Problems:

5.2 (c) and (d); 5.23 ; 5.22 (modified see below) ; 5.25 (see hints in problem 3 below) ; 5.30 (see hints in 4 below) ; (5.27 + problem five below) ; Practice Test #4

1. 5.22 (**Graded**)

   (a) Replace (c) with the following: Calculate how the classical turning points (the place where the particle would bounce off the well walls and turn back) depend on energy. Make shure your graphs in parts (a) and (b) reflect this dependence.

   (b) Replace (d) with estimate the size of the ground state wave function for an electon in this potential. Estimate the kinetic and potential energies associated with this wave function. Your answer should involve C, $\hbar$ and m_e.

2. For an even potential, $V(-x) = V(x)$ (take a harmonic oscillator for example $V(x) = \frac{1}{2}kx^2$) argue that the wave functions must either be even or odd, i.e.

$$\Psi_n(-x) = \pm\Psi_n(x). \tag{1}$$

Hint for a symmetric potential there is no preference to be either to the right or the left – say these words again and ask what that means. Sketch the lowest four wave functions of the harmonic oscillator oscillator verify that the wave functions have this property is the case.

3. (**Graded** based on problem 5.26 in book). Consider an electron in a box with a small additional potential shown below:

$$V(x)$$

Box potential + bump

bump from
-Δx to Δx

Hight of bump V_o

$-a/2$ $2\Delta x$ $a/2$
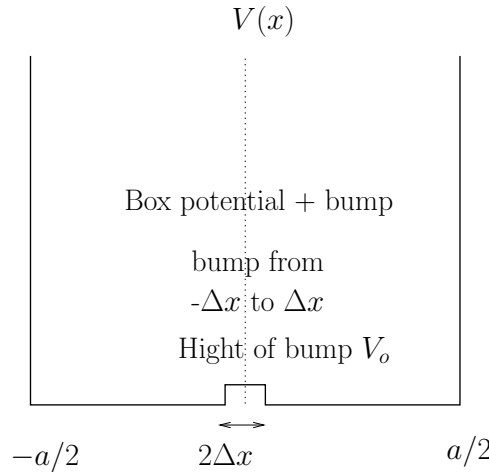
Here the width of the potential $2\Delta x$ is much-much smaller than the size of the box $\Delta x \ll a$ and the potential energy V_o is small.

   • A good student asks: What means small ? Small means that the V_o should be small compared to something? What is that something? Well, I will tell you. Small in this case means that V_o should be small compared to the typical energy $\sim \hbar^2/2Ma^2$. When such a small potential is added, the energies, which are orignally $E_n = \hbar^2\pi^2n^2/2Ma^2$, change by a relatively small amount of $\sim V_o$.

   • In fact, the change in energy is smaller than V_o, because the width of the potential is small compared to the size of the box. Clearly, in the limit that the potential has no width $\Delta x = 0$ the original energies are unmodified. This is the ultimate approximation. Thus we expect for small Δx the energies to change by an amount of order $\sim V_o(\frac{\Delta x}{a})^{\text{somepower}}$.

   • We will show shortly in class that in the presence of a small additional potential potential $\delta V(x)$ the energy of the n-th state is changed by the average of the additional potential. More specificially, $\delta E_n = \overline{\delta V(x)}$.

$$E_n \rightarrow E_n + \delta E_n \qquad \delta E_n = \overline{\delta V(x)} = \int_{-\infty}^{\infty} \psi_n^*(x)\,\delta V(x)\,\psi_n(x) \tag{2}$$

where $\psi_n(x)$ are the unpertubed wave functions, i.e. Eq. (29)

- (*hint on 5.25*) When sketching the wave function, keep in mind how $E - V$ influences the bending of the wave function.

(a) For the unperturbed wavefunctions of the particle in the box, show that close to the center of the box the probability density is approximately

$$P(x) \simeq \begin{cases} \frac{2}{a}\left[1 - (n\pi)^2 \left(\frac{x}{a}\right)^2\right] & n = 1, 3, 5 \dots \\ \frac{2}{a}(n\pi)^2 \left(\frac{x}{a}\right)^2 & n = 2, 4, 6 \dots \end{cases} \tag{3}$$

The taylor series of sin and cos should be useful here.

(b) Show that the shift in energy is

$$\delta E_n \simeq \begin{cases} \frac{4V_o \Delta x}{a}\left[1 - \frac{(n\pi)^2}{3}\frac{(\Delta x)^2}{a^2} + \dots\right] & n = 1, 3, 5 \dots \\ \frac{4V_o}{3}(n\pi)^2 \left(\frac{\Delta x}{a}\right)^3 & n = 2, 4, 6 \dots \end{cases} \tag{4}$$

Draw two energy level diagrams side by side. The first showing the unperturbed energy levels. The second showing the perturbed energy levels.

(c) Explain why the spatially odd wave functions (to wit $n = 2, 4, 6 \dots$) experience less shift then the spatially even wave functions (to wit $n = 1, 3, 5 \dots$) What would happen if the perturbing potential was placed at the end of the box. Draw a schematic level diagram in this case.

(d) Explain why the energy shift for the spatially even wave functions decrease with increasing n, while the energy shift for the spatially odd wave functions increases with n.

4. (*hints on 5.30*)

(a) In part (a) think carefully about the concavity of the wave function in different regions.

(b) For part(b) remember that the wave will be localized where the potential is lowest. Remember that since the potentials are even, the wave functions are even or odd. You might think carefully about Problem 3 to decide what configuration would have the lowest energy. This last hint applies to (d) and (e).

5. Using the probability density corresponding to the wave function in problem 27, determine the distance D over which $\Psi^*\Psi$ is smaller than its value at the edge by a factor of $1/e$. Without looking up numbers, evaluate D in angstroms when the the electron is energy $1\,\mathrm{eV}$ under the potential, i.e. $E - V = -1eV$.

Wavefunctions

1. The electron wave function squared $|\Psi(x,t)|^2 = \mathrm{P}(x,t)$ is *a probability per unit length* to find the particle at time t. Thus the probability $\mathrm{d}\mathscr{P}$ to find a particle between x and $x + dx$ at time t

$$\mathrm{d}\mathscr{P} = \mathrm{P}(x,t)dx = |\Psi(x,t)|^2 dx \tag{5}$$

2. The electron must be somewhere so

$$\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = 1 \tag{6}$$

3. The average position at time t

$$\bar{x} = \int dx\, x\, |\Psi(x,t)|^2 \tag{7}$$

4. The average position squared at time t is

$$\overline{x^2} = \int dx\, x^2\, |\Psi(x,t)|^2 \tag{8}$$

5. The uncertainty squared in position $(\Delta x)^2$ (or standard deviation squared) is defined to be

$$(\Delta x)^2 \equiv \overline{x^2} - \bar{x}^2 = \overline{(x - \bar{x})^2} \tag{9}$$

If the average position is zero $\bar{x} = 0$ then $(\Delta x) \equiv \sqrt{\overline{x^2}}$ is the "root mean square" position. This gives a measure of how spread out is the wave function

Momentum Averages

1. We use a notation for "Operators"

$$\bar{x} = \int_{-\infty}^{+\infty} dx\, \Psi^*(x)\mathbb{X}\Psi(x) \tag{10}$$

$$= \int_{-\infty}^{+\infty} dx\, \Psi^*(x)x\Psi(x) \tag{11}$$

Here $\mathbb{X}$ is an simply an "operator" which takes the function $\Psi(x)$ and spits out the new function $x\Psi(x)$. It just gives a notation to things that we alaready understand, for example $\mathbb{X}^2\Psi(x) = \mathbb{X}\,x\Psi(x) = x^2\Psi(x)$

2. The average momentum is

$$\bar{p} = \int_{-\infty}^{+\infty} dx\, \Psi^*(x)\mathbb{P}\Psi(x) \tag{12}$$

$$= \int_{-\infty}^{+\infty} dx\, \Psi^*(x)\left(-i\hbar\frac{d}{dx}\right)\Psi(x) \tag{13}$$

$$= \int_{-\infty}^{+\infty} dx\, \Psi^*(x)\left(-i\hbar\frac{d\Psi}{dx}\right) \tag{14}$$

Here the momentum operator is

$$\mathbb{P} = -i\hbar\frac{d}{dx}$$

takes the function $\Psi(x)$ and spits out the derivative $-i\hbar\frac{d\Psi}{dx}$.

3. The average momentum squared is

$$\overline{p^2} = \int_{-\infty}^{+\infty} \Psi^*(x) \mathbb{P}^2 \Psi(x) \tag{15}$$

$$= \int_{-\infty}^{+\infty} \Psi^*(x) \left(-\hbar^2 \frac{d^2}{dx^2} \right) \Psi(x) \tag{16}$$

4. The uncertainty squared in momentum (or standard deviation squared) is defined like for $(\Delta x)^2$

$$(\Delta p)^2 \equiv \overline{p^2} - \overline{p}^2 \tag{17}$$

Again if $\overline{p}$ is zero then $\Delta p \equiv \sqrt{\overline{p^2}}$ is the "root mean square" momentum.

5. The average kinetic energy is

$$\overline{KE} = \int_{-\infty}^{+\infty} \Psi^*(x) \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \Psi(x) \tag{18}$$

6. The formal statement of the uncertainty principle is

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2} \tag{19}$$

where the standard deviation in position Δx and momentum Δp are defined as above. (You can see why its a good thing that we know how to use it before we can state it precisely)

Quantum Mechanics

1. As with momentum, the average energy of a particle is

$$\overline{E} = \int \Psi^*(x,t) \mathbb{E} \Psi(x,t) \tag{20}$$

$$= \int_{-\infty}^{\infty} dx \Psi^*(x,t) \left[+i\hbar \frac{\partial}{\partial t} \right] \Psi(x,t) \tag{21}$$

and the energy operator is

$$\mathbb{E} = +i\hbar \frac{\partial}{\partial t} \tag{22}$$

Note the difference in sign between this and the momentum operator $\mathbb{P}$ which ultimately is a reflection of the fact that waves are written $e^{+i(kx-\omega t)}$ with opposite signs for k and ω

2. The Schrödinger equation can be written

$$\left[\frac{\mathbb{P}^2}{2M} + V(\mathbb{X}) \right] \Psi(x,t) = \mathbb{E}\Psi(x,t) \tag{23}$$

$$\left[-\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + V(x) \right] \Psi(x,t) = +i\hbar \frac{\partial \Psi}{\partial t} \tag{24}$$

where V(x) is the potential energy (think $V = 1/2\,kx^2$)

3. The stationary wave functions (or eigenfunctions) have the following form

$$\Psi(x,t) = e^{-i\frac{E_n t}{\hbar}} \Psi_n(x) \tag{25}$$

And are called stationary because the square does not depend on time

$$|\Psi(x,t)|^2 = \left| e^{-i\frac{E_n t}{\hbar}} \right|^2 |\Psi_n(x)|^2 \tag{26}$$

$$= |\Psi_n(x)|^2 \tag{27}$$

Since the wave funcion does not depend on time we can take a long time to determine the energy. So stationay have functions exactly the energy $E = E_n$. There is no uncertainty in the energy. $\Delta E^2 = \overline{\mathbb{E}^2} - \overline{\mathbb{E}}^2$

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4. Stationary wave functions (also known as eigenfunctions) obey the time independent Schrödinger equation.

$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + V(x)\right]\Psi_n(x) \;=\; E_n\Psi_n(x) \tag{28}$$

Here the E_n are are the energy levels (as in the $E_n = -13.6eV/n^2$ in the Bohr Model) are the E_n in the stationary wave functions

Particle in the Box

1. For an electron bouncing around in a box of size a the stationary wave functions (eigen-functions) are

$$\Psi_n(x) \;=\; \begin{cases} \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi x}{a}\right) & n = 1,3,5,\ldots \\ \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) & n = 2,4,6,\ldots \end{cases} \tag{29}$$

while the stationary energies are

$$E_n = \frac{\hbar^2 k_n^2}{2M} = \frac{\hbar^2\pi^2}{2Ma^2}\,n^2 \qquad n = 1,2,3,4,5,\ldots \tag{30}$$

Qualitative Features of Schrödinger Equation

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi_n(x) = E_n\Psi_n(x) \tag{31}$$

1. In the classically allowed region the egein-functions oscillates. In the classically forbidden region the wave function decays exponentially. For a given potential you should be able to roughly sketch the wave functions.

2. In the classically allowed region $E > V$, you be able to show (by assuming that the potential V is constant) that the wave function oscillates with wave number $k = 2\pi/\lambda$ as

$$\Psi(k) \propto A\cos(kx) + B\sin(kx) \qquad \text{where} \qquad k \sim \sqrt{\frac{2m(E-V)}{\hbar^2}} \tag{32}$$

3. In the classically forbidden region $E < V$, we say that the particle is "under the barrier" because $E < V$. Assuming that the potential is constant you should be able to show wave function decreases as

$$\Psi \sim Ce^{-\kappa x} \qquad \text{where} \qquad \kappa \sim \sqrt{\frac{2m(V-E)}{\hbar^2}}, \tag{33}$$

as one goes deeper into the classically forbidden region. The length $D \equiv 1/(2\kappa)$ is known as the "penetration" depth. It is the length over which the probability decreases by a factor $1/e$.

4. Looking at the Schrödinger equation

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-V)\psi \tag{34}$$

we conclude:

   (a) In the classically allowed region ($E - V > 0$) the wave function is concave down if $\psi > 0$ and concave up if $\psi < 0$. The strength of the curvature (how rapidly it oscillates) is controlled by $2m(E-V)/\hbar^2$.

   (b) In the classically forbidden region ($E - V < 0$) the wave function is concave up if $\psi > 0$ and concave down if $\psi < 0$. The strength of the curvature is controlled by $2m(V-E)/\hbar^2$.

5. The energy is determined in the Schrödinger Equation by demanding that the wave function Ψ decreases as $x \to \infty$. This is why we neglect exponentially increasing solutions $e^{+\kappa x}$ in the preceding item.

6. Generally there is one more "half" wavelength in the "box" (or more properly the classically allowed region) each time the particle in the potential is excited from one energy state (i.e. Ψ_n) to the next higher one (i.e. Ψ_{n+1}). Look at Box wave functions or simple harmonic oscillator wave functions for examples.

7. The wave function is always continuous and has continuous first derivatives.

8. An example of these trends is given by the set of simple harmonic oscillator wave functions handed out in class. You should be able to see these features in the figures handed out in class.

Perturbations

1. In the presence of a small additional potential potential $\delta V(x)$ the energy of the n-th state is changed by the average of the additional potential. More specifically, $\delta E_n = \overline{\delta V(x)}$, i.e.

$$E_n \rightarrow E_n + \delta E_n \qquad \overline{\delta V(x)} = \int_{-\infty}^{\infty} \psi_n^*(x)\,\delta V(x)\,\psi_n(x) \tag{35}$$

where $\psi_n(x)$ is the unperturbed wave functions.

2. The wave functions are orthogonal. Orthogonal means in the context of quantum mechanics:

$$\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x) = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases} \tag{36}$$