Quantum Mechanics and Atomic Physics

Lecture 11:

The Harmonic Oscillator: Part I

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Prof. Sean Oh

The Classical Harmonic Oscillator

- Classical mechanics examples
  - Mass on a spring
  - Mass swinging as a simple pendulum
- These examples all correspond to a situation where we have a linear restoring force:

$$F = -kx \qquad -\infty \leq x \leq \infty$$

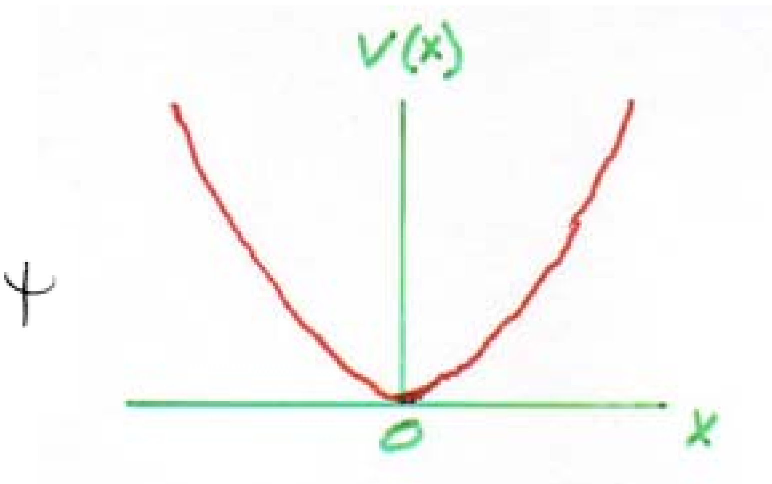
- And the harmonic oscillator potential is then:

$$V(x) = -\int F(x)\,dx = \int kx\,dx = \frac{kx^2}{2} + C$$

The S.E. for the harmonic oscillator potential

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

$$F(x) = -\frac{dV}{dx} = -kx$$



- S.E.: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} k x^2 \psi = E\psi$
- Angular Frequency of oscillator:

$$\omega = \sqrt{\frac{k}{m}} \Rightarrow k = m\omega^2$$

- So,

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi - \frac{m^2\omega^2}{\hbar^2} x^2 \psi = 0$$

S.E. of H.O., con't

- Let's define: $\xi = \alpha x$

  and $\alpha \equiv \sqrt{\frac{m\omega}{\hbar}}$, $\beta \equiv \frac{2mE}{\hbar^2}$

- Think of ξ as a dimensionless measure of x

So: $\frac{d\psi}{dx} = \frac{d\psi}{d\xi}\frac{d\xi}{dx} = \alpha \frac{d\psi}{d\xi}$

$$\frac{d^2\psi}{dx^2} = \alpha \frac{d}{dx}\left(\frac{d\psi}{d\xi}\right) = \alpha \frac{d^2\psi}{d\xi^2}\frac{d\xi}{dx} = \alpha^2 \frac{d^2\psi}{d\xi^2}$$

- Insert back into S.E. ….

S.E. of H.O., con't

$$\alpha^2 \frac{d^2\psi}{d\xi^2} + (\beta - \alpha^4 x^2)\psi = 0$$

$$\alpha^2 \frac{d^2\psi}{d\xi^2} + \left(\beta - \alpha^4 \left(\frac{\xi}{\alpha}\right)^2\right)\psi = 0$$

$$\frac{d^2\psi}{d\xi^2} + \left(\frac{\beta}{\alpha^2} - \xi^2\right)\psi = 0$$

- Let's define:

$$\lambda = \frac{\beta}{\alpha^2} = \frac{2mE}{\hbar^2} \cdot \frac{\hbar}{m\omega} = \frac{2}{\hbar\omega} E$$

$$\varepsilon = \frac{2}{\hbar\omega} \Rightarrow \lambda = \varepsilon E$$

- <u>Think of λ as a dimensionless measure of E</u>

S.E. of H.O., con't

- Finally we have:

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0$$

- This is called Weber's Differential Equation

Dimensional Analysis

- Let's check that ξ is a dimensionless measure of x

$$\xi = \alpha x$$

$$[\alpha]_{units} = m^{-1}$$

Let's check

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} = \left(\frac{mk}{\hbar^2}\right)^{1/4}$$

$$m^{-1} \stackrel{?}{=} \left[kg \cdot \frac{N}{m} \; \frac{1}{(J \cdot s)^2} \right]^{1/4}$$

$$= \left[kg \frac{1}{m} kg \frac{m}{s^2} \cdot \frac{1}{kg^2 \frac{m^4}{s^4} \cdot s^2} \right]^{1/4}$$

$$= \left[\frac{kg^2}{s^2} \cdot \frac{s^2}{kg^2 m^4} \right]^{1/4}$$

$$= \left(\frac{1}{m^4} \right)^{1/4}$$

$$= m^{-1} \quad \checkmark$$

Dimensional Analysis

- Let's check that λ is a dimensionless measure of E

$$\lambda = \varepsilon E$$

$$\varepsilon = \frac{2}{\hbar\omega} \longrightarrow [\varepsilon]_{\text{units}} = \frac{1}{J}$$

$$\frac{1}{J} \stackrel{?}{=} \frac{1}{J \cdot s \cdot Hz}$$

$$= \frac{1}{J \cdot s \cdot s^{-1}}$$

$$= \frac{1}{J} \quad \checkmark$$

The Asymptotic Solution

- Let's solve for $\Psi(\xi)$ and then revert back to x.
- First, let's consider Ψ at large ξ, i.e. large x
  - λ stays finite so:

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2} - \xi^2\psi = 0 \qquad \text{for } \xi \to \pm\infty$$

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi$$

  - Trial solution at large ξ: $\psi(\xi) = A e^{(\beta \xi^n)}$

$$\psi' = A\left[\beta n \xi^{n-1} e^{(\beta \xi^n)}\right] = \beta n \xi^{n-1}\psi$$

$$\psi'' = \beta n(n-1)\xi^{n-2}\psi + \beta n \xi^{n-1}\psi'$$

$$= \beta n(n-1)\xi^{n-2}\psi + (\beta n \xi^{n-1})^2\psi$$

Cont'd

$$\psi'' = [\beta n(n-1)\,\xi^{n-2} + \beta^2 n^2 \xi^{2n-2}]\,\psi$$

$$= [\beta n(n-1) + \beta^2 n^2 \xi^n]\,\xi^{n-2}\psi$$

$$\approx (\beta^2 n^2 \xi^n)\,\xi^{n-2}\psi$$

$\xi \to \infty$ limit with $n > 0$

For this to be the same as $\psi'' = \xi^2 \psi$

$\Rightarrow \quad \beta^2 n^2 = 1, \quad 2n-2 = 2 \quad \Rightarrow \quad n = 2, \ \beta = \pm\frac{1}{2}$

$$\Rightarrow \psi = A e^{-\frac{1}{2}\xi^2} + B e^{+\frac{1}{2}\xi^2}$$

at $\xi \to \infty$ limit

The Asymptotic Solution, con't

- Just like finite square well, we want that $\Psi(\xi) \rightarrow 0$ as $\xi \rightarrow \infty$
  - We establish the ***asymptotic form*** of the wavefunction
  - So if we require finiteness at $\xi = \infty$, then we must require B=0, so:

$$\psi(\xi) \approx A e^{-\xi^2/2} \qquad \text{for } \xi \rightarrow \pm\infty$$

The Series Solution

- For a more general solution, valid at any ξ, let's try

$$\psi(\xi) = H(\xi)\, e^{-\frac{1}{2}\xi^2}$$

- $H(\xi)$:
  - is a yet unknown function.
  - It must vary more slowly than $\exp(\xi^2/2)$ at large ξ in order to prevent ψ from diverging

The Series Solution, con't

- How do we know if this is a valid assumption?
  - We don't know yet, but let's see if it works.

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\xi^2-1)H\right)e^{-\xi^2/2}$$

$$\frac{d^2\psi}{d\xi^2} + (\lambda-\xi^2)\psi = 0$$

$$\Rightarrow \left(\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\xi^2-1)H\right)e^{-\xi^2/2} + (\lambda-\xi^2)He^{-\xi^2/2} = 0$$

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\lambda-1)H = 0$$

The Series Solution, con't

- Let's try series solution:

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

  - *(We omit negative powers since they would blow up at $x=\xi=0$)*

$$\frac{dH}{d\xi} = \sum_{n=0}^{\infty} n\, a_n \xi^{n-1}$$

$$\frac{d^2H}{d\xi^2} = \sum_{n=0}^{\infty} n(n-1)\, a_n \xi^{n-2}$$

The Series Solution, con't

- Plug back into eqn on p. 12:

$$\sum_{n=0}^{\infty} n(n-1)\,a_n\,\xi^{n-2} - 2\sum_{n=0}^{\infty} n\,a_n\,\xi^{n} + \sum_{n=0}^{\infty}(\lambda-1)\,a_n\,\xi^{n} = 0$$

$$\sum_{n=0}^{\infty} n(n-1)\,a_n\,\xi^{n-2} + \sum_{n=0}^{\infty}(\lambda-1-2n)\,a_n\,\xi^{n} = 0$$

$$\sum_{n=0}^{\infty} n(n-1)\,a_n\,\xi^{n-2} = \overset{n=0}{0} + \overset{n=1}{0} + \sum_{n=2}^{\infty} n(n-1)\,a_n\,\xi^{n-2}$$

The Series Solution, con't

- Let's define j=n-2:

$$\sum_{n=0}^{\infty} n(n-1)a_n \xi^{n-2} = \sum_{n=2}^{\infty} n(n-1)a_n \xi^{n-2}$$

$$= \sum_{j=0}^{\infty} (j+2)(j+1)a_{j+2} \xi^{j}$$

- j or n are dummy indices so,

$$\sum_{n=0}^{\infty} \left[(n+1)(n+2)a_{n+2} + (\lambda-1-2n)a_n\right] \xi^n = 0$$

The Series Solution, con't

$$\sum_{n=0}^{\infty} \left[(n+1)(n+2)\, a_{n+2} + (\lambda - 1 - 2n)\, a_n \right] \xi^n = 0$$

- The terms in the square brackets are pure numbers
  - No dependence on ξ
- ξ is not equal to zero yet the sum evaluates to zero
  - This can only happen for all possible values of ξ if what is in square brackets vanishes in general.
  - Therefore:

$$a_{n+2} = \frac{(2n+1-\lambda)}{(n+1)(n+2)}\, a_n$$

Recursion Relation

$$a_{n+2} = \frac{(2n+1-\lambda)}{(n+1)(n+2)} a_n$$

This is called a ***recursion relation***

- Specifies a given expansion coefficient ***recursively*** in terms of a preceding coefficient in the series.
- To get a complete solution, we also need to supply values for the first two coefficients, a_0 and a_1
- All subsequent even-indexed coefficients can then be expressed in terms of a_0
- All subsequent odd-indexed coefficients can then be expressed in terms of a_1

The Series Solution, con't

- The need to supply two coefficients can be understood since to solve second-order differential equation (S.E.) we have two constants of integration to be set by the boundary conditions.
- In this case, we have one boundary condition:
  - Finiteness: we want $\Psi(\xi) \to 0$ as $\xi \to \infty$
  - Recall our wavefunction

$$\psi(\xi) = H(\xi)\, e^{-\frac{1}{2}\xi^2}$$

    - Exp term converges
    - We want $H(\xi)$ convergent or if it diverges to do so more slowly than $\exp(\xi^2/2)$
    - Unfortunately though:

For large ξ, $H(\xi) \to e^{2\xi^2}$

See Reed for a nice explanation of this.

The Series Solution, con't

- So the series solution: $H(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$

  and since For large ξ, $H(\xi) \rightarrow e^{2\xi^2}$

- We must force the series to terminate after a finite number of terms.
  - *This has the physical consequence of quantizing the energy levels of the system*
- That will happen if all $a_j=0$ for $j>n$, then the recursion relation demands:
  - $\lambda=2n+1$

Initial coefficients

- But we have <u>two</u> initial coefficients a_0 and a_1
- We can't simultaneously terminate both even and odd sets of coefficients. So we must arbitrarily demand that either a_0 or a_1 be zero.
- So, we pick one of them to be zero and force the series termination of the other:
  - $\lambda=2n+1$
  - If $a_0=0$, n=1, 3, 5, …. Odd Parity
  - If $a_1=0$, n=0, 2, 4, …. Even Parity

Hermite Polynomials

- The general result is a family of functions $H_n(\xi)$, with each member being a polynomial involving only even or odd powers of ξ (but not both!) up to order ξ^n.

$H_0(\xi) = 1$, $H_1(\xi) = 2\xi$,

$H_2(\xi) = 4\xi^2 - 2$, $H_3(\xi) = 8\xi^3 - 12\xi$, etc.

Table 5.1 Hermite Polynomials

$H_0(\xi) = 1$	$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$
$H_1(\xi) = 2\xi$	$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$
$H_2(\xi) = 4\xi^2 - 2$	$H_6(\xi) = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120$
$H_3(\xi) = 8\xi^3 - 12\xi$	$H_7(\xi) = 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi$

Reed: Chapter 5

Normalized H.O. wavefunctions

- We can normalize, and go back to using x:

$$\psi_n(x) = A_n H_n(\xi)\, e^{-\xi^2/2} \qquad \xi = \alpha x$$

$$= A_n H_n(\alpha x)\, e^{-\alpha^2 x^2/2}$$

$$\alpha^2 = \sqrt{\frac{mk}{\hbar^2}}$$

$$A_n = \sqrt{\frac{\alpha}{\sqrt{\pi}\, 2^n n!}} \qquad \alpha = \left(\frac{mk}{\hbar^2}\right)^{1/4}$$

- Ground state energy of H.O. (n=0):

$$\psi_0(x) = \frac{\sqrt{\alpha}}{\pi^{1/4}}\, e^{-\alpha^2 x^2/2}$$

$$E_0 = \frac{1}{2}\hbar\omega$$

Example

- Verify the normalization factor of the groundstate wavefunction:

$$\psi_0(x) = A_0 e^{-\alpha^2 x^2/2}$$

$$H_0 = 1$$

$$\int_{-\infty}^{\infty} \psi_0^* \psi_0 \, dx = 1$$

$$\int_{-\infty}^{\infty} A_0^2 e^{-\alpha^2 x^2} dx = A_0^2 \underbrace{\int_{-\infty}^{\infty} e^{-\alpha^2 x^2} dx}_{\sqrt{\frac{\pi}{\alpha^2}}} = 1$$

see Appendix C

$$A_0^2 \frac{\sqrt{\pi}}{\alpha} = 1$$

$$A_0 = \sqrt{\frac{\alpha}{\sqrt{\pi}}} = \frac{\sqrt{\alpha}}{\pi^{1/4}} \checkmark$$

Wavefunctions

Reed: Chapter 5

- 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 maxima
  - Probability for finding the oscillator "outside" of the well is greatest for n=0.
  - By "outside" I mean beyond the classical turning point.

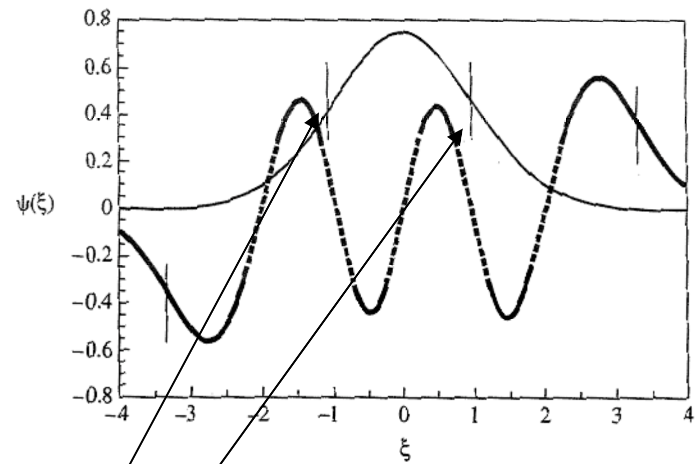
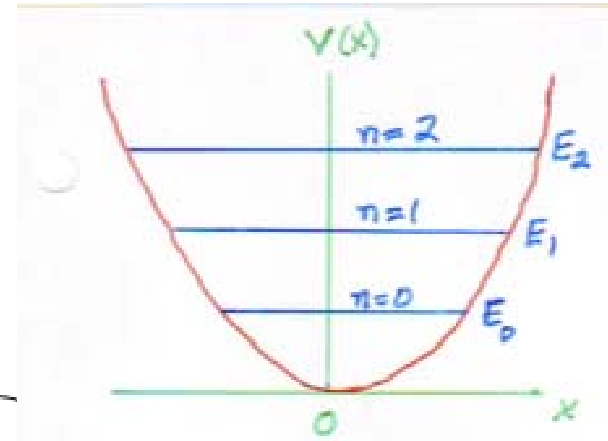


FIGURE 5.2 Harmonic oscillator wavefunctions for $n = 0$ (solid line) and $n = 5$ (dashed line). The vertical lines designate the classical turning points for each curve; $\xi_{turn} = \pm 1$ and $\pm\sqrt{11}$ for $n = 0$ and 5, respectively. See Problem 5–8.

Let's calculate this …

Classical Turning Point

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



$$\frac{1}{2} k x_n^2 = \hbar\omega\left(n+\frac{1}{2}\right)$$

$$x_n = \pm\sqrt{2\frac{\hbar\omega}{k}\left(n+\frac{1}{2}\right)}$$

$$= \pm\sqrt{\frac{\hbar\omega}{k}(2n+1)}$$

or

$$x_n = \pm\sqrt{\frac{\hbar}{m\omega}(2n+1)}$$

Or as function of $\xi = \alpha x$: $\alpha = \sqrt{\frac{k}{\hbar\omega}}$

$$\xi_n = \alpha\sqrt{\frac{\hbar\omega}{k}(2n+1)} = \sqrt{\frac{k}{\hbar\omega}}\sqrt{\frac{\hbar\omega}{k}(2n+1)} = \sqrt{2n+1}$$

$$\xi_n = \sqrt{2n+1}$$

- So in QM, we get penetration of Ψ_n into $|x|>|x_n|$

Harmonic-potential energy levels

- We can determine the energy corresponding to quantum number n:

$$\lambda = 2n+1 = \frac{2E}{\hbar\omega}$$

$$E = (n+\tfrac{1}{2})\hbar\omega = (n+\tfrac{1}{2})\hbar\sqrt{\frac{k}{m}} \quad , n = 0,1,2,3,\ldots$$

- Note, that E ∝ n
- **The energy levels are equally spaced!**
  - Called vibrational levels
  - Mimics attractive forces between molecules
  - Equal spacing of molecular spectral lines
- **The zero point energy (n=0) is:**

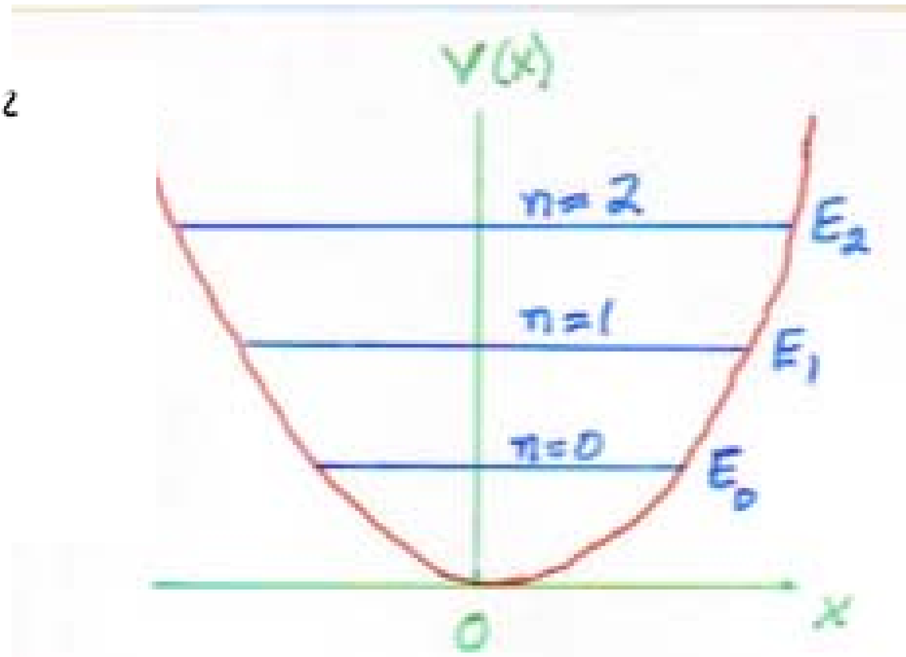
$$E_0 = \frac{1}{2}\hbar\omega$$

Energy Levels

$V(x) = \frac{1}{2} k x^2 = \frac{1}{2} m \omega^2 x^2$

$E_n = \hbar \omega \left(n + \frac{1}{2} \right)$

$\omega = \sqrt{\frac{k}{m}}$



- **Equally spaced energy levels**

Summary/Announcements

- Next time: Harmonic Oscillator continued
  - Probability, raising and lowering operators

- Next homework due on Mon. Oct 17.
- Midterm exam Mon. Oct. 19 in class - it will be **closed book** with one letter size formula-only sheet.