**5.61 Fall 2017**
**Problem Set #3**

**1. A.** McQuarrie, page 120, #3-3 Show $\hat{A}f(x) = \lambda f(x)$, for $\lambda$ constant. Find the eigenvalue $\lambda$.

---

**B.** McQuarrie, page 120, #3-4

---

**C.** McQuarrie, page 182, #4-11

---

## 2. McQuarrie, pages 121-122, #3-11. Continuity of $\psi'$

---

**3. A.** McQuarrie, page 123, #3-17

---

**B.** McQuarrie, page 127, #3-36

---

## 4. Particle in an infinite 1-D Well

**A.** McQuarrie, page 122, #3-12. Answer this problem qualitatively by drawing a cartoon for $n = 2$ and $n = 3$ states.

---

**B.** Is there a simple mathematical/physical reason why the probabilities are not 1/4 for all four regions: $0 \leq x \leq a/4$, $a/4 \leq x \leq a/2$, $a/2 \leq x \leq 3a/4$, and $3a/4 \leq x \leq a$?

[**HINT**: where are the nodes in $\psi_n(x)$?]

---

## 5. Particle on a Ring

Solve for the energy levels of the particle confined to a ring as a crude model for the electronic structure of benzene. The two dimensional Schrödinger Equation, in polar coordinates, is

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + U(r,\phi)\right]\psi = E\psi.$$

For this problem, $U(r,\phi) = \infty$ for $r \neq a$, but when $r = a$, $U(a,\phi) = 0$.

**A.** This implies that $\psi(r,\phi) = 0$ for $r \neq a$. Why?

---

**B.** If $\psi(r, \phi) = 0$ for $r \neq a$, then $\frac{\partial \psi}{\partial r} = 0$. What is the simplified form of the Schrödinger Equation that applies when the particle is confined to the ring?

---

**C.** Apply the "periodic" boundary condition that $\psi(a, \phi) = \psi(a, \phi + 2\pi)$ to obtain the $E_n$ energy levels.

---

## 6. 1-Dimensional Infinite Wells with Steps

Consider the potential

$$\begin{aligned} V(x) &= \infty && x < 0, x > a \\ V(x) &= 0 && 0 \leq x \leq a/2 \\ V(x) &= V_0 = \frac{h^2}{8ma^2}(2)^2 && a/2 < x \leq a \end{aligned}$$

(This is the energy of $n = 1$ of an infinite well of width $a/2$.)

**A.**

Sketch $V(x)$ vs. $x$.

---

**B.** What are the boundary conditions for $\psi(x)$ at $x = 0$ and $x = a$?

---

**C.** What requirements must be satisfied at $x = a/2$?

---

**D.** Solve for the $n = 2$ (one node) and $n = 3$ (two nodes) $\psi_n(x)$ eigenfunctions of $\widehat{H}$ and $E_n$ energy levels.

Hints:

(i) For $0 \leq x \leq a/2$, $\psi_{\text{I}}(x) = A \sin k_{\text{I}} x \qquad k_{\text{I}} = [2mE/\hbar^2]^{1/2}$

(ii) For $a/2 < x \leq a$, $\psi_{\text{II}} = B \sin k_{\text{II}}(a - x)$ $k_{\text{II}} = [2m(E - V_0)/\hbar^2]^{1/2}$

(iii) $\psi_{\text{I}}(a/2) = A \sin(k_{\text{I}} a/2)$

$\psi_{\text{II}}(a/2) = B \sin(k_{\text{II}} a/2)$

$\left.\frac{d\psi_{\text{I}}}{dx}\right|_{x=a/2} = Ak_{\text{I}} \cos(k_{\text{I}} a/2)$

$\left.\frac{d\psi_{\text{II}}}{dx}\right|_{x=a/2} = +Bk_{\text{II}} \cos(k_{\text{II}} a/2)$

---

**E.** Compare your values of $E_2$ and $E_3$ to what you obtain from the de Broglie quantization condition

$$(n/2) = \frac{a/2}{\lambda_{n,\mathrm{I}}} + \frac{a/2}{\lambda_{n,\mathrm{II}}}$$
$$\lambda = h/p = 2\pi/k = h[2m(E - V(x))]^{-1/2}$$

---

**F.** For the $n = 2$ and $n = 3$ energy levels, what are the probabilities, $P_2$ and $P_3$, of finding the particle in the $0 \leq x \leq a/2$ region?

---

**G.** (optional) Will the $n = 2$ and $n = 3$ energy levels of the $V_1(x)$ and $V_2(x)$ potentials (defined below) be identical, as suggested by part **E**? Why?

$$V_1(x): \quad \left.\begin{array}{ll} V_1(x) = \infty & x < 0, x > a \\ V_1(x) = 0 & 0 \leq x \leq a/2 \\ V_1(x) = V_0 & a/2 < x \leq a \end{array}\right] \text{barrier on right side}$$

versus

$$V_2(x): \quad \left.\begin{array}{ll} V_2(x) = \infty & x < 0, x > a \\ V_2(x) = 0 & 0 \leq x \leq a/4, 3a/4 \leq x \leq a \\ V_2(x) = V_0 & a/4 < x \leq 3a/4 \end{array}\right] \text{barrier in the center}$$

---

**H.** Solve for $n = 1$ $\psi_1(x)$ and $E_1$ for $V_1$.

HINTS: For $a/2 < x \leq a$,

$$\psi_{\mathrm{II}}(x) = Be^{\kappa_{\mathrm{II}}(a-x)} + Ce^{-\kappa_{\mathrm{II}}(a-x)}$$
$$\kappa_{\mathrm{II}} = [2m(V_0 - E)/\hbar^2]^{1/2}$$

---

**I.** *(optional)* Is $E_1$ for $V_1$ larger or smaller than $E_1$ for $V_2$? Why? A cartoon would be helpful.

---