## B.7 Uncertainty principle (supplementary)

You might be surprised that the famous Heisenberg uncertainty principle is not among the postulates of quantum mechanics. That is because it is not a postulate, but a theorem, which can be proved from the postulates. This section is optional, since the uncertainty principle is not required for quantum computation.

### B.7.a Informally

The uncertainty principle states a lower bound on the precision with which certain pairs of variables, called *conjugate variables*, can be measured. These are such pairs as position and momentum, and energy and time. For example, the same state can be represented by the wave function $\psi(x)$ as a function of space and by $\phi(p)$ as a function of momentum. The most familiar version of the Heisenberg principle, limits the precision with which location and momentum can be measured simultaneously: $\Delta x \, \Delta p \geq \hbar/2$, where the reduced Plank constant $\hbar = h/2\pi$, where $h$ is Planck's constant.

It is often supposed that the uncertainty principle is a manifestation of the *observer effect*, the inevitable effect that measuring a system has on it, but this is not the case. "While it is true that measurements in quantum mechanics cause disturbance to the system being measured, this is most emphatically *not* the content of the uncertainty principle."(Nielsen & Chuang, 2010, p. 89)

Often the uncertainty principle is a result of the variables representing measurements in two bases that are Fourier transforms of each other. Consider an audio signal $\psi(t)$ and its Fourier transform $\Psi(\omega)$ (its spectrum). Note that $\psi$ is a function of time, with dimension $t$, and its spectrum $\Psi$ is a function of frequency, with dimension $t^{-1}$. They are reciprocals of each other, and that is always the case with Fourier transforms. Simultaneous measurement in the time and frequency domains obeys the uncertainty relation $\Delta t \Delta \omega \geq 1/2$. (For more details on this, including an intuitive explanation, see MacLennan (prep, ch. 6).)

Time and energy are also conjugate, as a result of the de Broglie relation, according to which energy is proportional to frequency: $E = h\nu$ ($\nu$ in Hertz, or cycles per second) or $E = \hbar\omega$ ($\omega$ in radians per second). Therefore simultaneous measurement in the time and energy domains obeys the uncertainty principle $\Delta t \Delta E \geq \hbar/2$.

More generally, the observables are represented by Hermitian operators $P, Q$ that do not commute. That is, to the extent they do not commute, to that extent you cannot measure them both (because you would have to do either $PQ$ or $QP$, but they do not give the same result). The best interpretation of the uncertainty principle is that if you set up the experiment multiple times, and measure the outcomes, you will find

$$2\,\Delta P\,\Delta Q \geq |\langle[P,Q]\rangle|,$$

where $P$ and $Q$ are conjugate observables. (The commutator $[P,Q]$ is defined below, Def. B.2, p. 96.)

Note that this is a *purely mathematical* result (proved in Sec. B.7.b). Any system obeying the QM postulates will have uncertainty principles for every pair of non-commuting observables.

### B.7.b Formally

In this section we'll derive the uncertainty principle more formally. Since it deals with the variances of measurements, we begin with their definition. To understand the motivation for these definitions, 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, $\sum_{m=0}^{2} e_m|m\rangle\langle m|$.

**Definition B.1 (observable)** *An* observable *$M$ is a Hermitian operator on the state space.*

An observable $M$ has a spectral decomposition (Sec. A.2.g):

$$M = \sum_{m=1}^{N} e_m P_m,$$

where the $P_m$ are *projectors* onto the eigenspaces 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.d.) Since an observable is described by a Hermitian operator $M$, it has a spectral decomposition with real eigenvalues, $M = \sum_{m=1}^{N} e_m |m\rangle\langle m|$, where $|m\rangle$ is the measurement basis. Therefore we can write $M = UEU^\dagger$, where $E = \text{diag}(e_1, e_2, \ldots, e_N)$, $U = (|1\rangle, |2\rangle, \ldots, |N\rangle)$, and

$$U^\dagger = (|1\rangle, |2\rangle, \ldots, |N\rangle)^\dagger = \begin{pmatrix} \langle 1| \\ \langle 2| \\ \vdots \\ \langle N| \end{pmatrix}.$$

$U^\dagger$ expresses the state in the measurement basis and $U$ translates back. In the measurement basis, the matrix for an observable is a diagonal matrix: $E = \text{diag}(e_1, \ldots, e_N)$. The probability of measuring $e_m$ is

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

We can derive the mean or expectation value of an energy measurement for a given quantum state $|\psi\rangle$:

$$\begin{aligned} \langle E \rangle &\stackrel{\text{def}}{=} \mu_E \stackrel{\text{def}}{=} \mathcal{E}\{E\} \\ &= \sum_m e_m p(m) \\ &= \sum_m e_m \langle \psi \mid m \rangle \langle m \mid \psi \rangle \\ &= \sum_m \langle \psi |\, e_m |m\rangle\langle m|\, |\psi\rangle \\ &= \langle \psi | \left( \sum_m e_m |m\rangle\langle m| \right) |\psi\rangle \\ &= \langle \psi \mid E \mid \psi \rangle. \end{aligned}$$

This formula can be used to derive the standard deviation $\sigma_E$ and variance $\sigma_E^2$, which are important in the uncertainty principle:

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

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

We now proceed to the derivation of the uncertainty principle.[2]

**Definition B.2 (commutator)** *If $L, M : \mathcal{H} \rightarrow \mathcal{H}$ are linear operators, then their* commutator *is defined:*

$$[L, M] = LM - ML. \tag{III.6}$$

***Remark B.1*** *In effect, $[L, M]$ distills out the non-commutative part of the product of $L$ and $M$. If the operators commute, then $[L, M] = \mathbf{0}$, the identically zero operator. Constant-valued operators always commute ($cL = Lc$), and so $[c, L] = \mathbf{0}$.*

**Definition B.3 (anti-commutator)** *If $L, M : \mathcal{H} \rightarrow \mathcal{H}$ are linear operators, then their* anti-commutator *is defined:*

$$\{L, M\} = LM + ML. \tag{III.7}$$

*If $\{L, M\} = \mathbf{0}$, we say that $L$ and $M$* anti-commute*, $LM = -ML$.*

See B.2.c (p. 82) for the justification of the following definitions.

**Definition B.4 (mean of measurement)** *If $M$ is a Hermitian operator representing an observable, then the mean value of the measurement of a state $|\psi\rangle$ is*

$$\langle M \rangle = \langle \psi \mid M \mid \psi \rangle.$$

**Definition B.5 (variance and standard deviation of measurement)** *If $M$ is a Hermitian operator representing an observable, then the variance in the measurement of a state $|\psi\rangle$ is*

$$\text{Var}\{M\} = \langle (M - \langle M \rangle^2) \rangle = \langle M^2 \rangle - \langle M \rangle^2.$$

*As usual, the* standard deviation $\Delta M$ *of the measurement is defined*

$$\Delta M = \sqrt{\text{Var}\{M\}}.$$

[2]The following derivation is from MacLennan (prep, ch. 5).

**Proposition B.1** *If $L$ and $M$ are Hermitian operators on $\mathcal{H}$ and $|\psi\rangle \in \mathcal{H}$, then*

$$4\langle\psi \mid L^2 \mid \psi\rangle \, \langle\psi \mid M^2 \mid \psi\rangle \geq |\langle\psi \mid [L,M] \mid \psi\rangle|^2 + |\langle\psi \mid \{L,M\} \mid \psi\rangle|^2.$$

*More briefly, in terms of average measurements,*

$$4\langle L^2\rangle\langle M^2\rangle \geq |\langle[L,M]\rangle|^2 + |\langle\{L,M\}\rangle|^2.$$

**Proof**: Let $x + iy = \langle\psi \mid LM \mid \psi\rangle$. Then,

$$\begin{aligned} 2x &= \langle\psi \mid LM \mid \psi\rangle + (\langle\psi \mid LM \mid \psi\rangle)^* \\ &= \langle\psi \mid LM \mid \psi\rangle + \langle\psi \mid M^\dagger L^\dagger \mid \psi\rangle \\ &= \langle\psi \mid LM \mid \psi\rangle + \langle\psi \mid ML \mid \psi\rangle \quad \text{since } L, M \text{ are Hermitian} \\ &= \langle\psi \mid \{L,M\} \mid \psi\rangle. \end{aligned}$$

Likewise,

$$\begin{aligned} 2iy &= \langle\psi \mid LM \mid \psi\rangle - (\langle\psi \mid LM \mid \psi\rangle)^* \\ &= \langle\psi \mid LM \mid \psi\rangle - \langle\psi \mid ML \mid \psi\rangle \\ &= \langle\psi \mid [L,M] \mid \psi\rangle. \end{aligned}$$

Hence,

$$\begin{aligned} |\langle\psi \mid LM \mid \psi\rangle|^2 &= 4(x^2 + y^2) \\ &= |\langle\psi \mid [L,M] \mid \psi\rangle|^2 + |\langle\psi \mid \{L,M\} \mid \psi\rangle|^2. \end{aligned}$$

Let $|\lambda\rangle = L|\psi\rangle$ and $|\mu\rangle = M|\psi\rangle$. By the Cauchy-Schwarz inequality, $\||\lambda\rangle\| \, \||\mu\rangle\| \geq |\langle\lambda \mid \mu\rangle|$ and so $\langle\lambda \mid \lambda\rangle \, \langle\mu \mid \mu\rangle \geq |\langle\lambda \mid \mu\rangle|^2$. Hence,

$$\langle\psi \mid L^2 \mid \psi\rangle \, \langle\psi \mid M^2 \mid \psi\rangle \geq |\langle\psi \mid LM \mid \psi\rangle|^2.$$

The result follows.

□

**Proposition B.2** *Prop. B.1 can be weakened into a more useful form:*

$$4\langle\psi \mid L^2 \mid \psi\rangle \, \langle\psi \mid M^2 \mid \psi\rangle \geq |\langle\psi \mid [L,M] \mid \psi\rangle|^2,$$

*or* $4\langle L^2\rangle\langle M^2\rangle \geq |\langle[L,M]\rangle|^2$

**Proposition B.3 (uncertainty principle)** *If Hermitian operators $P$ and $Q$ are measurements (observables), then*

$$\Delta P\ \Delta Q \geq \frac{1}{2}|\langle \psi \mid [P, Q] \mid \psi \rangle|.$$

*That is, $\Delta P\ \Delta Q \geq |\langle [P, Q] \rangle|/2$. So the product of the variances is bounded below by the degree to which the operators do not commute.*

**Proof**: Let $L = P - \langle P \rangle$ and $M = Q - \langle Q \rangle$. By Prop. B.2 we have

$$\begin{aligned} 4\,\mathrm{Var}\{P\}\,\mathrm{Var}\{Q\} &= 4\langle L^2 \rangle \langle M^2 \rangle \\ &\geq |\langle [L, M] \rangle|^2 \\ &= |\,\langle [P - \langle P \rangle, Q - \langle Q \rangle] \rangle\,|^2 \\ &= |\langle [P, Q] \rangle|^2. \end{aligned}$$

Hence,

$$2\ \Delta P \Delta Q \geq |\langle [P, Q] \rangle|$$

$\square$