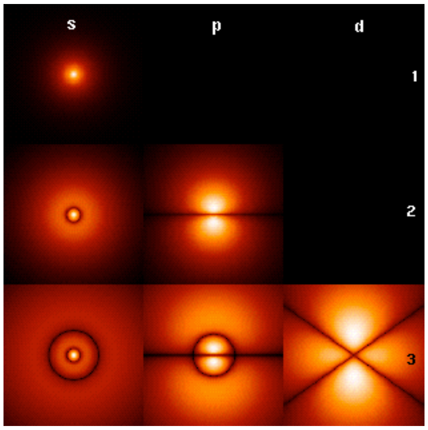

Figure III.1: Probability density of first six hydrogen orbitals. The main quantum number ($n = 1, 2, 3$) and the angular momentum quantum number ($\ell = 0, 1, 2 =$ s, p, d) are shown. (The magnetic quantum number $m = 0$ in these plots.) [fig. from wikipedia commons]

B Basic concepts from quantum theory

B.1 Postulates of QM

Quotes are from Nielsen, Michael A. & Chuang, Isaac L. *Quantum Computation and Quantum Information* (10th Anniversary Edition, Cambridge, 2010) unless otherwise specified.

B.1.a Postulate 1: state space

¶1. Associated with any isolated physical system is a *state space*, which is a Hilbert space.

¶2. The state of the system "is completely defined by its *state vector*, which is a unit vector in the system's state space."

¶3. The state $|\psi\rangle$ is understood as a *wavefunction*.

¶4. A wavefunction for a particle defines the *probability amplitude* distribution (actually probability density function) of some quantity. For example, $|\psi\rangle$ may define the complex amplitude $\psi(x)$ associated with

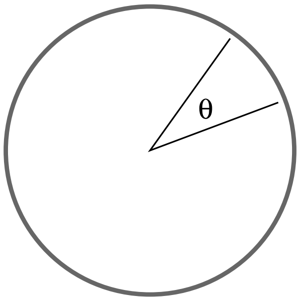

Figure III.2: Relative phase vs. global phase. What matters in QM is relative phases between state vectors (e.g., θ in the figure). Global phase "has no physical meaning"; i.e., we can choose to put the 0° point any where we like.

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each location x, and $|\phi\rangle$ may define the complex amplitude of $\phi(p)$ associated with each momentum p. See Fig. III.1.

¶5. **Normalization:** The state vector has to be normalized so that the total probability is 1.

¶6. **Inner product:** The inner product of wavefunctions is defined:

$$\langle \phi \mid \psi \rangle = \int_{\mathbb{R}^3} \overline{\phi(\mathbf{r})}\psi(\mathbf{r})\mathrm{d}\mathbf{r}.$$

For this example we are assuming the domain is 3D space.

¶7. **Global vs. relative phase:** In QM, global phase has no physical meaning; all that matters is relative phase.
In other words, if you consider all the angles around the circle, there is no distinguished 0°. See Fig. III.2.
Likewise, in a continuous wave (such as sine), there is no distinguished starting point (see Fig. III.3).

¶8. To say all pure states are normalized is another way to say that their absolute length has no physical meaning.
That is, only their *form* (shape) matters, not their absolute size. This is a characteristic of *information*.

¶9. **Projective Hilbert space:** Pure states correspond to the *rays* in a *projective Hilbert space*.

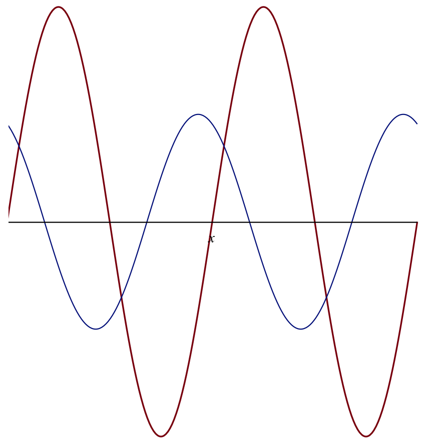

Figure III.3: Relative phase vs. global phase of sine waves. There is no privileged point from which to start measuring absolute phase, but there is a definite relative phase between the two waves.

A *ray* is an equivalence class of nonzero vectors under the relation, $\phi \cong \psi$ iff $\exists z \neq 0 \in \mathbb{C} : \phi = z\psi$, where $\phi, \psi \neq \mathbf{0}$.
However, it is more convenient to use normalized vectors in ordinary Hilbert spaces, ignoring global phase.

B.1.b POSTULATE 2: EVOLUTION

¶1. "The evolution of a closed quantum system is described by a unitary transformation."

Therefore a closed quantum system evolves by complex rotation of a Hilbert space.

¶2. That is, the state $|\psi\rangle$ of the system at time t is related to the state $|\psi'\rangle$ of the system at time t' by a unitary operator U which depends only on the times t and t',

$$|\psi'\rangle = U(t, t')|\psi\rangle = U|\psi\rangle.$$

¶3. See Sec. B.6, below.

¶4. This describes the evolution of systems that don't interact with the rest of the world.

B.1.c POSTULATE 3: QUANTUM MEASUREMENT

¶1. What happens if the system is no longer closed, i.e., it interacts with the larger environment?

¶2. **Postulate 3:** Quantum measurements are described by a collection of *quantum measurement operators*, M_m, for each possible measurement outcome m.

¶3. The probability of measurement m of state $|\psi\rangle$ is:

$$p(m) = \|M_m|\psi\rangle\|^2 = \langle\psi \mid M_m^\dagger M_m \mid \psi\rangle. \tag{III.1}$$

¶4. **Born's Rule:** After measurement the state of the system is (unnormalized) $M_m|\psi\rangle$, or normalized:

$$\frac{M_m|\psi\rangle}{\|M_m|\psi\rangle\|}.$$

¶5. Measurement operations satisfy the *completeness relation*: $\sum_m M_m^\dagger M_m = I$.

¶6. That is, the measurement probabilities sum to 1:

$$1 = \sum_m p(m) = \sum_m \langle\psi \mid M_m^\dagger M_m \mid \psi\rangle.$$

¶7. **Observable:** An *observable* M is a Hermitian operator on the state space.

¶8. **Projective measurements:** An observable M has a spectral decomposition

$$M = \sum_m e_m P_m,$$

where the P_m are *projectors* onto the eigenspace of M, and the eigenvalues e_m are the corresponding measurement results.
The projector P_m projects into the eigenspace corresponding to eigenvalue e_m.
(For projectors, see Sec. A.2.i, ¶6.)

¶9. Since a projective measurement is described by a Hermitian operator M, it has a spectral decomposition with real eigenvalues, $M = \sum_j e_j |\eta_j\rangle\langle\eta_j|$, where η_j is the measurement basis.

¶10. Therefore we can write $M = UEU^\dagger$, where $E = \text{diag}(e_1, e_2, \ldots)$, $U = (|\eta_1\rangle, |\eta_2\rangle, \ldots)$, and

$$U^\dagger = (|\eta_1\rangle, |\eta_2\rangle, \ldots)^\dagger = \begin{pmatrix} \langle\eta_1| \\ \langle\eta_2| \\ \vdots \end{pmatrix}.$$

$U^\dagger$ expresses the state in the measurement basis and U translates back.

¶11. In the measurement basis, the matrix for an observable is a diagonal matrix: $E = \text{diag}(e_1, \ldots, e_m)$.

¶12. This is a special case of Postulate 3 in which the "M_m are orthogonal projectors, that is, the M_m are Hermitian, and $M_m M_{m'} = \delta_{m,m'} M_{m'}$."
That is $M_m M_m = M_m$ (idempotent), and $M_m M_{m'} = \mathbf{0}$ for $m \neq m'$ (orthogonal).
Also, since M_m is Hermitian, $M_m^\dagger M_m = M_m M_m = M_m$.

¶13. The probability of measuring e_m is

$$p(m) = \langle\psi \mid M_m^\dagger M_m \mid \psi\rangle = \langle\psi \mid M_m \mid \psi\rangle = \langle\psi \mid P_m \mid \psi\rangle.$$

¶14. Suppose $P_m = |m\rangle\langle m|$ and $|\psi\rangle = \sum_j c_j |j\rangle$ (i.e., write it in the measurement basis). Then

$$\begin{aligned} p(m) &= \langle\psi \mid P_m \mid \psi\rangle \\ &= \langle\psi \mid m\rangle\langle m \mid \psi\rangle \\ &= \langle m \mid \psi\rangle^* \langle m \mid \psi\rangle \\ &= |\langle m \mid \psi\rangle|^2 \\ &= |c_m|^2. \end{aligned}$$

¶15. More generally, the same hold if P_m projects into an eigenspace, $P_m = \sum_k |k\rangle\langle k|$.
Alternatively, we can "zero out" the c_j for the orthogonal subspace, i.e., for the $|j\rangle$ omitted by P_m.

¶16. To maintain total probability = 1, the state after measurement is

$$\frac{P_m|\psi\rangle}{\sqrt{p(m)}} = \frac{P_m|\psi\rangle}{\|P_m|\psi\rangle\|}.$$

¶17. **Motivation:** To understand the motivation for this, suppose we have a quantum system (such as an atom) that can be in three distinct states $|\text{ground}\rangle$, $|\text{first excited}\rangle$, $|\text{second excited}\rangle$ with energies e_0, e_1, e_2, respectively. Then the energy observable is the operator

$$\begin{aligned} E &= e_0|\text{ground}\rangle\langle\text{ground}| + e_1|\text{first excited}\rangle\langle\text{first excited}| \\ &\quad + e_2|\text{second excited}\rangle\langle\text{second excited}|, \end{aligned}$$

or more briefly, $\sum_{j=0}^{2} e_j|j\rangle\langle j|$.

¶18. **Mean or expectation value:** We can derive the mean or expectation value of an energy measurement for a given quantum state:

$$\begin{aligned} \langle E\rangle &\overset{\text{def}}{=} \mu_E \overset{\text{def}}{=} \mathcal{E}\{E\} \\ &= \sum_j e_j p(j) \\ &= \sum_j e_j \langle\psi \mid j\rangle\langle j \mid \psi\rangle \\ &= \sum_j \langle\psi|\; e_j|j\rangle\langle j|\; |\psi\rangle \\ &= \langle\psi| \left(\sum_j e_j|j\rangle\langle j|\right) |\psi\rangle \\ &= \langle\psi \mid E \mid \psi\rangle. \end{aligned}$$

¶19. **Variance and standard deviation:** This yields the formula for the standard deviation σ_E and variance, which are important in the uncertainty prinsiple:

$$\begin{aligned} \sigma_E^2 &\overset{\text{def}}{=} (\Delta E)^2 \overset{\text{def}}{=} \text{Var}\{E\} \\ &= \mathcal{E}\{(E - \langle E\rangle)^2\} \\ &= \langle E^2\rangle - \langle E\rangle^2 \\ &= \langle\psi \mid E^2 \mid \psi\rangle - (\langle\psi \mid E \mid \psi\rangle)^2. \end{aligned}$$

Note that E^2, the matrix E multipled by itself, is also the operator that measures the square of the energy, $E^2 = \sum_j e_j^2 |j\rangle\langle j|$. (This is because E is diagonal in this basis; alternately, E^2 can be interpreted as an operator function.)

B.1.d Postulate 4: composite systems

¶1. "The state space of a composite physical system is the tensor product of the state spaces of the component physical systems."

¶2. If there are n subsystems, and subsystem j is prepared in state $|\psi_j\rangle$, then the composite system is in state

$$|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_n\rangle = \bigotimes_{j=1}^{n} |\psi_j\rangle.$$