Solutions for assignment 2:

1. Beiser; Chap. 5: Prob 9: Show that the expectation values $\langle xp \rangle$ and $\langle px \rangle$ are related by

$$\langle px \rangle - \langle xp \rangle = \frac{\hbar}{i}$$

This result is described by saying that p and x do not commute and it is intimately related to the uncertainty principle,

Ans. The quantity shown is the expectation value of a special operator called a commutator of operators $\hat{p}$ and $\hat{x}$ and is defined as

$$[\hat{p},\ \hat{x}] = \hat{p}\hat{x} - \hat{x}\hat{p}$$

Let us calculate the expectation values for a normalised wavefunction $\psi(x)$,

$$\langle px \rangle - \langle xp \rangle = \int \psi(x)^* \hat{p}\hat{x}\psi(x)dx - \int \psi(x)^* \hat{x}\hat{p}\psi(x)dx$$

Using $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$, we have,

$$\langle px \rangle - \langle xp \rangle = \frac{\hbar}{i}\left[\int \psi(x)^* \frac{\partial}{\partial x}[x\psi(x)]dx - \int \psi(x)^* x \frac{\partial}{\partial x}\psi(x)dx\right]$$

$$= \frac{\hbar}{i}\left[\int \psi(x)^* x \frac{\partial}{\partial x}\psi(x) + \int \psi(x)^*\psi(x)dx - \int \psi(x)^* x \frac{\partial}{\partial x}\psi(x)dx\right] = \frac{\hbar}{i}$$

The first and the third term cancel out and the second term is equal to one (since the function is normalised.

2. Atkins: 9.12: Confirm that a function of the form e^{-gx^2} is a solution of the Schrodinger equation for the ground state of a harmonic oscillator and find an expression for g in terms of the mass and force constant of the oscillator.

Ans. We need to show : $\hat{H}e^{-gx^2} = (\text{eigen value})e^{-gx^2}$

$$\hat{H}e^{-gx^2} = \left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}kx^2\right)e^{-gx^2} = -\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2}\left(e^{-gx^2}\right) + \frac{1}{2}kx^2e^{-gx^2}$$

$$= -\frac{\hbar^2}{2\mu}(-2g)\left[\frac{d}{dx}\left(xe^{-gx^2}\right)\right] + \frac{1}{2}kx^2e^{-gx^2} = -\frac{\hbar^2}{2\mu}\left[4g^2x^2\left(e^{-gx^2}\right) - 2g\left(e^{-gx^2}\right)\right] + \frac{1}{2}kx^2e^{-gx^2}$$

If we can get rid of the $x^2\left(e^{-gx^2}\right)$ term, then we have proved our case. For this

$$\frac{4g^2\hbar^2}{2\mu}=\frac{1}{2}k \implies g=\frac{1}{2}\sqrt{\frac{\mu k}{\hbar^2}}$$

Verify if this is correct by looking back at what we got in the class.

3. Atkins: 9.20: Evaluate the z-component of the angular momentum and the kinetic energy of a particle on a ring that is described by the (unnormalized) wavefunctions (a) $e^{i\phi}$(b) $e^{-2i\phi}$, (c) cosϕ, and (d) cos$\chi e^{i\phi}+\sin\chi e^{-i\phi}$.

Ans. The operator for z-component of the angular momentum, $\hat{l}_z=\frac{\hbar}{i}\frac{\partial}{\partial\phi}$

The values for a system with wavefunction ψ, $\langle\hat{l}_z\rangle=\frac{\int\psi^*(\phi)\hat{l}_z\psi(\phi)d\phi}{\int\psi^*(\phi)\psi(\phi)d\phi}$ are as follows:

(a) $\frac{\int_0^{2\pi}e^{-i\phi}\frac{\hbar}{i}\frac{\partial}{\partial\phi}\left(e^{i\phi}\right)d\phi}{\int_0^{2\pi}e^{-i\phi}e^{i\phi}d\phi}=\hbar$; (b) $\frac{\int_0^{2\pi}e^{2i\phi}\frac{\hbar}{i}\frac{\partial}{\partial\phi}\left(e^{-2i\phi}\right)d\phi}{\int_0^{2\pi}e^{2i\phi}e^{-2i\phi}d\phi}=-2\hbar$;

(c) $\cos\phi=\frac{e^{i\phi}+e^{-i\phi}}{2}$, Thus we can see $\cos\phi$ as a superposition of two different functions. Even though we have an unnormalized function, we can see easily that the contribution of the two components is equal, since each appears with a coefficient of $\frac{1}{2}$. We can also see from part (a) that for the state $e^{-i\phi}$, the value of $\langle\hat{l}_z\rangle=-\hbar$. Thus, for $\cos\phi$, we can write,

$\langle\hat{l}_z\rangle=\frac{1}{2}\left[\langle\hat{l}_z\rangle_{e^{i\phi}}+\langle\hat{l}_z\rangle_{e^{-i\phi}}\right]=0.$

Part (d) is a generlised situation from part (c), where the the contributions of the two components $e^{i\phi}$ and $e^{-i\phi}$ are not equal, but is the ratio of $\sin^2\chi$ and $\cos^2\chi$ (remember the property depends on the probability density and the density is the square of the function).

$\therefore\langle\hat{l}_z\rangle=\cos^2\chi\langle\hat{l}_z\rangle_{e^{i\phi}}+\sin^2\chi\langle\hat{l}_z\rangle_{e^{-i\phi}}=\hbar(\cos^2\chi-\sin^2\chi)=\hbar\cos 2\chi.$

4. Atkins: 9.22: This problem was about writing/using a code. We can discuss this in class.

5. Atkins: 9.26: Show that the function f = cos ax cos by cos cz is an eigenfunction of ∇^2 and determine its eigenvalue.

Ans. $\nabla^2 f=\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\cos ax.\cos by.\cos cz=-(a^2+b^2+c^2)\cos ax.\cos by.\cos cz.$