deep questions as you, should read, although it's not easy!

- > This brings me also to my next question:
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- > 6) What is the reason for distinguishing in the Schroedinger equation between the Hamiltonian and total Energy? Is this related to the view that Planck's constant can be considered to be the fundamental unit of action? Under what circumstances is it valid to substitute total energy for the Hamiltonian?

In which sense was this distinguished in your lecture? A reason might be the following:

The total energy (i.e., kinetic + potential energy) has only a certain fixed value for systems, which are prepared in an energy-eigenstate. For all other states, the Hamiltonian has not a fixed value.

Nevertheless, the Hamiltonian H represents the observable "total energy", and it is the generator of time evolution, because according to Noether's theorem it's the conserved quantity from the symmetry of the physical laws under time translations.

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- > 7) What examples, other than the simple harmonic oscillator, can be
- > used to illustrate the correspondence principle, that is, the idea
- > that in the limit of large scales quantum mechanics reduces to
- > classical mechanics? In particular, how can we get from the
- > Schroedinger equation to the classical Hamiltonian (or vice versa)?

Look in a good textbook under "WKB approximation" or semi-classical approximation. It's again a little bit difficult to squeeze the interesting answer into a newsgroup posting, which becomes already quite lengthy ;-)).

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- > 8) Is there any experimental evidence which would answer the following
- > question: does the probability of finding a particle in a volume
- > element ($\psi^*\psi$) change if the shape of the volume element is changed
- > (but the volume is kept the same as before)? Have any experiments been
- > conducted which examine the predicted and actual probabilities of
- > finding particles in volume-elements that are not cubical?

I don't know. For sure, one has not found a contradiction of quantum theory with experiment. To the contrary: The more hard the quantum theory is tested by experiment, the more accurate we find its consistency with the outcomes of these experiments. A lot of experiments, which one could think of only as "gedanken experiments" some years ago, can now be done with real experiments in the lab, thanks to the advancement in quantum optics. That's the reason, why a quite new branch of quantum studies has arisen in the last view years like "quantum computing" and "nano technology".

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- > 9) Does ψ have a dimension (like length?) Can ψ itself ever end up
- > being orthogonal to the imaginary axis (i.e. be real, rather than
- > complex)? If so, under what circumstances? Would that have any effect
- > on what we observe? I ask this question because if its phase shift
- > ever caused ψ to lie exactly on the real axis, this would seem to
- > introduce a dimensional problem when we square it: A complex number
- > with some dimension multiplied by its complex conjugate gives a real
- > number with same dimension. A real number with some dimension squared
- > obviously gives a number with the square of the dimension.

The wave function, i.e., the states in the position representation

$$\psi(x) = \int \langle x | \psi \rangle \delta(x - x') dx'$$

must have dimension $\text{length}^{-d/2}$, where d is the number of position observables needed to describe the system (i.e., 3 for one particle, 6 for two particles and so on), both, real and imaginary part. Of course $|\psi(x)|^2$ is always a real number $\int \psi^* \psi dx = 1$, as it must be for a probability distribution.

This must be so, since $|\psi(x)|^2 dx$ is the probability distribution

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to find the particles in a little volume element $d^d x$ around x . The shape of the volume element is unimportant. As I stated above, I am not aware whether this prediction of quantum theory ever has been tested in the lab.

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> 10) Some versions of the postulates also mention this one:

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> The total wavefunction must be antisymmetric with respect to the
> interchange of all coordinates of one fermion with those of another.

> Electronic spin must be included in this set of coordinates

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> I understand that this postulate leads to the Pauli exclusion
> principle, but I don't know how it does so (i.e. how do you derive the

> Pauli exclusion principle from this postulate?). Also, the postulate
> itself is not clear to me, can someone explain this to me?.

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> Again, I know this is a lot, so answering just a part at a time would
> be fine.

Well, I take the opportunity to leave the last question unanswered, since this would again be a long one. The answer, using path-integral methods, can be found in the original paper

M. G. G. Laidlaw, C. M. DeWitt, Feynman Functional Integrals for Systems of Indistinguishable Particles, Phys. Rev. D 3 (1970) 1375, URL <http://link.aps.org/abstract/PRD/v3/i6/p1375>

but that's REALLY a tough one!

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◆ **Re: 10 questions on QM postulates**

◇ From: Arnold Neumaier

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