Name________________________________ Student #__________________________

Quiz 1
CHEM 3PA3; Fall 2018

This quiz has 6 problems worth 17 points each. There are 2 "free" bonus points.

1. **Write the time-independent Schrödinger equation (TISE) for a particle with mass *m* in one dimension bound by a time-independent potential $V(x)$?**

2. **Write the time-dependent Schrödinger equation (TDSE) for particle with mass *m* in one dimension bound by a time-dependent potential $V(x,t)$?**

The following text pertains to problems 3, 4, and 5.

You are given a photon with wave number $k = 10^7 m^{-1}$. Planck's constant is $h = 6.626 \cdot 10^{-34}\ \frac{\text{kg}\cdot\text{m}^2}{\text{s}}$ and the speed of light is $c = 2.998 \cdot 10^8\ \frac{\text{m}}{\text{s}}$.

3. **What is the wavelength of the photon?**

4. **What is the momentum of the photon?**

5. **What is the energy of the photon?**

The following text pertains to problems 6, and 7.

The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\kappa x^2$$

You are told that its ground-state wavefunction is

$$\Psi(x) = \left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{\sqrt{\kappa m}x^2}{2\hbar}\right)$$

6. **What is the probability density for observing a particle in the middle of the harmonic well, $x = 0$?**

Bonus (5 pt) What is the zero-point energy of the quantum harmonic oscillator?

Name________________________________ Student #__________________________

Quiz 1
CHEM 3PA3; Fall 2018

This quiz has 7 problems worth 14 points each. There are 2 "free" bonus points.

1. **Write the time-independent Schrödinger equation (TISE) for a 1-dimensional particle bound by a time-independent potential $V(x)$?**

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\Psi_n(x)=E_n\Psi_n(x)$$

2. **Write the time-dependent Schrödinger equation (TDSE) for particle with mass *m* in one dimension bound by a time-dependent potential $V(x,t)$?**

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,t)\right)\Psi_n(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

The following text pertains to problems 3, 4, and 5.

You are given a photon with wave number $k=10^7 m^{-1}$. Planck's constant is $h=6.626\cdot 10^{-34}\ \frac{\text{kg}\cdot\text{m}^2}{\text{s}}$.

3. **What is the wavelength of the photon?**

Using the definition of wavenumber, $k=2\pi/\lambda$, $\lambda=2\pi/k=6.283\cdot 10^{-7}\,\text{m}=628.3\text{ nm}$.

4. **What is the momentum of the photon?**

Using the De Broglie relation, $p=h/\lambda$, $p=\left(6.626\cdot 10^{-34}\ \frac{\text{kg}\cdot\text{m}^2}{\text{s}}\right)\Big/\left(6.283\cdot 10^{-7}\,\text{m}\right)=1.055\cdot 10^{-27}\ \frac{\text{kg}\cdot\text{m}}{\text{s}}$

5. **What is the energy of the photon?**

Using the Planck relation, $E=h\nu=hc/\lambda=pc$,

$$E=\left(1.055\cdot 10^{-27}\ \tfrac{\text{kg}\cdot\text{m}}{\text{s}}\right)\cdot\left(2.998\cdot 10^{8}\ \tfrac{\text{m}}{\text{s}}\right)=3.162\cdot 10^{-19}\ \tfrac{\text{kg}\cdot\text{m}^2}{\text{s}^2}=3.162\cdot 10^{-19}\,\text{J}$$

The following text pertains to problems 6, and 7.

The Hamiltonian for the quantum harmonic oscillator is

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}\kappa x^2$$

You are told that its ground-state wavefunction is

$$\Psi(x)=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{\kappa m}x^2}{2\hbar}\right)$$

6. **What is the probability density for observing a particle in the middle of the harmonic well, $x=0$?**

$$p(x=0)=\left|\Psi(x=0)\right|^2=\sqrt{\frac{\sqrt{\kappa m}}{\pi\hbar}}$$

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Bonus (5 pt) What is the zero-point energy of the quantum harmonic oscillator?

Because the Hamiltonian is the Hermitian operator for the energy, the eigenvalue associated with its ground-state energy is the zero-point energy. To find the eigenvalue, we just substitute the wavefunction in the Schrödinger equation and simplify. Then:

$$\hat{H}\Psi(x)=\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}\kappa x^2\right)\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)$$

$$=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\left(-\frac{\hbar^2}{2m}\left[\frac{d^2}{dx^2}\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\right]+\frac{1}{2}\kappa x^2\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\right)$$

$$=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\left(-\frac{\hbar^2}{2m}\left[\frac{d}{dx}\left(-\frac{x\sqrt{\kappa m}}{\hbar}\right)\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\right]+\frac{1}{2}\kappa x^2\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\right)$$

$$=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\left(\begin{array}{l}-\frac{\hbar^2}{2m}\left[\left(-\frac{\sqrt{\kappa m}}{\hbar}\right)\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)+\left(-\frac{x\sqrt{\kappa m}}{\hbar}\right)^2\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\right]\\ +\frac{1}{2}\kappa x^2\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\end{array}\right)$$

$$=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\left(-\frac{\hbar^2}{2m}\left[\left(-\frac{\sqrt{\kappa m}}{\hbar}\right)+\left(-\frac{x\sqrt{\kappa m}}{\hbar}\right)^2\right]+\frac{1}{2}\kappa x^2\right)$$

$$=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\left(-\frac{\hbar^2}{2m}\left[\left(-\frac{\sqrt{\kappa m}}{\hbar}\right)+\frac{\kappa m}{\hbar^2}x^2\right]+\frac{1}{2}\kappa x^2\right)$$

$$=\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)\left(\frac{\hbar}{2}\sqrt{\frac{\kappa}{m}}-\frac{1}{2}\kappa x^2+\frac{1}{2}\kappa x^2\right)$$

$$=\frac{\hbar}{2}\sqrt{\frac{\kappa}{m}}\left(\frac{\sqrt{\kappa m}}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{\sqrt{\kappa m}}{2\hbar}x^2\right)$$

$$=\frac{\hbar}{2}\sqrt{\frac{\kappa}{m}}\Psi(x)=E\Psi(x)$$

$$E_{\text{zero-point}}\equiv\frac{\hbar}{2}\sqrt{\frac{\kappa}{m}}$$