Worksheet 6 KEY

1. **The *units* of the ground-state wavefunction for the Hydrogen atom, $\psi_{1s}(x,y,z)$, are**

(a) $(\text{length})^{3}$
(b) $(\text{length})^{5/2}$
(c) $(\text{length})^{2}$
(d) $(\text{length})^{3/2}$
(e) $(\text{length})^{1}$
(f) $(\text{length})^{1/2}$
(g) $(\text{length})^{-3}$
(h) $(\text{length})^{-5/2}$
(i) $(\text{length})^{-2}$
(j) $(\text{length})^{-3/2}$
(k) $(\text{length})^{-1}$
(l) $(\text{length})^{-1/2}$
(m) the wavefunction is unitless.
(n) none of the above.

2. The Davisson-Germer experiment measured the electron diffraction pattern when a beam of electrons (a so-called "cathode ray," like in the old CRT monitors) impinged on a Nickel surface at a 90° angle. The spacing between planes of Nickel atoms is $d = .91\cdot 10^{-10}\text{ m}$. **In order to see a diffraction pattern, what is the (approximate) velocity of the electrons in the beam? Write your answer in meters/second.**

The wavelength of the light needs to be about twice the lattice spacing. Then, using the De Broglie relation,

$$\lambda = 2\left(.91\cdot 10^{-10}\text{ m}\right) = \frac{h}{p}$$

$$p = \frac{h}{2\left(.91\cdot 10^{-10}\text{ m}\right)} = 3.64\cdot 10^{-24}\ \tfrac{\text{m}}{\text{s}}$$

$$v = \frac{p}{m} = \frac{3.64\cdot 10^{-24}\ \frac{\text{kg}\cdot\text{m}}{\text{s}}}{9.1095\cdot 10^{-31}\text{ kg}}$$

$$= 4.00\cdot 10^{6}\ \frac{\text{m}}{\text{s}}$$

3. An experimental study of the photoelectric effect is performed on a sample of Cesium, which has the work function $\Phi = 2.14\text{ eV}$ and electrons with a kinetic energy of 1.00 eV are emitted. **What is the wavelength of the light that is shining on the Cesium surface? Write your answer in nanometers.**

The total energy of the light that is impinging on the surface must be $2.14\text{ eV} + 1.00\text{ eV} = 3.14\text{ eV}$. Then, using Planck's law,

$$h\nu = 3.14\text{ eV}$$

$$\nu = \frac{3.14\text{ eV}}{h} = \frac{(3.14\text{ eV})\cdot 1.602\cdot 10^{-19}\ \frac{\text{J}}{\text{eV}}}{6.6262\cdot 10^{-34}\text{ J}\cdot\text{s}} = 7.592\cdot 10^{14}\ \tfrac{1}{\text{s}}$$

$$\lambda = \frac{c}{\nu} = \frac{2.998\cdot 10^{8}\ \frac{\text{m}}{\text{s}}}{7.592\cdot 10^{14}\ \frac{1}{\text{s}}} = 3.949\cdot 10^{-7}\text{ m}$$

$$= 394.9\text{ nm}$$

4. Derive the "equation of motion" for the change in the expectation value of a time-dependent Hermitian operator:

$$i\hbar\frac{d\langle C(t)\rangle}{dt}=\int\Psi^*(\tau,t)\left[\hat{C}(\tau,t),\hat{H}(\tau,t)\right]\Psi(\tau,t)\,d\tau+\int\Psi^*(\tau,t)\frac{\partial\hat{C}(\tau,t)}{\partial t}\Psi(\tau,t)\,d\tau$$

Starting with the definition of the expectation value

$$\frac{d\langle C(t)\rangle}{dt}=\frac{d\int\Psi^*(\tau,t)\hat{C}(\tau,t)\Psi(\tau,t)\,d\tau}{dt}$$

We can pull the derivative inside the integral, and then we get:

$$\frac{d\langle C(t)\rangle}{dt}=\int\begin{pmatrix}\dfrac{\partial\Psi^*(\tau,t)}{\partial t}\hat{C}(\tau,t)\Psi(\tau,t)+\Psi^*(\tau,t)\dfrac{\partial\hat{C}(\tau,t)}{\partial t}\Psi(\tau,t)\\ +\Psi^*(\tau,t)\hat{C}(\tau,t)\dfrac{\partial\Psi(\tau,t)}{\partial t}\end{pmatrix}d\tau$$

Substitute in the time-dependent Schrödinger equations:

$$\frac{\partial\Psi(\tau,t)}{\partial t}=\frac{-i}{\hbar}\left(\hat{H}(\tau,t)\Psi(\tau,t)\right)$$

$$\frac{\partial\Psi^*(\tau,t)}{\partial t}=\frac{i}{\hbar}\left(\hat{H}^*(\tau,t)\Psi^*(\tau,t)\right)$$

to obtain

$$\frac{d\langle C(t)\rangle}{dt}=\frac{1}{i\hbar}\int\begin{pmatrix}-\left(\hat{H}^*(\tau,t)\Psi^*(\tau,t)\right)\left(\hat{C}(\tau,t)\Psi(\tau,t)\right)\\ +\Psi^*(\tau,t)\hat{C}(\tau,t)H(\tau,t)\Psi(\tau,t)\end{pmatrix}d\tau+\int\Psi^*(\tau,t)\frac{\partial\hat{C}(\tau,t)}{\partial t}\Psi(\tau,t)\,d\tau$$

$$=\frac{1}{i\hbar}\int\begin{pmatrix}-\left(\Psi^*(\tau,t)\right)\left(\hat{H}(\tau,t)\hat{C}(\tau,t)\Psi(\tau,t)\right)\\ +\Psi^*(\tau,t)\hat{C}(\tau,t)H(\tau,t)\Psi(\tau,t)\end{pmatrix}d\tau+\int\Psi^*(\tau,t)\frac{\partial\hat{C}(\tau,t)}{\partial t}\Psi(\tau,t)\,d\tau$$

$$i\hbar\frac{d\langle C(t)\rangle}{dt}=\int\Psi^*(\tau,t)\left(\hat{C}(\tau,t)\hat{H}(\tau,t)-\hat{H}(\tau,t)\hat{C}(\tau,t)\right)\Psi(\tau,t)\,d\tau$$

$$+i\hbar\int\Psi^*(\tau,t)\frac{\partial\hat{C}(\tau,t)}{\partial t}\Psi(\tau,t)\,d\tau$$

$$i\hbar\frac{d\langle C(t)\rangle}{dt}=\int\Psi^*(\tau,t)\left[\hat{C}(\tau,t),\hat{H}(\tau,t)\right]\Psi(\tau,t)\,d\tau+i\hbar\int\Psi^*(\tau,t)\frac{\partial\hat{C}(\tau,t)}{\partial t}\Psi(\tau,t)\,d\tau$$

We used the Hermitian property of the operator to obtain the next-to-last line,

$$\int\Psi_1^*(\tau,t)\hat{C}(\tau,t)\Psi_2(\tau,t)\,d\tau=\int\left(\hat{C}^*(\tau,t)\Psi_1^*(\tau,t)\right)\Psi_2(\tau,t)\,d\tau\,.$$

5. The Hamiltonian for an electron moving in a harmonic well with force constant k is

$$\hat{H}(x)=-\frac{\hbar^2}{2m_e}\frac{d^2}{dx^2}+\frac{k}{2}x^2\,.$$

Verify that the following functions are eigenfunctions of this operator.

$$\psi_0(x) = \exp\left(-\left(\frac{\sqrt{mk}}{2\hbar}\right)x^2\right)$$

$$\psi_1(x) = \exp\left(-\left(\frac{\sqrt{mk}}{2\hbar}\right)x^2\right)\cdot x$$

$$\psi_2(x) = \exp\left(-\left(\frac{\sqrt{mk}}{2\hbar}\right)x^2\right)\cdot\left[\left(2\cdot\sqrt{\frac{mk}{\hbar}}\right)x^2 - 1\right]$$

6. **What are the eigenvalues that correspond to the eigenfunctions in problem #5?**

7. **What is the expectation value of the kinetic energy and the potential energy for each of the eigenfunctions in problem #5?** Notice that this will require you to normalize the eigenfunctions.

Problems 5-7 are rather tedious practice exercises. You plug the eigenfunctions into the Hamiltonian in parts 5 and 6. In part 7, you evaluate the kinetic-energy and potential-energy integrals,

$$\langle T\rangle = \int_{-\infty}^{\infty}\psi_k(x)\left(-\frac{\hbar^2}{2m_e}\frac{d}{dx^2}\right)\psi_k(x)\,dx$$

$$\langle V\rangle = \int_{-\infty}^{\infty}\psi_k(x)\left(\tfrac{1}{2}kx^2\right)\psi_k(x)\,dx$$

8. Consider the following potential,

$$V(x)=\begin{cases}+\infty & x<0\\ x & x\geq 0\end{cases} \tag{1}$$

Which of the following sketches is a possible <u>ground-state</u> wavefunction for a particle bound by the potential in Eq. (1).

D and F are the answers.

A and B are not normalizable.

C is not zero where the potential diverges.

E has a node, and thus corresponds to an excited state.