

Handout Contents

- Golden Equations for Lectures 18 to 22
- Answers to examples on Handout 5
- Tricks of the Quantum trade (revision hints)

Golden Equations (Lectures 18 to 22)

$$\langle \psi | \hat{A} | \phi \rangle = \int \psi^*(\mathbf{x}) \hat{A} \phi(\mathbf{x}) dx^n$$

$$\hat{I} = \int |x\rangle \langle x| dx = \int |p\rangle \langle p| dp$$

Answers to Handout 5

Lecture 18

1. (a) If $|b\rangle$ is normalised we expect $\langle b|b\rangle = 1$. Evaluating it explicitly

$$\int_{-\infty}^{\infty} b^*(x)b(x) dx = \int_0^{\infty} \frac{dx}{(1+x)^2} = \left[\frac{-1}{1+x} \right]_0^{\infty} = 0 - \frac{-1}{1+0} = 1.$$

(b) $|xb\rangle = \hat{x}|b\rangle$ becomes $x/(1+x)$ (for $x > 0$) in the x -representation. Clearly this tends to 1 at large x and therefore its square integral

$$\langle xb|xb\rangle = \int_0^{\infty} \frac{x^2}{(1+x)^2} dx$$

obviously diverges.

(c) It's probably clear that the integrand in $\langle b|x|b\rangle$, i.e. $x/(1+x)^2$, tends to $1/x$ at large x and therefore its integral diverges logarithmically. If you wanted to do this carefully, integrate by parts with a finite upper limit a and then consider $a \rightarrow \infty$:

$$\begin{aligned} \langle b|x|b\rangle &= \lim_{a \rightarrow \infty} \int_0^a \frac{x}{(1+x)^2} dx = \left[\frac{-x}{1+x} \right]_0^a + \int_0^a \frac{dx}{1+x} \\ &= \frac{-a}{a+1} + 0 + [\ln(1+x)]_0^a = \ln(1+a) - \frac{a}{1+a}. \end{aligned}$$

As $a \rightarrow \infty$ the logarithmic term diverges while the fraction tends to 1, so the expected value of x diverges as predicted.

2. **(a)** We know $\delta(x - x') = \langle x|x' \rangle$. But $\langle x|x' \rangle = \langle x'|x \rangle^*$ as for any inner product. Hence, since $\delta(x)$ is real,

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

as required.

(b) Both $\delta(x)$ and $\delta(ax)$ equal zero when $x \neq 0$, so the crucial definition is the integral. If $c < 0 < d$, then $\int_c^d \delta(x) dx = 1$. Now if $a > 0$ then

$$\int_c^d \delta(ax) dx = \int_{ac}^{ad} \delta(y) \frac{dy}{a} = \frac{1}{a} = \frac{1}{|a|}.$$

where we write $y = ax$, and note that $ac < 0 < ad$. On the other hand, if $a < 0$ then $ad < 0 < ac$ and

$$\int_{ac}^{ad} \delta(y) \frac{dy}{a} = - \int_{ad}^{ac} \delta(y) \frac{dy}{a} = \int_{ad}^{ac} \delta(y) \frac{dy}{|a|} = \frac{1}{|a|}.$$

Therefore, in either case,

$$\int_c^d |a| \delta(ax) dx = |a| \int_{ac}^{ad} \delta(y) \frac{dy}{a} = 1,$$

showing that $|a| \delta(ax) = \delta(x)$ as required.

- 3.

$$\frac{d}{dx} \theta(x - x') = \lim_{\delta x \rightarrow 0} \frac{\theta(x + \delta x - x') - \theta(x - \delta x - x')}{\delta x}$$

If $x > x'$, both terms in the numerator equal 1 for sufficiently small δx , so their difference is zero. Similarly if $x < x'$, both terms are zero for sufficiently small δx . If $x = x'$, the numerator equals $(1 - 0)$ for any $\delta x > 0$ and so the fraction tends to positive infinity. Moreover, if $a < b$,

$$\int_a^b \frac{d}{dx} \theta(x - x') dx = \int_{\theta(a-x')}^{\theta(b-x')} d\theta(x - x') = \theta(b - x') - \theta(a - x').$$

This equals 1 if $a < x' \leq b$ and zero otherwise, so the function meets all the requirements for the delta function: equal to zero if $x \neq x'$ and integral of unity if the range covers x' .

Lecture 19

1.

$$\langle p|\psi(0)\rangle = \int_{-\infty}^{\infty} \langle p|x\rangle \langle x|\psi(0)\rangle dx = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/4\sigma^2} dx,$$

which is a Fourier transform:

$$\begin{aligned} \langle p|\psi(0)\rangle &= \frac{1}{\sqrt{\hbar\sigma}(2\pi)^{3/4}} \int dx \exp\left[-\frac{ipx}{\hbar} - \frac{x^2}{4\sigma^2}\right] \\ &= \frac{1}{(2\pi)^{3/4}(\hbar\sigma)^{1/2}} \int dx \exp\left[-\left(\frac{x}{2\sigma} + ip\frac{\sigma}{\hbar}\right)^2 - \frac{p^2\sigma^2}{\hbar^2}\right] \end{aligned}$$

(completing the square as suggested in the hint). Put $z = (x/2\sigma) + i(p\sigma/\hbar)$:

$$\begin{aligned} \langle p|\psi(0)\rangle &= \frac{1}{(2\pi)^{3/4}(\hbar\sigma)^{1/2}} \exp\left[-\frac{p^2\sigma^2}{\hbar^2}\right] \int 2\sigma dz e^{-z^2} = \frac{2\sigma\pi^{1/2}}{(2\pi)^{3/4}(\hbar\sigma)^{1/2}} \exp\left[-\frac{p^2\sigma^2}{\hbar^2}\right] \\ &= \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/4} e^{-p^2\sigma^2/\hbar^2}. \end{aligned}$$

2. (a) Time evolution operator of the free particle: $\hat{H} = \hat{p}^2/2m$, which is independent of time, so

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \exp\left[\frac{-i\hat{p}^2t}{2m\hbar}\right]$$

In the momentum representation,

$$\hat{p} \xrightarrow{p} p, \quad \text{i.e.} \quad \langle p|\hat{p}|\psi\rangle = p\langle p|\psi\rangle = p\psi(p)$$

By the usual rule for functions of operators, the time evolution operator is similarly just a multiplication of the momentum-space wave function:

$$\langle p|\hat{U}(t)|\psi\rangle = \exp[-ip^2t/2m\hbar]\langle p|\psi\rangle.$$

- (b) Momentum wave function is:

$$\langle p|\psi(t)\rangle = \langle p|\hat{U}(t)|\psi(0)\rangle = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/4} \exp\left[-\frac{p^2}{\hbar^2}\left(\sigma^2 + \frac{i\hbar t}{2m}\right)\right]$$

Fourier transforming back,

$$\langle x|\psi(t)\rangle = \int \langle x|p\rangle \langle p|\psi(t)\rangle dp,$$

Putting $y^2 = \sigma^2 + i\hbar t/2m$ and completing the square as in Q.1:

$$\begin{aligned}\langle x|\psi(t)\rangle &= \frac{1}{\sqrt{2\pi\hbar}} \int dp e^{ipx/\hbar} \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/4} \exp[-y^2 p^2/\hbar^2] \\ &= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{1/4} \int dp \exp[-((yp/\hbar) - ix/2y)^2 - (x/2y)^2] \\ &= \left(\frac{\sigma^2}{2\pi^3\hbar^4}\right)^{1/4} e^{-x^2/4y^2} \frac{\hbar}{y} \sqrt{\pi} = \frac{\sqrt{\sigma}}{(2\pi)^{1/4}y} e^{-x^2/4y^2}\end{aligned}$$

This is the given formula, since

$$\frac{y}{\sqrt{\sigma}} = \sqrt{\sigma + \frac{i\hbar t}{2m\sigma}}$$

(c) By inspection, $|\langle x|\psi\rangle|^2$ and $|\langle p|\psi\rangle|^2$ are symmetric about the origin, so the mean in both cases is zero. Thus

$$\Delta p = \sqrt{\langle p^2\rangle}; \quad \Delta x = \sqrt{\langle x^2\rangle}.$$

$$\Delta p^2 = \int dp p^2 |\langle p|\psi\rangle|^2 = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/2} \int dp p^2 \exp\left[-\frac{2p^2\sigma^2}{\hbar^2}\right]$$

Writing $\sigma_p = \hbar/2\sigma$ this gives

$$\Delta p^2 = \frac{1}{\sqrt{2\pi\sigma_p^2}} \int dp p^2 e^{-p^2/2\sigma_p^2}$$

You should recognise this as a standard normalised gaussian integral which will give $\Delta p = \sigma_p$. Alternatively the recurrence relation in the hints shows that

$$\int dp p^2 \exp[-ap^2] = -\frac{d}{da} \sqrt{\frac{\pi}{a}} = \sqrt{\frac{\pi}{4a^3}}$$

With $a = 1/2\sigma_p^2$ we have

$$\Delta p^2 = \sqrt{\frac{(\pi 8\sigma_p^6/4)}{2\pi\sigma_p^2}} = \sigma_p^2.$$

The probability distribution in x is

$$\begin{aligned}|\langle x|\psi\rangle|^2 &= \frac{\sigma}{\sqrt{2\pi}|y|^2} \exp\left[-\frac{x^2}{4}\left(\frac{1}{y^2} + \frac{1}{(y^*)^2}\right)\right] = \frac{\sigma}{\sqrt{2\pi\left(\sigma^4 + \left(\frac{\hbar t}{2m}\right)^2\right)}} \exp\left[-\frac{x^2}{4} \frac{y^2 + (y^*)^2}{|y|^4}\right] \\ &= \frac{1}{\sqrt{2\pi(\sigma^2 + (\hbar t/2m\sigma^2)^2)}} \exp\left[-\frac{x^2}{2} \frac{\sigma^2}{|y|^4}\right].\end{aligned}$$

Comparing with the momentum case, we have a gaussian with

$$\Delta x = \sigma_x = (|y|^2/\sigma) = \sigma \sqrt{1 + \left(\frac{\hbar^2 t^2}{4m^2 \sigma^4}\right)}.$$

When $t = 0$

$$\Delta x \Delta p = \sigma \sigma_p = \sigma \hbar / 2\sigma = \hbar / 2.$$

- (d) For Δx to increase by $\sqrt{2}$, $t = 2m\sigma^2/\hbar$. (i) $m_e \sim 10^{-30}$ kg, atomic size $\sigma \sim 1\text{\AA} = 10^{-10}$ m. So $t = 2 \times 10^{-16}$ s. (ii) 2×10^{10} s ≈ 600 yrs.

Lecture 20

1.

$$[a, a^\dagger] = \frac{m\omega}{2\hbar} \left[x + \frac{i}{m\omega} p, x - \frac{i}{m\omega} p \right] = \frac{m\omega}{2\hbar} \frac{i}{m\omega} ([x, -p] + [p, x]) = \frac{i}{2\hbar} (-i\hbar - i\hbar) = 1$$

$$\langle n | a a^\dagger | n \rangle = c_+^2 \langle n+1 | n+1 \rangle = c_+^2$$

$$= \langle n | (a^\dagger a + 1) | n \rangle = (n+1) \langle n | n \rangle = (n+1).$$

$$(a^\dagger)|0\rangle/\sqrt{1!} = \sqrt{1}|1\rangle = |1\rangle; \quad (a^\dagger)^2|0\rangle/\sqrt{2!} = a^\dagger|1\rangle/\sqrt{2} = \sqrt{2}|2\rangle/\sqrt{2} = |2\rangle$$

Assume true for $n-1$:

$$(a^\dagger)^n|0\rangle/\sqrt{n!} = a^\dagger|n-1\rangle/\sqrt{n} = \sqrt{n-1+1}|n\rangle/\sqrt{n} = |n\rangle$$

true by induction for all n .

2. $\hat{p} = \sqrt{2m\hbar\omega}(\hat{a} - \hat{a}^\dagger)/2i$, so

$$\hat{p} \xrightarrow{\text{Energy}} \frac{\sqrt{2m\hbar\omega}}{2i} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & \dots \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & -\sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Using the matrix representation of \hat{x} given in the lectures, the commutator is:

$$[\hat{x}, \hat{p}] \xrightarrow{\text{Energy}} \frac{\hbar}{2i} (XP - PX)$$

where X, P are the matrices. Since each row and each column have only one or two non-zero values, multiplication is very easy. For diagonal elements we get terms like:

$$(XP)_{33} = \sqrt{2}\sqrt{2} - \sqrt{3}\sqrt{3} = -1$$

$$(PX)_{33} = -\sqrt{2}\sqrt{2} + \sqrt{3}\sqrt{3} = 1$$

$$([\hat{x}, \hat{p}])_{33} = \frac{\hbar}{2i}(-1 - 1) = i\hbar$$

All the diagonal terms give the same answer as we always get $n - (n + 1)$ from each matrix product. Off diagonal terms $(XP)_{i,i+1}$ etc are clearly all zero and for an offset of two from the diagonal $(XP)_{i,i+2} = (PX)_{i,i+2}$ and the same for $(i,i-2)$ elements. Larger offsets give no overlap between the “inhabited” strip near the diagonal. Thus $[\hat{x}, \hat{p}] \longrightarrow i\hbar I$, where I is the identity matrix.

We can be more methodical using index notation:

$$X_{ij} = \sqrt{j}\delta_{i,j-1} + \sqrt{j+1}\delta_{i,j+1}; \quad P_{ij} = \sqrt{j}\delta_{i,j-1} - \sqrt{j+1}\delta_{i,j+1}$$

$$\begin{aligned} (XP)_{ij} &= \sum_k X_{ik}P_{kj} = \sum_k \left(\sqrt{i+1}\delta_{i,k-1} + \sqrt{i}\delta_{i,k+1} \right) \left(\sqrt{j}\delta_{k,j-1} - \sqrt{j+1}\delta_{k,j+1} \right) \\ &= \sum_k \left(\sqrt{(i+1)j}\delta_{i,k-1}\delta_{k,j-1} - \sqrt{(i+1)(j+1)}\delta_{i,k-1}\delta_{k,j+1} \right. \\ &\quad \left. + \sqrt{ij}\delta_{i,k+1}\delta_{k,j-1} - \sqrt{i(j+1)}\delta_{i,k+1}\delta_{k,j+1} \right) \\ &= \sqrt{(i+1)j}\delta_{i,j-2} - \sqrt{(i+1)(j+1)}\delta_{i,j} + \sqrt{ij}\delta_{i,j} - \sqrt{i(j+1)}\delta_{i,j+2} \\ &= (i - (i+1))\delta_{i,j} + \sqrt{(i+1)(i+2)}\delta_{i,j-2} - \sqrt{i(i-1)}\delta_{i,j+2} \\ (PX)_{ij} &= \sum_k (-\sqrt{i}\delta_{i,k+1} + \sqrt{i+1}\delta_{i,k-1})(\sqrt{j+1}\delta_{k,j+1} + \sqrt{j}\delta_{k,j-1}) \\ &= \delta_{i,j} + \sqrt{(i+1)(i+2)}\delta_{i,j-2} - \sqrt{i(i-1)}\delta_{i,j+2} \end{aligned}$$

Thus

$$(XP)_{ij} - (PX)_{ij} = -2\delta_{ij} = -2I_{ij}.$$

3.

$$\langle E \rangle = \frac{\langle p^2 \rangle}{2m} + \frac{1}{2}m\omega \langle x^2 \rangle$$

since $\Delta A^2 = \langle A^2 \rangle - \langle A \rangle^2$, this is what we want. Now $\langle x \rangle = k \langle n | (a + a^\dagger) | n \rangle$, where $k = \sqrt{\hbar/2m\omega}$. Hence

$$\langle x \rangle = k(\sqrt{n} \langle n | n - 1 \rangle + \sqrt{n+1} \langle n | n + 1 \rangle) = 0,$$

since different $|n\rangle$ are orthogonal. Similarly for $\langle p\rangle$. Thus

$$\begin{aligned}\Delta x^2 = \langle x^2 \rangle &= \frac{\hbar}{2m\omega} \langle n|(a + a^\dagger)^2|n\rangle = k^2 \langle n|(a^2 + aa^\dagger + a^\dagger a + (a^\dagger)^2)|n\rangle \\ &= k^2 \langle n|(a^2 + (a^\dagger a + 1) + a^\dagger a + (a^\dagger)^2)|n\rangle \\ &= k^2(0 + 2\langle n|N|n\rangle + 1\langle n|n\rangle + 0) = (n + \frac{1}{2})\frac{\hbar}{m\omega} \\ \Delta p^2 &= -\frac{m\hbar\omega}{2} \langle n|(a - a^\dagger)^2|n\rangle = k'^2 \langle n|(-a^2 + aa^\dagger + a^\dagger a - (a^\dagger)^2)|n\rangle \\ &= k'^2(-0 + 2\langle n|N|n\rangle + 1\langle n|n\rangle - 0) = (n + \frac{1}{2})m\hbar\omega.\end{aligned}$$

Lecture 21

1. See notes on Lecture 23
2. Trend 1: With switches set to B at both ends, the SG experiments measure S_n , and we need to prove that we sometimes get spin-up (green) at both ends, i.e. that:

$$\langle \langle +n|_1 \langle +n|_2 | \psi \rangle \rangle > 0$$

Substituting the given expression for $|\psi\rangle$ we get

$$\sqrt{\frac{3}{8}} \{ \langle \langle +n| \langle +n| \rangle \rangle \langle \langle \downarrow | \downarrow \rangle \rangle + \langle \langle +n| \langle +n| \rangle \rangle \langle \langle \uparrow | \downarrow \rangle \rangle \} - \frac{1}{2} \langle \langle +n| \langle +n| \rangle \rangle \langle \langle \uparrow | \uparrow \rangle \rangle$$

Using the formula for inner products between direct products:

$$= \sqrt{\frac{3}{8}} \{ \langle \langle +n | \downarrow \rangle \rangle \langle \langle +n | \uparrow \rangle \rangle + \langle \langle +n | \uparrow \rangle \rangle \langle \langle +n | \downarrow \rangle \rangle \} - \frac{1}{2} \langle \langle +n | \uparrow \rangle \rangle \langle \langle +n | \uparrow \rangle \rangle$$

Expanding $\langle +n|$ for the left-hand term, we get:

$$= \sqrt{\frac{3}{8}} \left\{ \left(\sqrt{\frac{3}{5}} \langle \uparrow | \downarrow \rangle + \sqrt{\frac{2}{5}} \langle \downarrow | \downarrow \rangle \right) \left(\sqrt{\frac{3}{5}} \langle \uparrow | \uparrow \rangle + \sqrt{\frac{2}{5}} \langle \downarrow | \uparrow \rangle \right) + \langle \langle +n | \uparrow \rangle \rangle \langle \langle +n | \downarrow \rangle \rangle \right\} - \frac{1}{2} \langle \langle +n | \uparrow \rangle \rangle \langle \langle +n | \uparrow \rangle \rangle$$

This shows you how the whole thing will go (too long to write out!). Taking only the non-zero terms, i.e. involving $\langle \uparrow | \uparrow \rangle$ or $\langle \downarrow | \downarrow \rangle$ (both equal to 1), we get

$$= \sqrt{\frac{3}{8}} \left\{ \sqrt{\frac{2}{5}} \sqrt{\frac{3}{5}} + \sqrt{\frac{3}{5}} \sqrt{\frac{2}{5}} \right\} - \frac{1}{2} \sqrt{\frac{3}{5}} \sqrt{\frac{3}{5}} = \sqrt{\frac{3}{8}} \frac{2\sqrt{6}}{5} - \frac{3}{10} = \frac{3}{10}$$

which is > 0 as required.

Trend 2: If we measure S_z at one end and S_n at the other, we never find both are spin up. $|\psi\rangle$ is obviously symmetric if we swap the two ends, so we get the

same result whichever end we measure S_z . Let's measure it for particle 1, i.e. our task is to show that

$$(\langle \uparrow | \langle +n |) |\psi\rangle = 0$$

Expanding:

$$\begin{aligned} &= \sqrt{\frac{3}{8}} \{ \langle \uparrow | \downarrow \rangle \langle +n | \uparrow \rangle + \langle \uparrow | \uparrow \rangle \langle +n | \downarrow \rangle \} - \frac{1}{2} \langle \uparrow | \uparrow \rangle \langle +n | \uparrow \rangle \\ &= \sqrt{\frac{3}{8}} \langle +n | \downarrow \rangle - \frac{1}{2} \langle +n | \uparrow \rangle = \sqrt{\frac{3}{8}} \sqrt{\frac{2}{5}} - \frac{1}{2} \sqrt{\frac{3}{5}} = \sqrt{\frac{3}{20}} - \sqrt{\frac{3}{20}} = 0. \end{aligned}$$

Finally, if we choose mode A (measure S_z) at both ends, we never get both red lights (both spin down), i.e.:

$$(\langle \downarrow | \langle \downarrow |) |\psi\rangle = 0$$

since there is no $|\downarrow\rangle|\downarrow\rangle$ component in $|\psi\rangle$. Therefore (cf. result of previous question) there must be some non-local “cooperation” between the measurements at the two ends!

Tricks of the quantum trade

The main reason for learning the Dirac notation is that it makes it *much easier* to do quantum mechanics. Not just because it tends to be shorter, but because it lets you make a number of ‘sanity checks’ on the equations you write. This document tries to spell this out, and also to highlight points where you have to take care because the notation does not help you.

Making the notation work for you

You are used to checking that all the terms in an equation have the same physical dimensions/units. You also know that every term in a vector equation must be a vector, every term in a matrix equation must be a matrix with the same number of columns and rows, etc.

In the same way, in QM, the terms in equations may be bras, kets, operators, or scalars (i.e. numbers, often complex numbers). Each side of an equation must be the same kind of thing, and only things of the same kind can be added or subtracted. Also, you shouldn’t mix terms which apply to different vector spaces. Checking this avoids a lot of potential mistakes... here are some examples:

$ a\rangle = b\rangle + d\rangle$	OK: all terms are kets, presumably in the same space
$\hat{R} a\rangle = h\rangle$	OK: operators act to the right on a ket to make a new ket
$ d\rangle = \sum_i c_i a_i\rangle$	OK: scalar (here, c_i) times a ket is a ket
$\hat{T} = \hat{p}^2/2m$	OK: all terms are operators (op divided by scalar is an op)
$\hat{P}_a = a\rangle\langle a $	OK: outer products are one type of operator
$\langle b h\rangle = \langle b \hat{R} a\rangle = 3 + 4i$	OK: inner products are complex numbers.
$\langle b \hat{R} = \langle e $	OK: operators act to the left on a bra to make a new bra
$ 1\rangle = \uparrow\rangle \otimes \uparrow\rangle$	OK: direct products of kets are kets (but in a bigger vector space)
$\langle b \hat{G} a\rangle = \langle b a\rangle\hat{G}$	WRONG: LHS is a complex number, RHS is an operator
$\langle b + a\rangle - \langle b a\rangle = 0$	WRONG: can’t add bras, kets and/or scalars to each other
$ 2\rangle = \uparrow\rangle \otimes \uparrow\rangle + \downarrow\rangle$	WRONG: all kets in an equation must belong to the same space
$\hat{A} a_0\rangle = 0$	OK: here ‘0’ means the zero (ket) vector, not scalar zero
$\hat{M} = \hat{S}_z^2 + 2\hbar^2$	OK(ish): what is really meant is $\hat{M} = \hat{S}_z^2 + 2\hbar^2\hat{I}$...i.e. scalars are implicitly multiplied by the identity operator
$\hat{J} = \hat{L} + \hat{S}$	OK(ish): the operators act on three different spaces, but we mean...
$\hat{J} = \hat{L} \otimes \hat{I} + \hat{I} \otimes \hat{S}$	OK: all terms are ops acting on the $L \otimes S$ product space

A second check is that each equation should refer to just one level of description. So far we have been talking about the level of abstract vectors for which we use Dirac notation. When we pick a particular basis, we get a ‘representation’ of these abstract quantities as a set of numbers in a less abstract (so-called ‘concrete’) notation; in this

course we have used matrices and wave functions. These should not be mixed, with each other or with abstract bras and kets. Here are some examples:

Abstract	ket $ a\rangle$	bra $\langle a $	operator \hat{O}	number $\langle a b\rangle$
Matrix rep	column $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$	row (a_1^*, a_2^*)	square $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$(a_1^*, a_2^*) \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = a_1^* b_1 + a_2^* b_2$
Wave fn rep	$a(x)$	$a^*(x)$	$x \times \dots, -i\hbar d/dx$, etc.	$\int a^*(x)b(x) dx$

Here are some no-no's:

$$\langle \uparrow | \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} | \downarrow \rangle = 0$$

This mixes abstract & matrix levels, although it's pretty clear what's meant.

$$\langle p \rangle = \int \langle \psi | \frac{\hbar}{i} \frac{d}{dx} | \psi \rangle dx$$

This mixes abstract vectors & wave functions and is wrong in two ways. First, one of the main reasons Dirac notation is shorter & neater than using wave functions is that it *avoids* having to write out such integrals; they are implicit in expressions like $\langle \psi | \hat{p} | \psi \rangle$. Second, the differential operator for \hat{p} applies to wave functions, $\psi(x) = \langle x | \psi \rangle$, not to kets $|\psi\rangle$. Notice that the momentum wave function $\psi(p)$, which is the Fourier transform of $\psi(x)$, is also encoded in $|\psi\rangle$: $\psi(p) = \langle p | \psi \rangle$. $|\psi\rangle$ is not a function of x — its value does not change as x changes, because it implicitly accounts for all values of x simultaneously:

$$|\psi\rangle = \hat{I}|\psi\rangle = \int_{-\infty}^{\infty} |x'\rangle \langle x' | \psi \rangle dx' = \int_{-\infty}^{\infty} |x'\rangle \psi(x') dx'$$

(notice that x' is a dummy variable). So you will get into trouble if you try to differentiate by x ! Note that, in contrast, kets representing quantum states *are* functions of time because they do change (i.e. rotate in their abstract vector space) with time, under the control of the Schrödinger equation.

Numbers in Quantum mechanics

In quantum mechanics, scalar numbers play several different roles, but unfortunately the notation does not help tell them apart, and many mistakes are due to getting these roles confused:

Values of observables: Operators representing physical observables have physical dimensions (usually) and therefore units. Their eigenvalues, which are the allowed values of the observables, have the same dimensions and units, for instance in the equation

$$\hat{H}|E_0\rangle = E_0|E_0\rangle,$$

the Hamiltonian \hat{H} and the scalar E_0 have dimensions of energy. Eigenvalues of Hermitian operators are always real numbers. Note that, in contrast, unitary operators (such as rotations) are dimensionless, and so are their eigenvalues, which may be complex. Expectation values of operators, e.g. $\langle \psi | \hat{p} | \psi \rangle$, are averages over eigenvalues and, of course, share the same units.

Useful check: If one term in an equation involves an operator with physical dimensions, all the other terms must also have those same physical dimensions and so the numbers multiplying the dimensionless kets (or bras) in any terms lacking operators must involve values of observables, at least implicitly.

Probability amplitudes: We represent physical states, and vectors in orthonormal bases, as normalised kets, e.g. $|\psi\rangle$, where $\langle \psi | \psi \rangle = 1$. These are therefore dimensionless. If we expand such a ket in terms of a basis

$$|\psi\rangle = \sum_i c_i |a_i\rangle$$

the scalars complex numbers $c_i = \langle a_i | \psi \rangle$ must also be dimensionless, and we must also have $|c_i| \leq 1$ (NB: only if $|\psi\rangle$ is normalised, of course). They are often called probability amplitudes. They can be thought of as ‘coordinates’ for the tip of the vector $|\psi\rangle$, in the chosen basis.

Probabilities: The absolute square of a probability amplitude, e.g. $|c_1|^2 = c_1^* c_1$ gives the probability that a suitable measurement will find the system in the state given by the corresponding basis vector, here $|a_1\rangle$. Probabilities are dimensionless real numbers between 0 and 1. (“Suitable” means we measure some observable for which $|a_1\rangle$ is an eigenstate).

Useful check: you never get equations where bras, kets, or operators are multiplied by probabilities.

Probability (amplitude) densities Bases like $\{|\mathbf{x}\rangle\}$, appropriate for a wave function in N spatial dimensions, are normalised to a delta-function instead of unity, i.e. $\langle x | x' \rangle = \delta(x - x')$. Instead of probabilities we get probability densities which can be converted to probabilities by integrating over a suitable N -dimensional volume, e.g. in 1-D

$$\text{Prob}(x \leq 0) = \int_{-\infty}^0 |\psi(x)|^2 dx.$$

Probability amplitude densities like $\psi(\mathbf{x}) = \langle \mathbf{x} | \psi \rangle$ have dimensions of length to the $(-N/2)$ power (e.g. $(\text{length})^{-1/2}$ for 1-D), so the above integral gives a dimensionless probability. Since $|\psi\rangle$ is dimensionless, $\langle \mathbf{x} |$ and $|\mathbf{x}\rangle$ must also have dimension $(\text{length})^{-N/2}$.

Many beginners confuse probability amplitudes with values of observables, since both are commonly found as multipliers of kets. The best way to tell them apart is to read

carefully the words surrounding the equations, especially the ones that go “where a_i are the eigenvalues of operator \hat{A} ” etc. Notice that sometimes you get both:

$$\hat{A}|\psi\rangle = \hat{A} \sum_i c_i |a_i\rangle = \sum_i c_i \hat{A} |a_i\rangle = \sum_i c_i a_i |a_i\rangle.$$

A last warning: mathematically, it is legitimate to write

$$c_2 a_2 |a_2\rangle = b_2 |a_2\rangle = |\Xi\rangle \quad (\text{DON'T DO THIS!})$$

but this is horrible because b_2 is a probability amplitude (likely complex) multiplied by something physical like an energy or position, and the final ket $|\Xi\rangle$ is not dimensionless but has the same units as the eigenvalue a_2 . Save yourself a lot of trouble by not writing things like this: keep the different kinds of numbers separate, and work out your own notation to help. For instance, in this document I've consistently used c_i for probability amplitudes, and deliberately not used 'C' to name any operator and hence eigenvalues.