HW #4 Solutions

Here is a trick for defining positive constants. Whenever Simplify or Integrate are used, these assumptions will be applied.

 $In[33]:= $Assumptions = {\hbar > 0, m > 0, \omega > 0, 1 > 0}$ $Out[33]= {\hbar > 0, m > 0, \omega > 0, 1 > 0}$

Since we will be calculating $\Delta x \Delta p$ several times over, it is convenient to define a general function for doing so. The Module command allows a function to use a number of different intermediate steps before returning its final value. In this case, the values of $\langle x^2 \rangle$, $\langle x \rangle$, and $\langle p^2 \rangle$ are first calculated and put in the local variable xsq, xx, and psq. Then $\Delta x \Delta p$ is calculated from those.

$$\ln[346]:= \Delta x \Delta p[psi_] := Module \left[\{xsq, xx, psq\}, \{xsq, xx, psq\} = \frac{\text{Integrate}[psi\{x^2 psi, x psi, -\hbar^2 D[psi, \{x, 2\}]\}, \{x, -\infty, \infty\}]}{\text{Integrate}[psi^2, \{x, -\infty, \infty\}]}; \sqrt{(xsq-xx^2) psq}$$

define the simple harmonic oscillator wavefunctions

$$\ln[6] := \operatorname{sho}[n_{]} := \operatorname{With}\left[\left\{y = \frac{x}{\sqrt{\frac{\hbar}{m\omega}}}\right\}, \operatorname{HermiteH}[n, y] \operatorname{Exp}\left[-y^{2}/2\right]\right]$$

Problem 1: uncertainty product for first 4 states of the harmonic oscillator

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In[46]:= Table [\Delta x \Delta p[sho[n]], {n, 0, 3}] // Simplify
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\text{Out[46]=} \left\{ \frac{\hbar}{2} , \frac{3 \hbar}{2} , \frac{5 \hbar}{2} , \frac{7 \hbar}{2} \right\}
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note that each successive state adds 1 \hbar to the uncertainty product

Problem 2: repeat for the particle in a box.

define the wavefunctions for the PIAB. This uses the Piecewise function to define the wavefunctions everywhere.

$$\ln[348] := piab[n_] := \begin{cases} 0 & x < 0 \\ Sin[n \pi x / 1] & 0 \le x < 1 \\ 0 & x \ge 1 \end{cases}$$

 $ln[349]:= Table[\Delta x \Delta p[piab[n]], \{n, 1, 4\}] // Simplify$

$$Out[349]= \left\{ \frac{1}{2} \sqrt{\frac{1}{3} (-6+\pi^2)} \ \breve{n}, \sqrt{\frac{1}{6} (-3+2\pi^2)} \ \breve{n}, \frac{1}{2} \sqrt{-2+3\pi^2} \ \breve{n}, \sqrt{\frac{1}{6} (-3+8\pi^2)} \ \breve{n} \right\}$$

In[350]:= % // N (*numerical values*)

Out[350]= {0.567862 Å, 1.67029 Å, 2.6272 Å, 3.55802 Å}

notice that the values are pretty close to those of the harmonic oscillator. Each successive energy level adds a little less than $1\hbar$.

Problem 3

note that the odd sho wavefunctions are solutions to the Schrodinger Eqn with $\psi(0)=0$, which is exactly what we need for this problem. Thus $E=(2n+1+1/2)\hbar\omega=(2n+3/2)\hbar\omega$. The corresponding eigenfunctions are $H_{2n+1}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega x^2}{2\hbar}}$.

Problem 4

now define the half-harmonic oscillator wavefunctions

$$\ln[354]:= \operatorname{sho2}[n_] :=$$

$$\operatorname{With}\left[\left\{y = \frac{x}{\sqrt{\frac{\hbar}{m\omega}}}\right\}, \operatorname{Piecewise}\left[\left\{\left\{\operatorname{HermiteH}[2n+1, y] \operatorname{Exp}\left[-y^2/2\right], y > 0\right\}, \{0, y \le 0\}\right\}\right]\right]$$

In[359]:= Table[ΔxΔp[sh02[n]], {n, 0, 3}] // N // Simplify
Out[359]:= {0.583216 ħ, 1.49105 ħ, 2.37291 ħ, 3.24886 ħ}

Problem 5

$$In[362]:= \frac{Integrate [x sho2[9]2, {x, 0, \infty}]}{Integrate [sho2[9]2, {x, 0, \infty}]} // Simplify // N$$
$$Out[362]= \frac{3.97634 \hbar}{\sqrt{m \omega \hbar}}$$

classical solution: $x(t) = x_T |\sin\omega t|$. Classical turning pt at energy E is $x_T = \sqrt{\frac{2E}{m\omega^2}} = \sqrt{\frac{2\hbar\omega(2n+3/2)}{m\omega^2}} = \sqrt{\frac{39\hbar}{m\omega}}$.

The time average is

In[365]:= Integrate
$$\left[\sqrt{\frac{39 \ \tilde{n}}{m \ \omega}} \frac{\sin\left[\omega \ t\right]}{\frac{\pi}{\omega}}, \left\{t, 0, \frac{\pi}{\omega}\right\}\right] // N$$

Out[365]= 3.97569 $\sqrt{\frac{\tilde{n}}{m \ \omega}}$

which is amazingly close. Both classical and quantum theories of harmonic oscillators give similar answers, except for the key difference which is only certain energies being allowed.