Problems:

5.12, 5.24, 6.6, 6.9, 6.11, 6.12, 6.24, 6.31, 6.32

Extend problems 6.31:

- Use the uncertainty principle to estimate the typical momentum of an electron with this wave function
- Determine the momentum space wave function for the $\psi(x)$ given in 6.31 and sketch a graph of $|\psi(p)|^2$. Use the Fourier transforms given in the handout.
- Working with the momentum space wave function argue that

$$\overline{p^n} = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} |\hat{\psi}(p)|^2 p^n \tag{1}$$

  with $n = 1, 2, ...$
- Argue that $\bar{p} = 0$
- Determine the probability that the electron will have momentum between $-\hbar/x_o$ and $+\hbar/x_o$. You may find the following integral helpful

$$\int du \frac{u^2}{(u^2+1)^2} = \frac{1}{2}\arctan(u) - \frac{u}{2(u^2+1)}$$

Basic notions of wave functions

1. The electron is described by a wave $\psi(x)$. DeBroglie says that the momentum is related to the wavelength

$$p = \frac{h}{\lambda} = \hbar\,\frac{2\pi}{\lambda} = \hbar k \tag{2}$$

2. If the typical size of the wave function is Δx then the typical spread is in the momentum Δp is determined by the uncertainty relation

$$\Delta x \Delta p \sim \hbar \tag{3}$$

3. The electron wave function $|\psi(x)|^2$ determines the probability that a particle is between x and $x + dx$

$$P(x)dx = |\psi(x)|^2 dx \tag{4}$$

4. The electron must be somewhere so

$$\int |\psi(x)|^2 = 1 \tag{5}$$

5. The momentum space wave function is

$$\hat{\psi}(p) = \int_{-\infty}^{\infty} dx\, e^{-i\frac{p\,x}{\hbar}} \qquad \Longleftrightarrow \qquad \psi(x) = \int_{-\infty}^{\infty} \frac{dp}{(2\pi\hbar)}\,\hat{\psi}(p)\,e^{+\frac{ip\,x}{\hbar}} \tag{6}$$

   The probability to find a particle with momentum between p and $p + dp$ is

$$P(p)dp = |\hat{\psi}(p)|^2 \frac{dp}{2\pi\hbar} \tag{7}$$

Static Quantum Mechanics

1. The Operators (position $\mathbb{X}$ and momentum $\mathbb{P}$) take functions and give back new functions

$$\mathbb{X}\psi(x) = x\psi(x) \tag{8}$$

$$\mathbb{P}\psi(x) = -i\hbar\frac{\partial}{\partial x}\psi(x) \tag{9}$$

   The book calls $\mathbb{P}$ and $\mathbb{X}$, $[p]$ and $[x]$ respectively.

2. The total energy operator is known as the Hamiltonian

$$\mathbb{H} = \frac{\mathbb{P}^2}{2M} + U(\mathbb{X}) \tag{10}$$
$$= -\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + U(x) \tag{11}$$

where U(x) is the potential energy.

3. The stationary wave functions $\psi_n(x)$ (which will correspond to the discrete Bohr orbits r_n) obey the stationary Schrödinger equation

$$\mathbb{H}\psi_n(x) = E_n\psi_n(x) \tag{12}$$
$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + U(x)\right]\psi_n(x) = E_n\psi_n(x) \tag{13}$$

where the E_n are are the energy levels (as in the $E_n = -13.6eV/n^2$ in the Bohr Model).

   - This is an equation for the ψ_n and the E_n. Only for certain E_n will the wave function obey boundary conditions that $\psi_n(x) \to 0$ as $x \to \infty$. For the particle in the box this says that the wave function vanishes at the edge of the box $\psi_n(0) = \psi_n(L) = 0$ which yields the condition that $k_n = n\pi/L$.

Particle in the Box

1. For an electron bouncing around in a box of size L the wave functions

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x) \qquad k_n = \frac{n\pi}{L} \qquad n = 1, 2, 3\ldots \tag{14}$$
$$= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \tag{15}$$

k_n here is different from (but similar to) the k_n used in Fourier series where it is $k_n = 2\pi n/L$

2. The energies are

$$E_n = \frac{\hbar^2 k_n^2}{2M} = \frac{\hbar^2\pi^2}{2ML^2}n^2 \tag{16}$$

Expectation Values

1. The average position is

$$\bar{x} = \langle\mathbb{X}\rangle = \int dx\, \psi^*(x)\mathbb{X}\psi(x) = \int dx\, x\, |\psi(x)|^2 \tag{17}$$

2. The average momentum is

$$\bar{p} = \langle\mathbb{P}\rangle = \int dx\, \psi^*(x)\mathbb{P}\psi(x) = \int dx\psi^*(x)\, -i\hbar\frac{\partial}{\partial x}\psi(x) \tag{18}$$

3. The average of any operator (call it $\mathbb{K}$ for kinetic energy for example) is

$$\bar{K} = \langle\mathbb{K}\rangle = \int dx\, \psi^*(x)\mathbb{K}\psi(x) \tag{19}$$

4. The variance (also called spread or standard deviation) of postion

$$(\Delta x)^2 = \overline{(x-\bar{x})^2} = \overline{x^2} - \overline{x}^2 \tag{20}$$
$$= \left\langle\mathbb{X}^2\right\rangle - \langle\mathbb{X}\rangle^2 \tag{21}$$
$$= \int dx\, (x-\bar{x})^2|\psi(x)|^2 \tag{22}$$

5. The variance or spread of any other operator (say momentum $\mathbb{P}$) is

$$(\Delta p)^2 \;=\; \left\langle \mathbb{P}^2 \right\rangle - \left\langle \mathbb{P} \right\rangle^2 \tag{23}$$

6. For example

$$\langle KE \rangle = \left\langle \frac{\mathbb{P}^2}{2M} \right\rangle = \int dx\, \psi^*(x) \left[-\frac{\hbar^2}{2M} \frac{d^2}{dx^2} \right] \psi(x) \tag{24}$$