Quantum Mechanics and Atomic Physics

Lecture 11:
The Harmonic Oscillator: Part II

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

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Summary: H.O.

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

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

- **Asymptotic solution:**
  \[ \psi(\xi) \sim A e^{-\xi^2/2} \text{ for } \xi \to \pm \infty \]

- **Series solution:** (valid at any x)
  \[ \psi(\xi) = H(\xi) e^{-\xi^2} \]
  \[ H(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \]
  \[ a_{n+2} = \frac{(2n+1-\lambda)}{(n+1)(n+2)} a_n \]

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

Recursion relation
Last time:

Wavefunctions

- Shows $n=0$ and $n=5$ wavefunctions

A few things to note:

- For even values of $n$, wavefunction is symmetric
- For odd values of $n$, wavefunction is anti-symmetric
- There are $n+1$ extrema (maxima/minima)
- Probability for finding the oscillator “outside” of the well is greatest for $n=0$.
- By “outside” I mean beyond the classical turning point.

Let’s calculate this …
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 $|x| > |x_n|$

\[
\frac{1}{2} m x_n^2 = \hbar w \left(n + \frac{1}{2}\right)
\]

\[
x_n = \sqrt{\frac{\hbar w (n + \frac{1}{2})}{k}}
\]

\[
x_n = \sqrt{\frac{\hbar w (2n+1)}{k}}
\]

Or as function of $\xi$:
\[
\xi_n = \alpha \sqrt{\frac{\hbar w (2n+1)}{k}} = \sqrt{\frac{\hbar}{k}} \sqrt{\frac{\hbar w (2n+1)}{k}} = \sqrt{2n+1}
\]

\[
\alpha = \sqrt{\frac{k}{\hbar}}
\]

\[
\xi_n = \sqrt{2n+1}
\]
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 it’s 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:

\[ \psi_n(x) = \frac{\sqrt{a}}{\pi^{1/4}} e^{-\frac{a^2 x^2}{2}} \]

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

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

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

\[ |x| > c \quad c = \sqrt{\frac{\hbar^2}{k}} = \frac{1}{\alpha} \]

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

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

\[ = 2 \frac{\pi}{\sqrt{\pi}} \int_{0}^{c} e^{-x^2} \, dx \]
- Change variables:

\[ 3 = \alpha x \quad dx = \frac{1}{\alpha} d\xi \]

\[ P_{\text{inside}} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-\frac{\xi^2}{4}} d\xi \]

\[ \text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\frac{x^2}{2}} dx \]

- This integral is known as the error function

\[ \Rightarrow \quad \text{here} \quad z = \alpha \cdot c = \alpha \cdot \frac{1}{2} = 1 \]

\[ \Rightarrow \quad P_{\text{inside}} = \text{erf}(1) \]

\[ = 0.843 \]

\[ \Rightarrow \quad P_{\text{outside}} = 1 - P_{\text{inside}} = 1 - 0.843 = 0.157 \]

\[ \Rightarrow \quad P_{\text{outside}} = 15.7\% \]
Harmonic Oscillator
Uncertainties

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

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, $<p_n> = 0$

Not a surprise!
Harmonic Oscillator
Uncertainties, con’t

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

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

\[
= \frac{X_{\text{turning point}}}{\sqrt{\alpha}}
\]

Since \( X_{\text{turning point}} = \sqrt{\frac{\hbar}{m \omega} (2n+1)} \)
For \( n=0 \) it just barely satisfies uncertainty principle!

- If you wish to carry out full integrals, use:

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

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

\[ P_{\phi} = -i\hbar \frac{\partial}{\partial x} \Rightarrow KE_{\phi} = \frac{p_x^2}{2m} = \frac{1}{2m} \left( - \hbar^2 \frac{\partial^2}{\partial x^2} \right) \]

\[ \langle KE \rangle = \int_{-\infty}^{\infty} \psi^*_{0} K \psi_{0} x^2 dx = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi^*_{0} x^2 \frac{\partial^2}{\partial x^2} \psi_{0} dx \]

\[ = -\frac{\hbar^2}{2m} \frac{\alpha}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\alpha^2} \frac{\partial^2}{\partial x^2} e^{-x^2/\alpha^2} dx \]

\[ = -\frac{\hbar^2}{2m} \frac{\alpha}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\alpha^2} \left( e^{-x^2/\alpha^2} \right) dx \]
\[
\Rightarrow -\frac{\hbar^2}{2m} \left( \frac{a}{\sqrt{\pi}} \right) \left[ -x^2 \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\alpha^2}} \, dx + \alpha \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2\alpha^2}} \, dx \right] \quad \frac{\sqrt{\pi}}{2\alpha^3}
\]

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

\[
= \frac{\hbar^2}{4m} \frac{a^2}{\sqrt{\pi}} = \frac{\hbar^2}{4m} \left( \frac{\pi m}{\hbar} \right) = \frac{\hbar \omega}{4}
\]

So,
\[
\langle \mathbf{r} \mathbf{E} \rangle = \frac{\hbar \omega}{4}
\]

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

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:

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

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

\[
\alpha = \sqrt{\frac{m}{\hbar}}
\]

- Called **Raising and Lowering Operators**
Let’s look at some of their properties

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

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

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

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

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

After canceling terms

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

Look familiar?

Hamiltonian

\[
H_0p = \frac{\hbar \omega}{2} (A^- A^+ + A^+ A^-)
\]

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

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

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

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

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

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

Similarly,

\[ H_{\text{op}} (A^- \psi) = (E - \hbar \omega)(A^- \psi) \]
Let’s dissect this

- When $A^+$ acts on $\Psi$, it gives rise to a new function $(A^+\Psi)$ whose energy eigenvalue is the same as that of $\Psi$ but more by $\hbar \omega$

- Similarly, when $A^-$ acts on $\Psi$, it gives rise to a new function $(A^-\Psi)$ whose energy eigenvalue is the same as that of $\Psi$ but less by $\hbar \omega$

- $A^+$ and $A^-$ are also called ladder operators
Let’s now go back to H.O. potential

- But first, let’s note that the lowering operator can’t generate a lower state than the ground state so:

\[ A^- \psi_0 = 0 \]

- Let’s use this to find that:

\[
\begin{align*}
H_0 \psi_0 &= \varepsilon_0 \psi_0 \\
\Rightarrow \hbar \omega (A^- A^+ + \frac{1}{2}) \psi_0 &= \hbar \omega (A^+(A^- \psi_0) + \frac{1}{2} \psi_0) \\
\hbar \omega \psi_0 &= \frac{\hbar \omega}{2} \psi_0 = \varepsilon_0 \psi_0 \quad \checkmark
\end{align*}
\]
A$^+$ and A$^-$ action on H.O. wavefunctions

- See proof in your book

\[ A^+ \psi_n = \sqrt{n+1} \psi_{n+1} \]
\[ A^- \psi_n = \sqrt{n} \psi_{n-1} \]

- We can also rearrange original equations to get:

\[ p_{op} = -i \hbar \frac{\partial}{\partial x} \]

\[ \Rightarrow p_{op} = \frac{\sqrt{\hbar}}{\sqrt{2}} (A^+ + A^-) \]

\[ \Rightarrow x_{op} = -i \frac{\sqrt{\hbar}}{\sqrt{2} \alpha} (A^+-A^-) \]

Momentum and position operators

In upcoming homework you will use these operators to verify the uncertainty principle!
Example

Let’s use this new knowledge to calculate $\langle x^2 \rangle$:

\[
\langle x^2 \rangle = \int \psi_n^* (x_0^2 \psi_n) \, dx
\]

\[
= \frac{i^2}{2\alpha^2} \int \psi_n^* \left[(A^+ - A^-)(A^+ \psi_n - A^- \psi_n)\right] \, dx
\]

\[
= -\frac{1}{2\alpha^2} \int \psi_n^* \left(A^+ A^+ \psi_n - A^+ A^- \psi_n - A^- A^+ \psi_n + A^- A^- \psi_n\right) \, dx
\]

\[
\propto \psi_{n+2}^2
\]

\[
\psi_n \psi_{n+2}
\]

\[
\psi_n^* \psi_{n-2}
\]
Recall, orthogonality:

\[ \langle \psi_k^* | \psi_n \rangle = \delta_{kn} \]

So,

\[ \langle x^2 \rangle = \frac{1}{2 \alpha^2} \int \psi_n^* (A^+ A^- + A^- A^+) \psi_n \, dx \]

\[ = \frac{1}{2 \alpha^2} \frac{2}{\hbar \omega} \int \psi_n^* \hat{H}_{\text{op}} \psi_n \, dx \]

\[ = \frac{1}{\alpha^2 \hbar \omega} \int \psi_n^* \hat{E}_n \psi_n \, dx = \frac{\hat{E}_n}{\alpha^2 \hbar \omega} \]

\[ \langle x^2 \rangle = \frac{1}{\alpha^2} (n + \gamma_2) \quad \checkmark \]

Similarly for \( \langle p^2 \rangle \).
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<th>Physical Example</th>
<th>Potential and Total Energies</th>
<th>Probability Density</th>
<th>Significant Feature</th>
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<td>$E$</td>
<td>$\psi \ast \psi$</td>
<td>Results used for other systems</td>
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<tr>
<td>Step potential (energy below top)</td>
<td>Conduction electron near surface of metal</td>
<td>$V(x)$</td>
<td>$\psi \ast \psi$</td>
<td>Penetration of excluded region</td>
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<tr>
<td>Step potential (energy above top)</td>
<td>Neutron trying to escape nucleus</td>
<td>$E$</td>
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<td>Partial reflection at potential discontinuity</td>
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<tr>
<td>Barrier potential (energy below top)</td>
<td>$\alpha$ particle trying to escape Coulomb barrier</td>
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<tr>
<td>Barrier potential (energy above top)</td>
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<td>$E$</td>
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<tr>
<td>Finite square well potential</td>
<td>Neutron bound in nucleus</td>
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<td>Zero-point energy</td>
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Midterm

Note:
The midterm will cover material through here.

(Reed Chapters 1-5 and homeworks 1-6)
Summary/Announcements

- Next time:
  - S.E. in 3D

- Next homework due Mon Oct 15.
  - You will have a homework due on Mon. Oct 22nd (before midterm) but none due Mon. Oct. 29th (after midterm)


- Now time for a quiz ....