1a) Let $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$. We need our wavefunction to be zero outside $x,y,z \in [0,a]$, and satisfy $\hat{H}\psi = E\psi$ inside $x,y,z \in [0,a]$

This equation becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) = E\psi \text{, or}$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = -\frac{2mE}{\hbar^2}\psi$$

Plugging in our guess $\psi = \psi_x\psi_y\psi_z$, we get

$$\psi_x''\psi_y\psi_z + \psi_x\psi_y''\psi_z + \psi_x\psi_y\psi_z'' = -\frac{2mE}{\hbar^2}\psi_x\psi_y\psi_z \text{, or}$$

$$\frac{\psi_x''}{\psi_x} + \frac{\psi_y''}{\psi_y} + \frac{\psi_z''}{\psi_z} = -\frac{2mE}{\hbar^2}$$

Setting each term equal to a constant, we have

$$\frac{\psi_x''}{\psi_x} = -C_x \qquad \frac{\psi_y''}{\psi_y} = -C_y \qquad \frac{\psi_z''}{\psi_z} = -C_z, \qquad C_x + C_y + C_z = \frac{2mE}{\hbar^2}$$

The solutions are

$$\psi_x(x) = A_x\sin(\sqrt{C_x}\,x) + B_x\cos(\sqrt{C_x}\,x)$$

$$\psi_y(y) = A_y\sin(\sqrt{C_y}\,y) + B_y\cos(\sqrt{C_y}\,y)$$

$$\psi_z(z) = A_z\sin(\sqrt{C_z}\,z) + B_z\cos(\sqrt{C_z}\,z)$$

We know at $x=0$, $y=0$, or $z=0$, we need $\psi=0$. Thus, $\psi_x(0)=0$, $\psi_y(0)=0$, and $\psi_z(0)=0$. So we have $B_x = B_y = B_z = 0$.

We also know @ $x=a$, $y=a$, or $z=a$, $\psi=0$. Thus $\psi_x(a) = \psi_y(a) = \psi_z(a) = 0$.

We <u>cant</u> have $A_x = 0$, so we must have $\sin(\sqrt{C_x}\,x) = 0$, or $\sqrt{C_x} = \frac{\pi n_x}{a}$. Similarly, we have $\sqrt{C_y} = \frac{\pi n_y}{a}$, $\sqrt{C_z} = \frac{\pi n_z}{a}$.

Thus, we have eigenstates

$$\psi(x,y,z) = A\sin\left(\frac{\pi n_x}{a}x\right)\sin\left(\frac{\pi n_y}{a}y\right)\sin\left(\frac{\pi n_z}{a}z\right)$$

w/ $E = \frac{\hbar^2}{2m}(C_x + C_y + C_z) = \frac{\hbar^2\pi^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$

We can determine the constant A by normalization.

$$1 = \int |\Psi(x,y,z)|^2 \,dx\,dy\,dz = A^2 \int_0^a\int_0^a\int_0^a \sin^2\left(\frac{n_x\pi}{a}x\right)\sin^2\left(\frac{n_y\pi}{a}y\right)\sin^2\left(\frac{n_z\pi}{a}z\right) dx\,dy\,dz$$

$$= A^2 \int_0^a \sin^2\left(\frac{n_x\pi}{a}x\right)dx \int_0^a \sin^2\left(\frac{n_y\pi}{a}y\right)dy \int_0^a \sin^2\left(\frac{n_z\pi}{a}z\right)dz$$

$$= A^2\left(\frac{a}{2}\right)\left(\frac{a}{2}\right)\left(\frac{a}{2}\right), \quad \text{so} \quad A = \sqrt{\frac{8}{a^3}} = \left(\frac{2}{a}\right)^{3/2}$$

b & c) $n_x, n_y,$ and n_z go from 1 to infinity. Each triple (n_x, n_y, n_z) labels a state. We have energies $\frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2)$.

E	States	Degeneracy
$\frac{\pi^2\hbar^2}{2ma}(3)$	(1,1,1)	1
$\frac{\pi^2\hbar^2}{2ma}(6)$	(1,1,2) (1,2,1) (2,1,1)	3
$\frac{\pi^2\hbar^2}{2ma}(9)$	(1,2,2) (2,1,2) (1,2,2)	3
$\frac{\pi^2\hbar^2}{2ma}(11)$	(1,1,3) (1,3,1) (3,1,1)	3
$\frac{\pi^2\hbar^2}{2ma}(12)$	(2,2,2)	1
$\frac{\pi^2\hbar^2}{2ma}(14)$	(1,2,3) (1,3,2) (2,1,3) (2,3,1) (3,1,2) (3,2,1)	6

Physics 486 – Discussion #10 Problem 2 Solution

Problem 2 : Momentum-Basis Operators

Last week we learned that a position-space wavefunction $\psi_\alpha(x)$ is really a *representation* of a state $|\alpha\rangle$ in a *particular basis*, namely the basis of position eigenstates $|e_x\rangle$:

$$\boxed{\psi_\alpha(x) = \langle e_x|\alpha\rangle}$$

The wavefunction $\psi_\alpha(x) = \langle e_x|\alpha\rangle$ is the set of *coefficients* of the state $|\alpha\rangle$ along the basis elements $\{\ |e_x\rangle\ \}$, in the same way that (v_x, v_y, v_z) is the set of *coefficients* of the vector $\vec{v}$ along the basis elements $\{\ \hat{x},\hat{y},\hat{z}\ \}$.

(a) We are therefore free to build many different wavefunctions to represent a state $|\alpha\rangle$!
Specifically, we can build a wavefunction $\psi_\alpha(q)$ in the eigenspace $\{\ |e_q\rangle\}$ of any Hermitian operator Q, since Hermitian operators always have complete eigenspaces. In class we concentrated on transforming wavefunctions from position-space to momentum-space. Show that the general rule to transform of an x-space wavefunction $\psi(x)$ to a q-space wavefunction $\phi(q)$ describing the same state is :

$$\boxed{\phi(q) = \int \psi_q^*(x)\,\psi(x)\,dx}$$

where $\{q\}$ are the eigenvalues of a Hermitian operator Q, and $\psi_q(x)$ denotes the eigenfunction of Q with eigenvalue q.

STRATEGY: Go to Dirac notation straight away, and make good use of the completeness relation

$$\sum_y |e_y\rangle\langle e_y| = 1 \text{ for a discrete set of eigenvalues } \{y\} \qquad \text{or} \qquad \int dy\ |e_y\rangle\langle e_y| = 1 \text{ for a continuous set .}$$

IMPORTANT FYI : Recall that this space-switching is not just a mathematical curiosity; the *extreme* usefulness of changing the space of a wavefunction $\psi(x)$ is that $\psi(x)^*\psi(x)$ gives you the **probability density** $P(x)$ of finding the system at position x … and so $\phi(q)^*\phi(q)$ gives you the probability density $P(q)$ of finding it at the value q of **any other observable** Q : i.e.

$$\boxed{P(q) = \left|\langle e_q|\alpha\rangle\right|^2 = |\phi_\alpha(q)|^2}$$

as we wrote down last week. No longer are we constrained to simply obtain expectation values and variances from quantum wavefunctions, we can now obtain complete probability distributions in terms of any observable.

(a) solution

The boxed relation at the bottom,

$$P(q) = \left|\langle e_q|\alpha\rangle\right|^2 = |\phi_\alpha(q)|^2,$$

gives us the definition of a generalized wavefunction $\phi(q)$, i.e. a wavefunction in a basis of eigenvalues q:

$$\phi_\alpha(q) = \langle e_q|\alpha\rangle$$

In words: the wavefunction of the state α is the projection of the state α onto the eigenstates of whatever operator whose eigenvalues q you want to use as a basis. (Ack, the math expression is simpler than the words!)

Now we must translate the above relation into one involving x-basis wavefunction $\psi(x)$ since all of our work has been done in that basis. To do so, we inject the completeness operator

$$1 = \int_{-\infty}^{+\infty} dx\, |x\rangle\langle x|$$

into the middle of the expression for $\phi(q)$:

$$\phi_\alpha(q) = \int_{-\infty}^{+\infty} dx\, \langle e_q|x\rangle\langle x|\alpha\rangle$$

Finally, we recognize that

$\langle x|\alpha\rangle$ is the *x*-basis wavefunction for the state $|\alpha\rangle$, with symbol $\psi_\alpha(x)$ and

$\langle x|e_q\rangle$ is the *x*=basis wavefunction for the state $|e_q\rangle$, with symbol $\psi_q(x)$

and so

$$\phi_\alpha(q) = \int_{-\infty}^{+\infty} dx\, \langle x|e_q\rangle^* \langle x|\alpha\rangle = \int\; dx\, \psi_q^*(x)\, \psi_\alpha(x)$$

which is what we were tasked to prove. ☺

(b) In position-space, the operators for position x, momentum p, and any dynamical property $Q(x,p)$ are :

$$\hat{x} = x\,, \qquad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}\,, \qquad \hat{Q} = Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right).$$

What are the corresponding operators in momentum-space ? The operator for momentum itself is clearly just p, but what is the p-space operator for x? What a mind-bending question! ☺ It turns out the answer is

$$\hat{p} = p\,, \qquad \hat{x} = -\frac{\hbar}{i}\frac{\partial}{\partial p}\,, \qquad \hat{Q} = Q\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}, x\right)$$

Where did that $\hat{x}$ come from?? To show that the position operator in momentum space is indeed the one given above, prove that the expectation value of position is

$$\langle x \rangle = \int \Phi^*(p)\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}\right)\Phi(p)\; dp$$

HINT #1: Start with the formula you *know* for <x>. HINT #2 : Notice that $x\,\exp(ipx/\hbar) = -i\hbar(d/dp)\,\exp(ipx/\hbar)$.
FYI: In principle, you can do *all* calculations in momentum space instead of position space (though not always as easily). It is an interesting mental exercise to look at the quantum world as if p, not x, is the independent variable for your wavefunctions i.e. the basis in which you *think*. View the world through momentum-coloured glasses! ☺

(b) solution

From Eq. 3.55: $\Psi(x,t) = \dfrac{1}{\sqrt{2\pi\hbar}}\displaystyle\int_{-\infty}^{\infty} e^{ipx/\hbar}\Phi(p,t)dp.$

$$\langle x \rangle = \int \Psi^* x \Psi dx = \int \left[\frac{1}{\sqrt{2\pi\hbar}}\int e^{-ip'x/\hbar}\Phi^*(p',t)dp'\right] x \left[\frac{1}{\sqrt{2\pi\hbar}}\int e^{+ipx/\hbar}\Phi(p,t)dp\right] dx.$$

But $xe^{ipx/\hbar} = -i\hbar\dfrac{d}{dp}(e^{ipx/\hbar})$, so (integrating by parts):

$$x\int e^{ipx/\hbar}\Phi\, dp = \int \frac{\hbar}{i}\frac{d}{dp}(e^{ipx/\hbar})\Phi\, dp = \int e^{ipx/\hbar}\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right] dp.$$

$$\text{So } \langle x \rangle = \frac{1}{2\pi\hbar}\iiint \left\{ e^{-ip'x/\hbar}\Phi^*(p',t)e^{ipx/\hbar}\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right]\right\} dp'\, dp\, dx.$$

Do the x integral first, letting $y \equiv x/\hbar$:

$$\frac{1}{2\pi\hbar}\int e^{-ip'x/\hbar}e^{ipx/\hbar}dx = \frac{1}{2\pi}\int e^{i(p-p')y}dy = \delta(p-p'), \text{ (Eq. 2.144), so}$$

$$\langle x \rangle = \iint \Phi^*(p',t)\delta(p-p')\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right] dp'\, dp = \int \Phi^*(p,t)\left[-\frac{\hbar}{i}\frac{\partial}{\partial p}\Phi(p,t)\right] dp. \quad \text{QED}$$