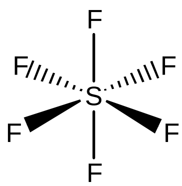
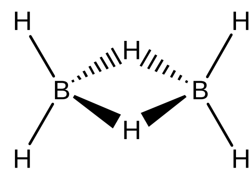
Quiz 5
CHEM 325
Spring 2009

Name: ____

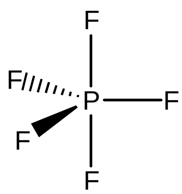
1. (5 Points) Assign the following molecules to the proper point group.



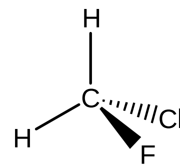
O_h



D_{2h}



D_{3h}



C_s

2. (5 Points) If the solution to the Schrödinger equation for a particular quantum mechanical system is given by $\psi = Ae^{im\phi}$, where A and m are constants and ϕ is the angle from the x axis. Show that $A = \frac{1}{\sqrt{2\pi}}$ by normalizing the wavefunction.

To be normalized the wavefunction must meet this criterion: $\int_0^{2\pi} A^2 e^{-im\phi} e^{im\phi} d\phi = 1$**. This can be rearranged to**

$$A^2 \int_0^{2\pi} e^{-im\phi} e^{im\phi} d\phi = A^2 \int_0^{2\pi} e^{-im\phi+im\phi} d\phi = A^2 \int_0^{2\pi} e^0 d\phi = A^2 \int_0^{2\pi} 1 d\phi = 1$$

Evaluating the definite integral gives $A^2(2\pi - 0) = 1$ **and** $A = \sqrt{\frac{1}{2\pi}}$**.**

3a. (5 Points) Demonstrate that the wavefunction for a particle in a one-dimensional box is not an eigenfunction of the momentum operator, $\hat{p}_x$.

Appling the operator to the wavefunction gives

$$\hat{p}_x \psi_n = -i\hbar \frac{\partial}{\partial x}\left[i\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\right] = \left(\sqrt{\frac{2}{L}}\hbar\right)\frac{\partial}{\partial x}\sin\left(\frac{n\pi x}{L}\right) = \left(\sqrt{\frac{2}{L}}\hbar\right)\left(\frac{n\pi}{L}\right)\cos\left(\frac{n\pi x}{L}\right)$$

Since this operation does not give the original function back times a constant, the wavefunction is not an eigenfunction of the operator.

b. (8 Points) Show that the wavefunction for a particle in one-dimensional box is the superposition of two wavefunctions, one for the particle traveling left to right and the other for the particle traveling right to left in the box. Hint: make a substitution and then show that each term in the sum is an eigenfunction of the momentum operator.

Using the relationship $\sin\theta = \frac{1}{2i}\left(e^{i\theta} - e^{-i\theta}\right)$**, we can rewrite the equation as**

$$\psi_n = i\hbar\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) = \left(\frac{\hbar}{2}\right)\left(\sqrt{\frac{2}{L}}\right)\left(e^{in\pi x/L} - e^{-in\pi x/L}\right)$$

This is clearly a linear combination of two functions $Ce^{in\pi x/L}$ **and** $Ce^{-in\pi x/L}$**, where** ***C*** **is a constant, which we could determine if we chose to.**

Applying the momentum operator on each function gives

$$\hat{p}_x\left(Ce^{in\pi x/L}\right) = -i\hbar C\frac{\partial}{\partial x}\left(e^{in\pi x/L}\right) = -i\hbar C\left(\frac{in\pi}{L}\right)\left(e^{in\pi x/L}\right) = \left(\frac{n\hbar\pi}{L}\right)\left(Ce^{in\pi x/L}\right)$$

and

$$\hat{p}_x\left(Ce^{-in\pi x/L}\right) = -i\hbar C\frac{\partial}{\partial x}\left(e^{-in\pi x/L}\right) = -i\hbar C\left(-\frac{in\pi}{L}\right)\left(e^{-in\pi x/L}\right) = -\left(\frac{n\hbar\pi}{L}\right)\left(Ce^{-in\pi x/L}\right)$$

In both cases the operation returns the original function times a constant. Therefore, these wavefunctions are eigenfunctions of the momentum operator. Since the eigenvalues $+\frac{n\hbar\pi}{L}$ **and** $-\frac{n\hbar\pi}{L}$ **have the same magnitude, but are opposite in sign, they must correspond the particle traveling in the positive** ***x*** **direction (the positive eigenfunction) or the negative** ***x*** **direction (the negative eigenfunction). Thus, the original wavefunction is a linear combination (superposition) of the two degenerate wavefunctions for the particle traveling in opposite directions in the box.**

c. (3 Points) What is the physical meaning of all this?

We can know the energy of the particle and we can know the magnitude of the momentum simultaneously, but we can't know the direction of travel. In other words, the momentum vector, but not its magnitude, is ill-defined when we know the energy.