

So, how do Alice and Bob figure out the computer is not a quantum computer? Suppose that Alice and Bob make a large number of measurements, independently and randomly choosing from directions  $0^\circ$ ,  $120^\circ$ , and  $-120^\circ$ . Since the spins have distinct values, according to Bell's Theorem,  $E(\text{opp spin}) > \frac{1}{2}$ . But, also according to Bell's theorem, a true quantum computer would yield  $E(\text{opp spin}) = \frac{1}{2}$ . So Alice and Bob are able to determine that the computer is not a quantum computer. (They could also just compare their spins and observe that half of them are not opposites.) ■

**Note.** In Example 4 we *currently* know of no experiment that distinguishes the computer. We know that Bell-like experiments are not sufficient but that is not to say that some clever person won't one day find a different experiment that does distinguish the computer.

## Chapter 8. Particles and Waves

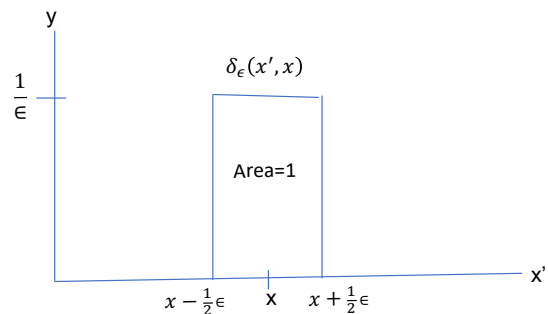
Quantum Mechanics is not so much about particles and waves as it is about the set of non-classical principles given in Chapter 3 that govern their behavior. We now extend the principles and concepts from the discrete systems we have so far studied to continuous systems (where we will at last develop wave examples.) See Table 8.1, below.

### Dirac Delta Note

Intuitively the Dirac delta function  $\delta(x - x')$  is a density function at some value  $x$ . In physics it is often defined informally as follows.

Let  $\epsilon > 0$ . Define

$$\delta_\epsilon(x', x) = \begin{cases} \frac{1}{\epsilon} & \text{if } x' \in \left(x - \frac{1}{2}\epsilon, x + \frac{1}{2}\epsilon\right) \\ 0 & \text{otherwise} \end{cases}.$$



The Dirac Delta function is the function  $\delta$  that satisfies

$$\int_{-\infty}^{\infty} \delta(x - x') dx' = \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \delta_\epsilon(x, x') dx'$$

where it is understood that the limit cannot be freely interchanged with the integral sign (which doesn't make sound mathematical sense since this violates Fubini's theorem).

**Table 8.1**

Concept	Discrete	Continuous
<b>Observable <math>L</math></b>	Discrete set of eigenvectors $\{ \lambda\rangle\}$	Continuous set of eigenvectors $\{ x\rangle\}$
<b>Hilbert Space of States</b>	$\{ \lambda\rangle\}$ forms algebraic orthonormal basis	$\{ x\rangle\}$ forms a complete (i.e., Schauder) basis
<b>State Vector</b>	$ \Psi\rangle = \sum_{\lambda} \psi(\lambda)  \lambda\rangle \quad (8.1)$	$ \Psi\rangle = \int_x \psi(x) dx \quad (8.1b)$
<b>Bra Vector</b>	$\langle\Psi  = \sum_{\lambda} \langle\lambda  \psi^*(\lambda)$	$\langle\Psi  = \int_x \psi^*(x) dx$
<b>Wave Function</b>	$\{\psi(\lambda)\}$	$\{\psi(x)\}$
<b>Inner Product</b>	$\langle\Psi \Phi\rangle = \sum_{\lambda} \psi^*(\lambda) \phi(\lambda)$	$\langle\Psi \Phi\rangle = \int_x \psi^*(x) \phi(x) dx \quad (8.2)$
<b>Probability</b>	$P(\lambda) = \psi^*(\lambda) \psi(\lambda)$	$P(a,b) = \int_a^b P(x) dx = \int_a^b \psi^*(x) \psi(x) dx$
<b>Normalization</b>	$\sum_{\lambda} \psi^*(\lambda) \psi(\lambda) = 1$	$\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1 \quad (8.3)$
<b>Kronecker &amp; Dirac Deltas</b>	$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$	$\delta(x-x')$ s.t. for any continuous $F$ $\int_{-\infty}^{\infty} \delta(x-x') F(x') dx' = F(x) \quad (8.4)$
<b>Integration By Parts</b>	$\int_a^b F dG = FG _a^b - \int_a^b G dF$	$\int_{-\infty}^{\infty} F \frac{dG}{dx} dx = \int_{-\infty}^{\infty} -G \frac{dF}{dx} dx \quad (8.4b)$ for wave functions $F$ and $G$

Three properties immediately follow:

$$(1) \int_{-\infty}^{\infty} \delta(x-x') dx' = 1: \quad (8.4c)$$

$$\int_{-\infty}^{\infty} \delta(x-x') dx' = \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \delta_{\epsilon}(x',x) dx' = \lim_{\epsilon \rightarrow 0} 1 = 1 \quad \checkmark$$

$$(2) \delta(x-x') = \begin{cases} \infty & \text{if } x' = x \\ 0 & \text{otherwise} \end{cases} :$$

$$\delta(x-x') = \lim_{\epsilon \rightarrow 0} \delta_{\epsilon}(x',x) = \begin{cases} \infty & \text{if } x' = x \\ 0 & \text{otherwise} \end{cases} \quad \checkmark$$

$$(3) \int_{-\infty}^{\infty} \delta(x-x') F(x') dx' = F(x) \text{ for continuous functions } F: \quad (8.4)$$

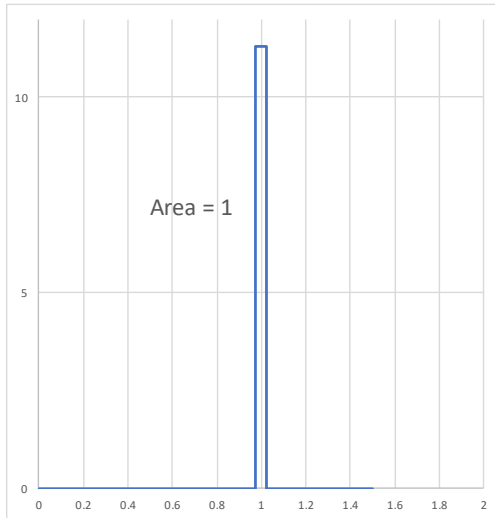
$$\begin{aligned}\int_{-\infty}^{\infty} \delta(x-x') F(x') dx' &\equiv \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \delta_{\epsilon}(x', x) F(x') dx' = \lim_{\epsilon \rightarrow 0} \int_{x-\frac{1}{2}\epsilon}^{x+\frac{1}{2}\epsilon} \frac{1}{\epsilon} F(x') dx' \\ &= F(x) \lim_{\epsilon \rightarrow 0} \int_{x-\frac{1}{2}\epsilon}^{x+\frac{1}{2}\epsilon} \frac{1}{\epsilon} dx' = F(x) \quad \checkmark \\ &\text{(because } \lim_{\epsilon \rightarrow 0} F(x') = F(x) \text{ since } F \text{ is continuous).}\end{aligned}$$

When referring to equation (2) in light of (1), we informally say that  $\delta$  **approaches infinity at a rate that keeps the area under the curve  $\delta(x-x')$  at unity**.

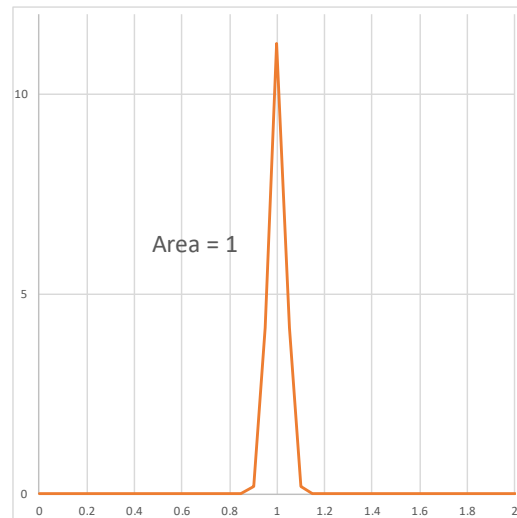
This informal definition of  $\delta(x-x')$  could also have been made in terms of

$\frac{n}{\sqrt{\pi}} e^{-(n[x'-x])^2}$  instead of  $\delta_{\epsilon}(x', x)$ . To see this, let  $\epsilon = \frac{\sqrt{\pi}}{n}$  and compare

$\delta_{\epsilon}(x', x) = \delta_{\frac{\sqrt{\pi}}{n}}(x', x)$  to  $\frac{n}{\sqrt{\pi}} e^{-(n[x'-x])^2}$ . The graphs below show the comparison for  $x = 1$  and  $n = 20$ .



$$\delta_{\frac{\sqrt{\pi}}{20}}(x', 1)$$



$$\frac{20}{\sqrt{\pi}} e^{-(20[x'-1])^2}$$

Unfortunately, the fact that the above definitions are informal and mathematically incorrect (e.g.,  $\delta$  is not a real-valued function; Fubini's Theorem) makes proving some of its properties difficult. See, for example, the argument below to normalize  $\psi_p$  in equation (8.17).

A mathematically rigorous definition of  $\delta$  requires the concept of measure, specifically Lebesgue measure. The Dirac delta “function” is not a function at all

but a measure. The argument of a measure, unlike a function, is a set. The Dirac delta function is defined for any measurable set containing “ $x$ ” to be 1, and 0 otherwise. Thus, the density  $\delta(\{x\}) = 1$  and also  $\delta(-\infty, \infty) = 1$ . The latter can be expressed in probability distribution terminology:  $\int_{-\infty}^{\infty} \delta(x - x') dx' = 1$

### Integration By Parts Note

We were able to drop the term  $FG|_a^b$  because wave functions are zero at  $\pm\infty$ .

### Linear Operators

Recall that observables are represented by Hermitian linear operators.

By definition,  $L$  is a **linear operator** if  $L(\alpha x + \beta y) = \alpha Lx + \beta Ly$ .

Recall that  $L$  is **Hermitian** if  $L^\dagger = L \stackrel{(3.06)}{\Leftrightarrow} \langle \Psi | L | \Phi \rangle = \langle \Phi | L | \Psi \rangle^* \forall \Psi, \Phi$ .

**Example 1. Multiplication Operator:**  $X \psi(x) = x\psi(x)$  (8.5)

$$\langle \Psi | X | \Phi \rangle = \int \psi^*(x) x \phi(x) dx$$

$$\langle \Phi | X | \Psi \rangle = \int \phi^*(x) x \psi(x) dx$$

$$\langle \Phi | X | \Psi \rangle^* = \int \phi(x) x^* \psi^*(x) dx = \int \phi(x) x \psi^*(x) dx = \langle \Psi | X | \Phi \rangle$$

(because  $x^* = x$  since  $x \in \mathbb{R}$ ).

Thus,  $X$  is Hermitian.

**Example 2. Differentiation Operator:**  $D \psi(x) = \frac{d\psi(x)}{dx}$  (8.6)

$$\langle \Psi | D | \Phi \rangle = \int \psi^*(x) \frac{d\phi(x)}{dx} dx$$

$$\langle \Phi | D | \Psi \rangle = \int \phi^*(x) \frac{d\psi(x)}{dx} dx \stackrel{(8.3b)}{=} - \int \psi^*(x) \frac{d\phi(x)}{dx} dx = -\langle \Psi | D | \Phi \rangle$$

Thus,  $D$  is anti-Hermitian. But, we next show that this means that both  $iD$  and  $-iD$  are Hermitian. In particular,  $i\hbar D$  is Hermitian.

**Theorem.** If  $M$  is anti-Hermitian, then both  $iM$  and  $-iM$  are Hermitian.

**Proof.** Let  $z, w \in \mathbb{C}$ . Then  $(zw)^* = z^* w^*$ . In particular,

$$(iz)^* = i^* z^* = -iz^* \quad (i)$$

$$(-iz)^* = (-i)^* z^* = iz^* \quad (\text{ii})$$

Let  $M = (m_{jk})$  be an  $(n \times n)$ -complex matrix. Then

$$[iM]^\dagger = (im_{jk})^{T*} = (im_{kj})^* = \left( [im_{kj}]^* \right)^{(i)} = (-im_{kj}^*) = -iM^\dagger \quad (\text{iii})$$

$$[-iM]^\dagger = (-im_{jk})^{T*} = (-im_{kj})^* = \left( [-im_{kj}]^* \right)^{(ii)} = (im_{kj}^*) = iM^\dagger \quad (\text{iv})$$

Suppose  $M$  is anti-Hermitian:

$$M^\dagger = -M \quad (\text{v})$$

Then

$$[iM]^\dagger \stackrel{(iii)}{=} -iM^\dagger \stackrel{(v)}{=} iM. \text{ That is, } iM \text{ is Hermitian. } \checkmark$$

$$[-iM]^\dagger \stackrel{(iv)}{=} iM^\dagger \stackrel{(v)}{=} -iM. \text{ That is, } -iM \text{ is Hermitian. } \checkmark$$



We show that the multiplication operator  $X$  is the Hermitian operator that represents the position observable. That is, Alice observes a particle at position  $x_0 \in \mathbb{R}$ . Let  $|\Psi\rangle$  be the state vector that represents the outcome  $x_0$  of the observable  $X$ . The states  $\{|x\rangle : x \in \mathbb{R}\}$  form a continuum so we represent  $|\Psi\rangle$  as an integral rather than a linear sum of basis vectors:

$$|\Psi\rangle \stackrel{(8.1b)}{=} \int_{x=-\infty}^{\infty} \psi(x) dx.$$

By Principle 2, the outcome  $x_0$  is an eigenvalue of  $X$ . That is,

$$X|\Psi\rangle = x_0|\Psi\rangle.$$

By the definition (8.5) of  $X$ , the LHS is

$$X|\Psi\rangle \stackrel{(8.1b)}{=} \int_{-\infty}^{\infty} X \psi(x) dx \stackrel{(8.5)}{=} \int_{-\infty}^{\infty} x \psi(x) dx.$$

The RHS is

$$x_0|\Psi\rangle \stackrel{(8.1b)}{=} \int_{-\infty}^{\infty} x_0 \psi(x) dx.$$

Thus,

$$x \psi(x) = x_0 \psi(x) \text{ a.e. (almost everywhere ; i.e., except on a set of measure$$

$$\Leftrightarrow (x - x_0) \psi(x) = 0 \text{ a.e.} \quad \text{zero)} \quad (8.11)$$

This means that except on some set of measure zero, if  $x \neq x_0$  then  $\psi(x) = 0$ .

We seek a function  $\psi$  that has this property (8.11) and which also satisfies the normalization requirement that  $\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx = 1$ . We claim that the Dirac delta function meets these requirements. Let

$$\psi(x) = \delta(x_0 - x) = \begin{cases} \infty & \text{if } x = x_0 \\ 0 & \text{Otherwise} \end{cases} \quad (8.11b)$$

If  $x \neq x_0$ ,  $\psi(x) = 0$ . Thus  $\psi$  satisfies (8.11). Also

$$\delta^2(x_0 - x) = \begin{cases} \infty^2 & \text{if } x = x_0 \\ 0 & \text{Otherwise} \end{cases} = \delta(x_0 - x).$$

So, intuitively

$$\int_{-\infty}^{\infty} \psi^*(x) \psi(x) dx \stackrel{(8.11b)}{=} \int_{-\infty}^{\infty} \delta^2(x_0 - x) dx = \int_{-\infty}^{\infty} \delta(x_0 - x) dx = 1$$

and  $\psi$  satisfies (8.3). This argument lacks rigor because we haven't shown that  $\delta^2(x_0 - x)$  is just infinite enough that the area under the curve is unity.

Another useful relationship is

$$\langle x_0 | \Psi \rangle \stackrel{(3.00)}{=} \psi(x_0). \quad (8.12)$$

Since this is true for all  $x_0$ , we can drop the subscript to get

$$\langle x | \Psi \rangle = \psi(x). \quad (8.13)$$

In other words, the wave function,  $\psi(x)$ , of a particle at position  $x$  is the projection of a state vector  $|\Psi\rangle$  onto the eigenvector of position.

**Definition.** We will refer to  $\psi(\mathbf{x})$  as the **wave function in the position representation**.

We move on to the concept of momentum. The **momentum operator** is defined in terms of the differentiation operator:

$$\mathbf{P} = -i\hbar\mathbf{D} \quad (8.14)$$

The  $\hbar$  factor is needed to provide units of mass times velocity ( $mv$ ).

For any function  $\psi(x)$ ,

$$\mathbf{P}\psi(x) \stackrel{(8.14)}{=} -i\hbar\mathbf{D}\psi(x) \stackrel{(8.6)}{=} -i\hbar \frac{d\psi(x)}{dx}. \quad (8.15)$$

Let  $|\Psi_p\rangle$  be a momentum state vector. Similar to  $X$ ,

$$|\Psi_p\rangle \stackrel{(8.1b)}{=} \int_{x=-\infty}^{\infty} \psi_p(x) dx$$

where  $x$  still represents position (rather than momentum) because  $D$  is defined in terms of position.

If  $p$  is an eigenvalue of  $P$  then

$$\mathbf{P}|\Psi_p\rangle = p|\Psi_p\rangle.$$

$$\text{LHS: } \mathbf{P}|\Psi_p\rangle \stackrel{(8.1b)}{=} \int_{-\infty}^{\infty} \mathbf{P}\psi_p(x) dx \stackrel{(8.15)}{=} \int_{-\infty}^{\infty} (-i\hbar) \frac{d\psi_p(x)}{dx} dx.$$

$$\text{RHS: } p|\Psi_p\rangle \stackrel{(8.1b)}{=} \int_{-\infty}^{\infty} p\psi_p(x) dx.$$

$$\therefore -i\hbar \frac{d\psi_p(x)}{dx} = p\psi_p(x) \text{ a.e.} \Rightarrow \frac{d\psi_p(x)}{dx} = \frac{ip}{\hbar} \psi_p(x) \text{ a.e.}$$

Solving the differential equation yields

$$\psi_p(x) = Ae^{\frac{ipx}{\hbar}} \text{ a.e.}$$

To solve for  $A$  we must apply normalization, but (8.3) doesn't work:

$$1 \stackrel{(8.3)}{=} \int_{-\infty}^{\infty} \psi_p^*(x) \psi_p(x) dx = \int_{-\infty}^{\infty} Ae^{-\frac{ipx}{\hbar}} Ae^{\frac{ipx}{\hbar}} dx = A^2 \int_{-\infty}^{\infty} dx = A^2(\infty) = \infty.$$

The difficulty in solving for  $A$  is due to the informality (i.e., the mathematical non-correctness) of the Dirac delta definition. The approach that works is to first assume that  $x$  is periodic with period  $2\pi R$ . This leads to discrete values  $p_n$  for  $p$ , and use of the discrete normalization equation in Table 8.1, above. Then taking

$R \rightarrow \infty$ , discrete  $p_n \rightarrow$  continuous  $p$ , and Kronecker  $\delta \rightarrow$  Dirac  $\delta$ , this finally

leads to  $A = \frac{1}{\sqrt{2\pi}}$ . Thus

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}} \text{ a.e.} \quad (8.17)$$

Of interest is the inner product of a position eigenvector  $|x\rangle$  and a momentum state vector  $|\Psi_p\rangle$ :

$$\left\{ \begin{array}{l} \langle x | \Psi_p \rangle \stackrel{(8.13)}{=} \psi_p(x) \stackrel{(8.17)}{=} \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}} \text{ a.e.} \\ \langle \Psi_p | x \rangle = \psi_p^*(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{ipx}{\hbar}} \text{ a.e.} \end{array} \right. \quad (8.18)$$

This relates to the Heisenberg Uncertainty Principle.