

Worksheet 6 KEY

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

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

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 $d = .91 \cdot 10^{-10}$ 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,

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

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

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

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

3. An experimental study of the photoelectric effect is performed on a sample of Cesium, which has the work function $\Phi = 2.14$ 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 eV + 1.00 eV = 3.14 eV. Then, using Planck’s law,

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

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

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

$$= 394.9 \text{ nm}$$

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

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

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:

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

Substitute in the time-dependent Schrödinger equations:

$$\begin{aligned} \frac{\partial \Psi(\tau, t)}{\partial t} &= \frac{-i}{\hbar} (\hat{H}(\tau, t) \Psi(\tau, t)) \\ \frac{\partial \Psi^*(\tau, t)}{\partial t} &= \frac{i}{\hbar} (\hat{H}^*(\tau, t) \Psi^*(\tau, t)) \end{aligned}$$

to obtain

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

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

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

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.

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

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

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

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,

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

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

8. Consider the following potential,

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

Which of the following sketches is a possible ground-state 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.



