Quantum Mechanics and Atomic Physics

Lecture 12:
Harmonic Oscillator II

http://www.physics.rutgers.edu/ugrad/361

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Last Time: Harmonic Oscillator

\[ V(x) = \frac{1}{2} k x^2 \quad \text{for all } x \]

\[ \tau(x) = -\frac{dV}{dx} = -k x \]

- **Asymptotic solution:**

\[ \psi(\xi) \approx A e^{-\xi^2/2} \quad \text{for } \xi \to \pm\infty \]

- **Series solution:** (valid at any \( x \))

\[ \psi(\xi) = H(\xi) e^{-\frac{1}{2} \xi^2} \]

\[ H(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \]

\( H(\xi) \) are really **Hermite polynomials**

Reed: Chapter 5

**FIGURE 5.2** Harmonic oscillator wavefunctions for \( n = 0 \) (solid line) and \( n = 5 \) (dashed line). The vertical lines designate the classical turning points for each curve: \( \xi_{\text{turn}} = \pm 1 \) and \( \pm \sqrt{11} \) for \( n = 0 \) and 5, respectively. See Problem 5-8.
Classical Turning Point

- The Classical “turning points” of the motion are at $x_n$ such that $V(x) = E_n$

- So in QM, we get penetration of $\Psi_n$ into $|x| > |x_n|$
Check Correspondence Principle

\[
\lim_{n \to \infty} \frac{\Delta E_n}{E_n} = \frac{E_{n+1} - E_n}{E_n} = \frac{\hbar \omega (n + \frac{3}{2}) - \hbar \omega (n + \frac{1}{2})}{\hbar \omega (n + \frac{1}{2})}
\]

\[
= \frac{1}{\hbar + \frac{1}{2}}
\]

\[
\lim_{n \to \infty} \frac{\Delta E_n}{E_n} \to 0
\]

- Recall, classically: continuum of energies so \(\Delta E/E = 0\)
- Classically, a particle spends much of its time near the turning points because it has low speed there.
  - Think of a mass on a spring
Classical vs. Quantum H.O.

- Probability density for classical harmonic oscillator (see Reed section 5.5) and for QM oscillator for \( n=15 \).

- \( P_{\text{classical}} \) diverges at the turning points
  - Oscillator is momentarily at rest at those points and has a high probability of being found there

- \( P_{\text{classical}} \) tracks closely the running average of \( P_{\text{QM}} \)
  - In the limit as \( n \to \infty \), these should agree more and more.
Probability of finding the oscillator “outside” the well

- Let’s do this calculation for the ground state wavefunction:

\[
\psi_n(x) = \frac{\sqrt{\alpha}}{\sqrt[n]{n!}} e^{-\alpha^2 x^2}
\]

\[
E_0 = \frac{\hbar^2}{2m}
\]

Classically forbidden region: \( V(x) > E_0 \)

\[
\Rightarrow \frac{1}{2} k x^2 > \frac{\hbar^2}{2m}
\]

\[
\Rightarrow |x| > c
\]

where \( c = \frac{\sqrt{\frac{\hbar^2}{m}}}{\alpha} \)

\[
P(\text{outside}) = 1 - P(\text{inside})
\]

\[
P(\text{inside}) = \int_{-c}^{c} \psi_0^2 \psi_0^* dx = 2 \int_{0}^{c} \psi_0^2 \psi_0^* dx
\]

\[
= \frac{2a}{\sqrt{\pi}} \int_{-c}^{c} e^{-ax^2} dx
\]
- Change variables:

$$\xi = \alpha \nu \quad d\xi = \frac{1}{2} d\nu$$

$$P(\text{inside}) = \frac{2}{\sqrt{\pi}} \int_{0}^{\alpha \cdot \zeta} e^{-\xi^2} d\xi$$

- This integral is known as the error function

$$\text{erf}(\zeta) = \frac{2}{\sqrt{\pi}} \int_{0}^{\zeta} e^{-x^2} dx$$

$$\Rightarrow \quad \text{here} \quad \zeta = \alpha \cdot \zeta = \alpha \cdot \frac{1}{2} = 1$$

$$\Rightarrow \quad P(\text{inside}) = \text{erf}(1)$$

$$= 0.843$$

$$\Rightarrow \quad P(\text{outside}) = 1 - P(\text{inside}) \quad 1 - 0.843 = 0.157$$

$$\Rightarrow \quad P(\text{outside}) = 15.7\%$$
Harmonic Oscillator
Uncertainties

- Because integrand is odd irrespective of parity of $\Psi_n(x)$.

\[
\langle x_n \rangle = \int_{-\infty}^{\infty} \psi_n^* x \psi_n \, dx = 0 \quad \text{for any } n
\]

- If $\Psi_n$ has even parity, $d\Psi_n/dx$ has odd parity
- If $\Psi_n$ has odd parity, $d\Psi_n/dx$ has even parity
- So, $\langle p_n \rangle = 0$
  - Not a surprise!
Harmonic Oscillator
Uncertainties, con’t

\[
\langle x_n^2 \rangle = \int_{-\infty}^{\infty} \psi_n^* x^2 \psi_n \, dx = \frac{t_n}{m w} (n+\frac{1}{2})
\]

\[
(\Delta x)_n = \sqrt{\langle x_n^2 \rangle - \langle x_n \rangle^2} = \sqrt{\frac{t_n}{m w} (n+\frac{1}{2})}
\]

\[
= \frac{x_{\text{turning point}}}{\sqrt{2}}
\]

Since \( x_{\text{turning point}} = \sqrt{\frac{t_n}{m w} (2n+1)} \)
For $n=0$ it just barely satisfies uncertainty principle!

If you wish to carry out full integrals, use:

$$\int_{-\infty}^{\infty} \xi^2 H_n^2(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} 2^n n! (n+\frac{1}{2})$$
Expectation Value of KE

For the H.O. in the ground state, let’s find the expectation value of the Kinetic Energy.

\[
\rho_{\psi} = -i \hbar \frac{\partial}{\partial \psi} \Rightarrow KE_{\psi} = \frac{\rho_{\psi}^2}{2m} = \frac{1}{2m} \left( -\hbar^2 \frac{d^2}{dx^2} \right)
\]

\[
\langle KE \rangle = \int_{-\infty}^{\infty} \psi^* KE \psi \, dx = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^* \frac{d^2}{dx^2} \psi \, dx
\]

\[
= -\frac{\hbar^2}{2m} \left( \frac{\alpha}{\sqrt{\pi}} \right) \int_{-\infty}^{\infty} e^{-x^2/2} \frac{d^2}{dx^2} e^{-x^2/2} \, dx
\]

\[
\frac{d^2}{dx^2} e^{-x^2/2} = -x^2 e^{-x^2/2} + x^2 e^{-x^2/2}
\]
\[
\Rightarrow -\frac{\hbar^2}{2m\sqrt{\pi}} \left[ -\int_{-\infty}^{\infty} x^2 e^{-x^2} dx + x^4 \int_{-\infty}^{\infty} x^2 e^{-x^2} dx \right]
\]

\[
\Rightarrow -\frac{\hbar^2}{2m\sqrt{\pi}} \left[ -\sqrt{\pi} + \frac{\sqrt{\pi}}{2} \right] = -\frac{\hbar^2}{2m\sqrt{\pi}} \left( -\frac{\sqrt{\pi}}{2} \right)
\]

\[
= \frac{\hbar^2 \alpha^2}{4m} = \frac{\hbar^2}{4m} \left( \frac{\mu \omega}{\hbar} \right) = \frac{\hbar \omega}{4}
\]

So,

\[
\langle k E \rangle = \frac{\hbar \omega}{4}
\]

Similarly:

\[
\langle V \rangle = \frac{1}{4} \frac{\hbar \omega}{4}
\]

where \[ V = \frac{1}{2} k x^2 = \frac{1}{2} m \omega^2 x^2 \]

and we've seen that \[ E_0 = \frac{\hbar \omega}{2} \].
Animation

http://phet.colorado.edu/simulations/sims.php?sim=Quantum_Bound_States
Raising and Lowering Operators

- Operator based solution to the H.O. potential developed by Paul Dirac
  - Can be applied to any potential
- Define two operators:
  \[
  A^+ = \frac{i}{\alpha \sqrt{2}} \left( -\frac{d}{dx} + \alpha^2 x \right) \\
  A^- = \frac{i}{\alpha \sqrt{2}} \left( -\frac{d}{dx} - \alpha^2 x \right) \\
  \alpha = \sqrt{\frac{m \omega}{\hbar}}
  \]
- Called **Raising and Lowering Operators**
Let’s look at some of their properties

\[ A^+ \psi = \frac{i}{\alpha \sqrt{2}} \left( -\frac{d\psi}{dx} + \alpha^2 x \psi \right) \]

\[ A^- (A^+ \psi) = \frac{i}{\alpha \sqrt{2}} \left( -\frac{d\psi}{dx} - \alpha^2 x \right) \]

\[ = -\frac{1}{2\alpha^2} \left( \frac{d^2\psi}{dx^2} - \alpha^2 \psi - \alpha^2 x \frac{d\psi}{dx} + \alpha^2 x^2 \frac{d\psi}{dx} - \alpha^2 x^2 \psi \right) \]

\[ = -\frac{1}{2\alpha^2} \left( \frac{d^2\psi}{dx^2} - \alpha^2 \psi - \alpha^2 x^2 \psi \right) \]
This is independent of the wavefunction being operated on.
Now let’s apply this operator on $\Psi$

\[
(A^-A^+ + A^+A^-)\Psi = -\frac{\hbar}{\alpha^2} \frac{d^2\psi}{dx^2} + \alpha^2 x^2 \psi
\]

After canceling terms

\[
= -\frac{\hbar}{m\omega} \frac{d^2\psi}{dx^2} + \frac{m\omega}{\hbar} \chi^2 \psi
\]

$\Rightarrow$ Becomes $KE_{\text{op}}$  $\Rightarrow$ Becomes $PE_{\text{op}}$

Look familiar? What if you multiply through by $\hbar$  $\alpha^2 \omega$? 2?
More on this next time....

\[ H_\text{op} \equiv \hbar \omega \left( A^+ A^- + \frac{1}{2} \right) \]

\[ \Rightarrow [H_\text{op}, A^+] \psi = (\hbar \omega A^+) \psi \]

\[ \Rightarrow [H_\text{op}, A^-] \psi = (\hbar \omega A^-) \psi \]

\[ [H_\text{op}, A^+] \psi = (H_\text{op} A^+) \psi - (A^+ H_\text{op}) \psi = \hbar \omega (A^+ \psi) \]

\[ \Rightarrow (H_\text{op} A^+) \psi - A^+ (E \psi) = \hbar \omega (A^+ \psi) \]

\[ \Rightarrow H_\text{op} (A^+ \psi) = (E + \hbar \omega) (A^+ \psi) \]

Similarly,

\[ H_\text{op} (A^- \psi) = (E - \hbar \omega) (A^- \psi) \]
Summary/Announcements

- Finished H.O. and raising/lowering operators
- Next time: S.E. in 3D

- Homework #5 due on Wednesday Oct 16.

- Midterm exam Wed. Oct. 23
  - chapters 1-4
  - homework 1-5
  - and related lectures
  - it will be closed book - check website for more information.

- Office hours:
  - I will hold office hours as usual this Tuesday from 3:30-4:30pm
  - No office hours next Tuesday
  - Instead I will hold office hours on Friday, Oct 18 from 1:30-2:30pm

- Now time for a quiz ....