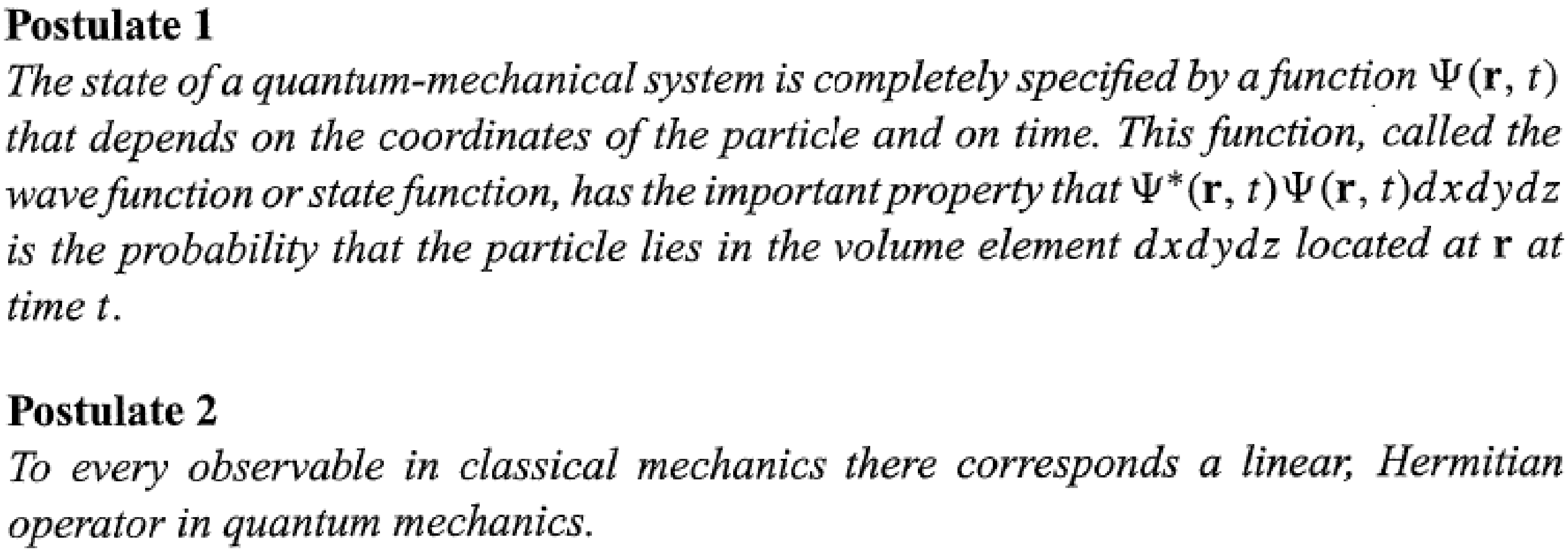
I. The Postulates of Quantum Mechanics

- There are different versions, but they amount to the same thing.
- Some versions are friendlier, some are more abstract.
- See "boxes" in Ch. XI on spin. The "boxes" are the key general concepts.
- Below are three sets of postulates from three books, starting from the friendliest one. The sources are:
  - D. McQuarrie, "Quantum Chemistry"
  - Rae, "Quantum Mechanics"
  - Bransden and Joachain, "Quantum Mechanics"

Postulates of QM: Taken from McQuarrie's *Quantum Chemistry*



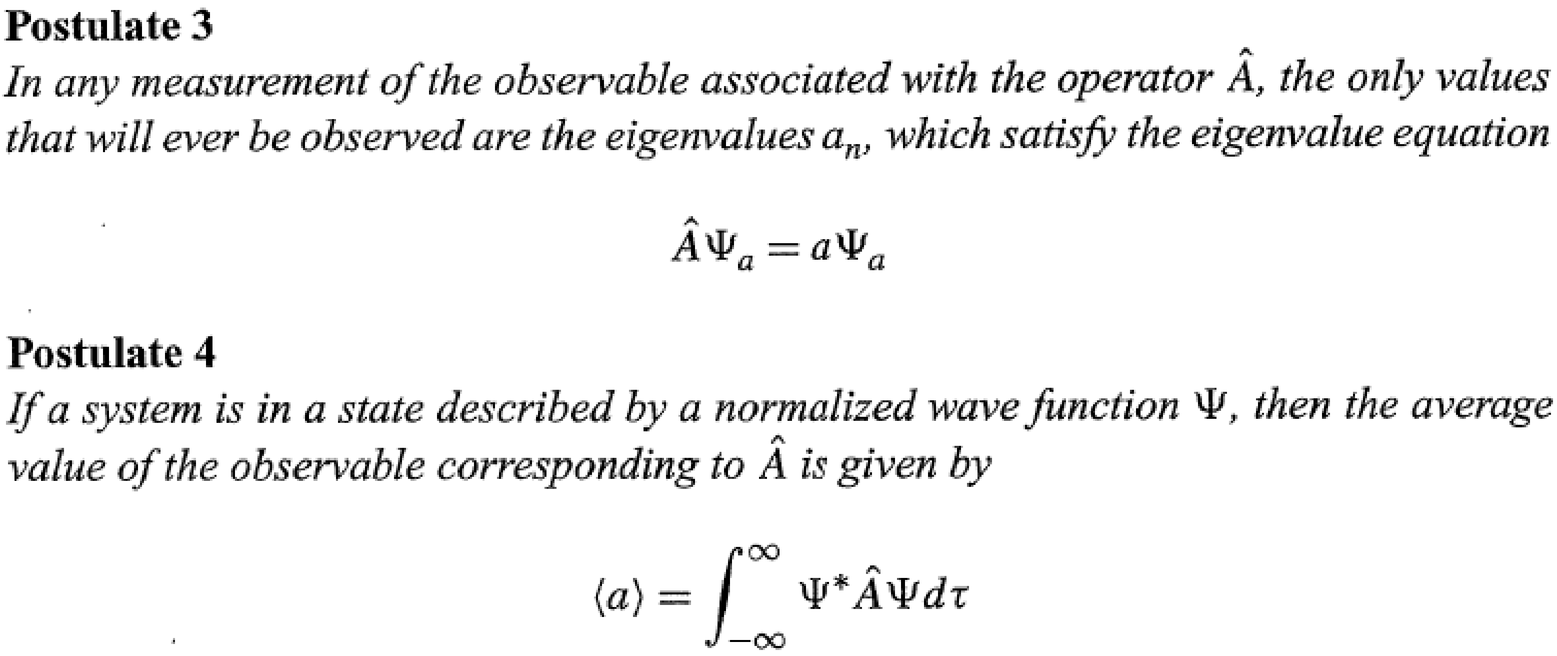
Postulate 1

The state of a quantum-mechanical system is completely specified by a function $\Psi(\mathbf{r}, t)$ *that depends on the coordinates of the particle and on time. This function, called the wave function or state function, has the important property that* $\Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)dxdydz$ *is the probability that the particle lies in the volume element* $dxdydz$ *located at* $\mathbf{r}$ *at time* t.

Postulate 2

To every observable in classical mechanics there corresponds a linear, Hermitian operator in quantum mechanics.

[Remark: This is the friendliest set because it is stated in terms of the more familiar wavefunction. But it also mentioned the state function.]



Postulate 3

In any measurement of the observable associated with the operator $\hat{A}$*, the only values that will ever be observed are the eigenvalues* a_n*, which satisfy the eigenvalue equation*

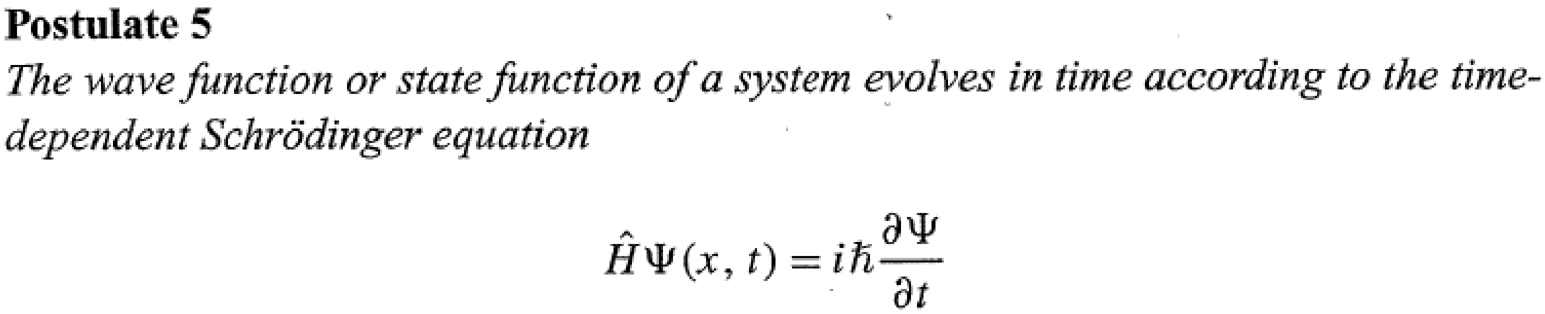
$$\hat{A}\Psi_a = a\Psi_a$$

Postulate 4

If a system is in a state described by a normalized wave function Ψ*, then the average value of the observable corresponding to* $\hat{A}$ *is given by*

$$\langle a \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi \, d\tau$$

[Remark: The average value is the expectation value. Using it as a postulate could infer the idea of expanding a general wavefunction in terms of the eigenstates of the operation A and the coefficient squared gives the probability of getting a particular eigenvalue *a*.



Postulate 5

The wave function or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$\hat{H}\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t}$$

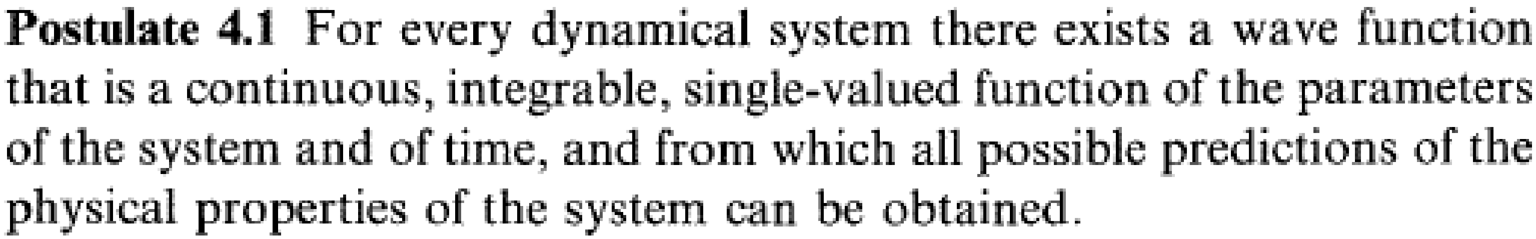
Remarks:

- This set of postulates is stated in plain language. This is the bare minimum for every student.

- But this set is sufficient for most students to move on to do problems and even research on QM. The book from which the version is taken is a standard beginning graduate-level Quantum Chemistry book. This is what one needs to move on to learn more techniques, e.g. perturbation theory, applications to atoms and molecules, and do computational quantum chemistry calculations.

Postulates of QM: Taken from Rae's *Quantum Mechanics*

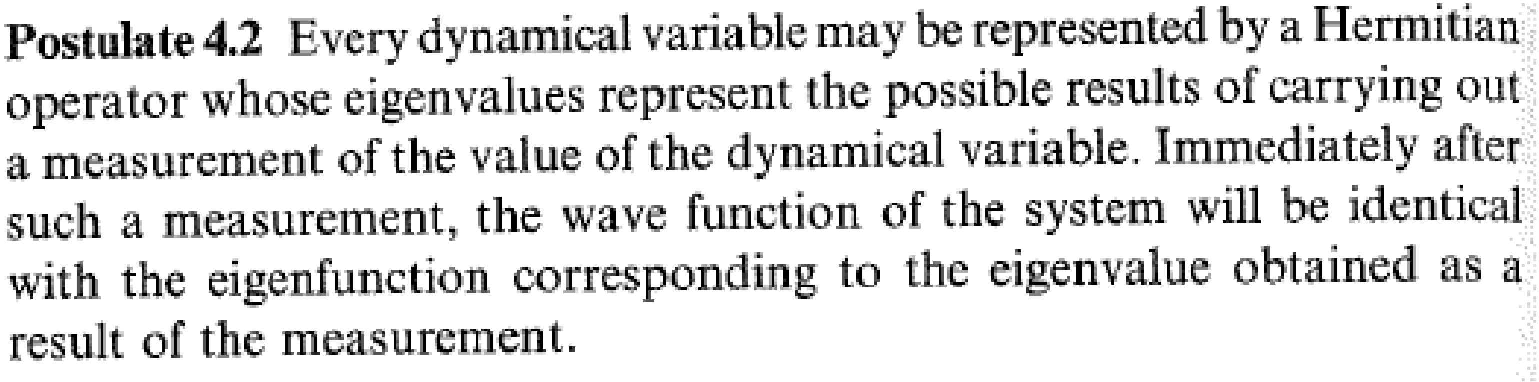
P1



Postulate 4.1 For every dynamical system there exists a wave function that is a continuous, integrable, single-valued function of the parameters of the system and of time, and from which all possible predictions of the physical properties of the system can be obtained.

[Remark: This is a typical physics book's statement. It emphasizes there is a wavefunction (or state function) that contains all the information that one can extract.]

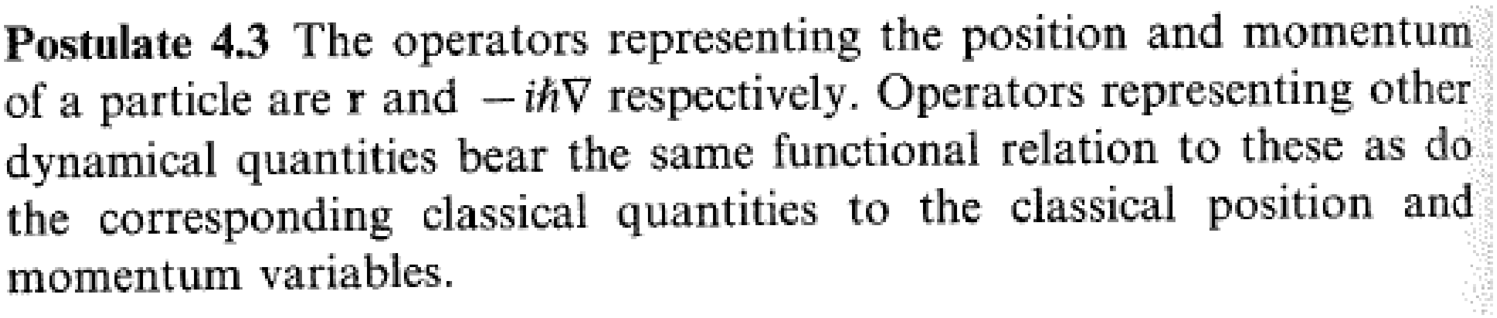
P2



Postulate 4.2 Every dynamical variable may be represented by a Hermitian operator whose eigenvalues represent the possible results of carrying out a measurement of the value of the dynamical variable. Immediately after such a measurement, the wave function of the system will be identical with the eigenfunction corresponding to the eigenvalue obtained as a result of the measurement.

[Remark: This actually contains several points: operators, measurement results, and collapse of wavefunction after measurement. Up to here, it is about what one can say about a measurement if there is no information about the state on which the measurement is done.]

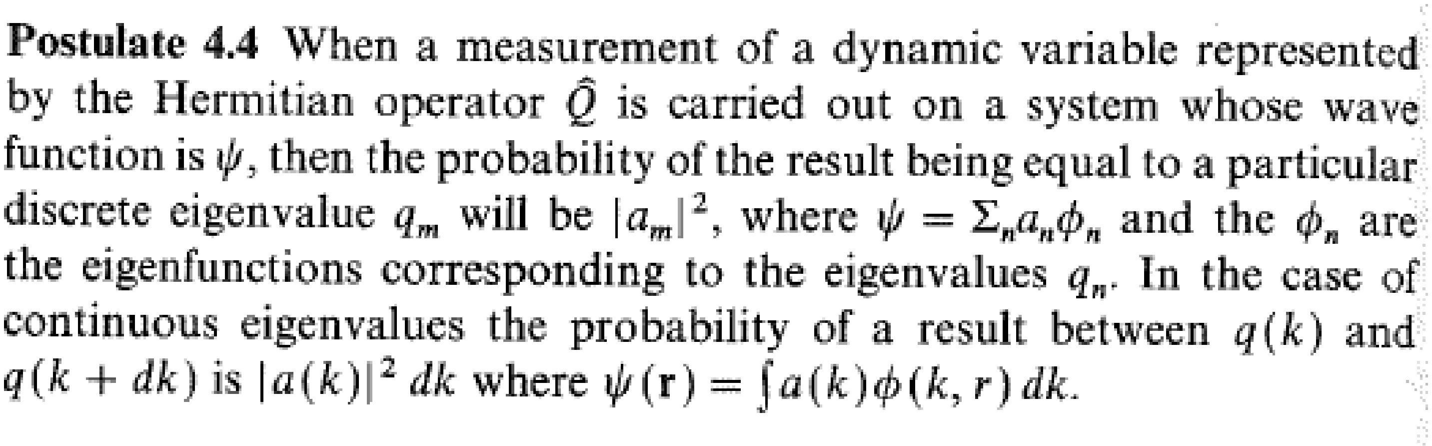
P3



Postulate 4.3 The operators representing the position and momentum of a particle are $\mathbf{r}$ and $-i\hbar\nabla$ respectively. Operators representing other dynamical quantities bear the same functional relation to these as do the corresponding classical quantities to the classical position and momentum variables.

[Remark: This sticks to the Schrodinger’s way of representing operators, i.e., in the position representation.]

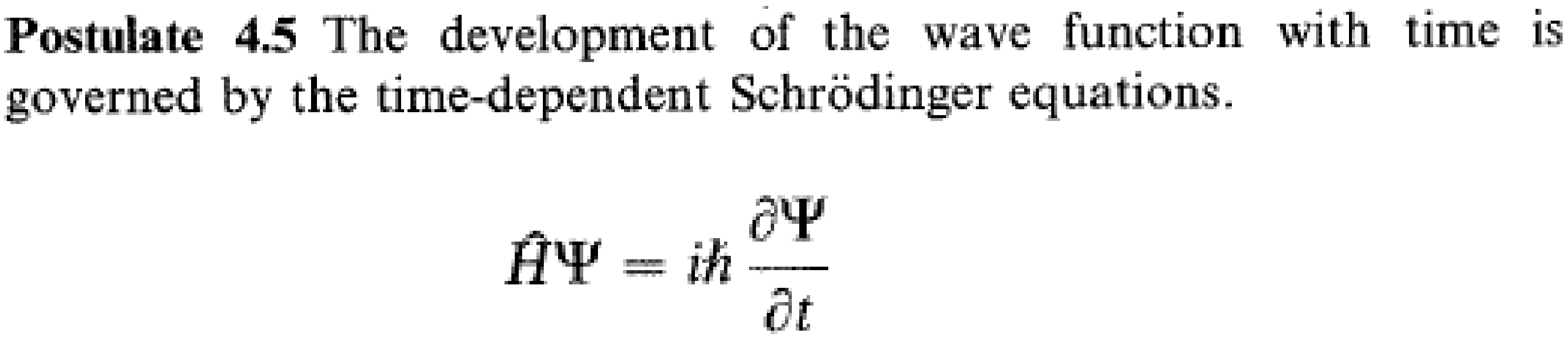
P4



Postulate 4.4 When a measurement of a dynamic variable represented by the Hermitian operator $\hat{Q}$ is carried out on a system whose wave function is ψ, then the probability of the result being equal to a particular discrete eigenvalue q_m will be $|a_m|^2$, where $\psi = \Sigma_n a_n \phi_n$ and the ϕ_n are the eigenfunctions corresponding to the eigenvalues q_n. In the case of continuous eigenvalues the probability of a result between $q(k)$ and $q(k + dk)$ is $|a(k)|^2\, dk$ where $\psi(\mathbf{r}) = \int a(k)\phi(k, r)\, dk$.

[Remark: This says more about measurement if we know the state on which measurements are to be done. From this one can infer how expectation values can be calculated.]

P5



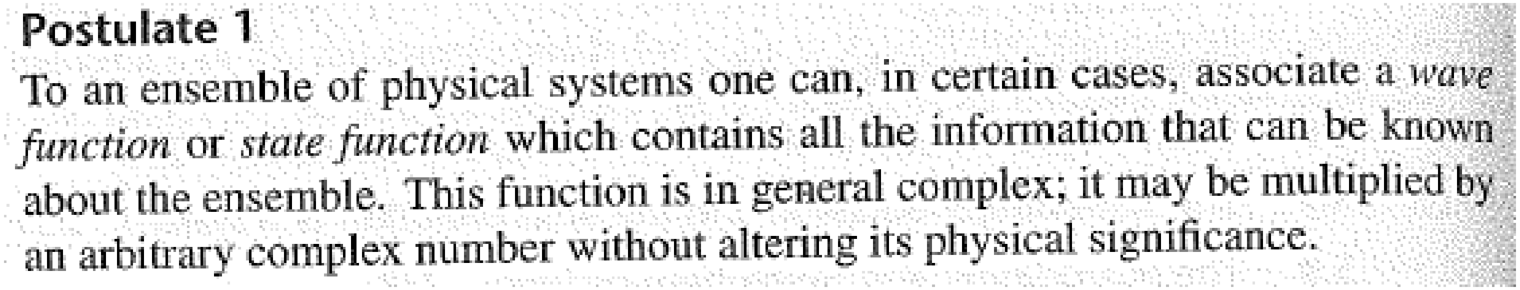
Postulate 4.5 The development of the wave function with time is governed by the time-dependent Schrödinger equations.

$$\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

Remarks:

- This set is more wordy, but amounts to the same contents.
- The book by Rae is a standard undergraduate physics textbook on QM.

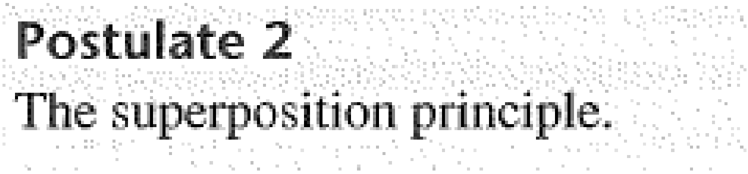
Postulates of QM: Taken from Bransden and Joachain’s *Quantum Mechanics*



Postulate 1

To an ensemble of physical systems one can, in certain cases, associate a *wave function* or *state function* which contains all the information that can be known about the ensemble. This function is in general complex; it may be multiplied by an arbitrary complex number without altering its physical significance.

[Remark: It is talking about an ensemble (collection) of systems in order to prepare for statements on measurement results. But the point here again is about the wavefunction or state function that contains all the information.]



Postulate 2

The superposition principle.

[Remark: This is about QM being a theory that is linear, i.e., if two state functions satisfy the time-dependent Schrodinger Equation, then their linear combination also satisfies TDSE.]

Postulate 3

With every dynamical variable is associated a linear operator.

Postulate 4

The only result of a precise measurement of the dynamical variable $\mathcal{A}$ is one of the eigenvalues a_n of the linear operator A associated with $\mathcal{A}$.

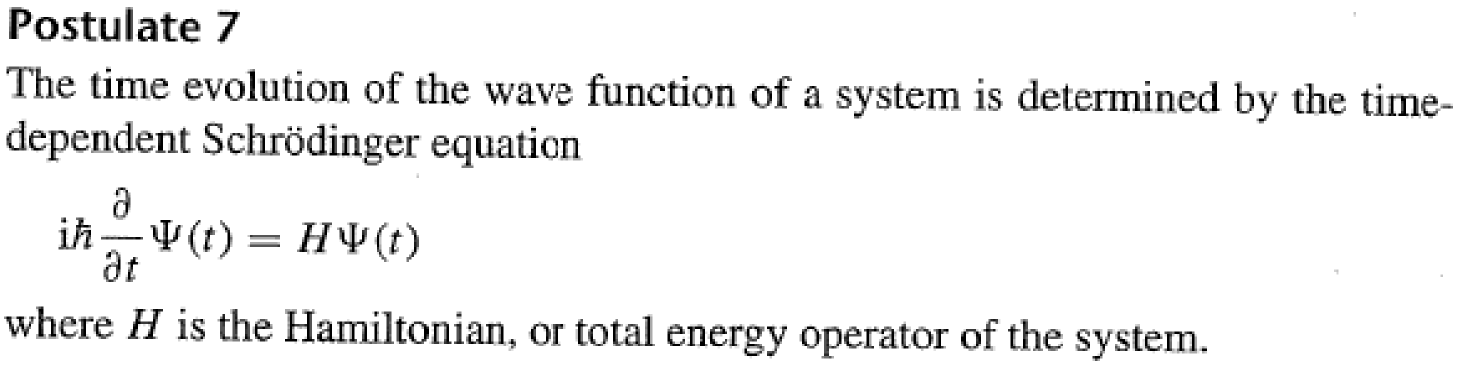
Postulate 5

If a series of measurements is made of the dynamical variable A on an ensemble of systems[2], described by the wave function Ψ, the expectation or average value of this dynamical variable is

$$\langle A \rangle = \frac{\langle \Psi | A | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

Postulate 6

A wave function representing any dynamical state can be expressed as a linear combination of the eigenfunctions of A, where A is the operator associated with a dynamical variable.



Postulate 7

The time evolution of the wave function of a system is determined by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = H \Psi(t)$$

where H is the Hamiltonian, or total energy operator of the system.

Remarks:

- Bransden and Joachain's book covers more quantum mechanics than undergraduate needs. It is full of equations and therefore good for students who want to see more mathematics. The same authors wrote a book on applying QM to atoms and molecules.

- You have seen the postulates of QM stated in three different books in different ways. At the end, the statements all cover the same ground.

- Depending on your taste and level of acceptance, pick one set that you find most comfortable and move on to the next course.