Quantum Mechanics and Atomic Physics

Lecture 12:

The Harmonic Oscillator: Part II

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

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Last time: H.O.

With $\xi = \alpha x$, $\alpha \equiv \sqrt{\frac{m\omega}{\hbar}}$, the H.O. S.E. reduces to

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

We found that the solution ψ should look like

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

, where $A_n = \sqrt{\frac{\alpha}{\sqrt{\pi}\, 2^n n!}}$

And λ should be $\lambda = 2n+1$

$H_n(\xi)$ are Hermite polynomials

→ even ftn if n is even

→ odd ftn if n is odd

Even and Odd functions

even odd

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

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

even odd

$f_{even} \times f_{odd} \Rightarrow odd$, $f_{odd} \times f_{odd} \Rightarrow even$

$$\int_{-\infty}^{\infty} f_{even}(x)\,dx = 2\int_0^{\infty} f_{even}(x)\,dx$$

$$\int_{-\infty}^{\infty} f_{odd}(x)\,dx = 0$$

Even and Odd functions

- Even functions

$f(x) = x^2$, $f(x) = e^{-x^2}$, $f(x) = x^4$

$f(x) = x^2 + 2x^6$, $f(x) = -x^4 + e^{x^2}$

$f(x) = \cos(x)$, $f(x) = \sin^2(x)$

- Odd functions

$f(x) = -x$, $f(x) = x^3$, $f(x) = x + 3x^3$

$f(x) = \sin(x)$

- Neither even nor odd

$f(x) = \cos(x) + \sin(x)$, $f(x) = e^x$, $f(x) = x + x^2$

Example

- How can the quantization of energy of a H.O. apply to the motion of a mass on a spring?
  - Classical example: Let's evaluate the discrete values of the allowed energy levels at the macroscopic level:

$m \approx 0.01\,kg \qquad k = 0.1\,N/m \qquad \omega = \sqrt{\frac{k}{m}} = 3.16\,rad/s.$

$T = \frac{2\pi}{\omega} = 1.99\,s$

$\Delta E = \hbar\omega = 6.58 \times 10^{-16}\ \text{eV} * \text{s}\ \ 3.16\,rad/s$

$= 2.08 \times 10^{-15}\ eV$

  - These energy levels are far too small to be detected.

Example, con't

- Now at the atomic level:

$$a_0 = 0.529\,\text{Å}$$

$$v = \frac{1}{137}c$$

$$\omega = \frac{v}{r} = \frac{v}{a_0} = \left(\frac{1}{137}\right)\left(3\times10^{18}\,\frac{\text{Å}}{s}\right)\Big/\left(0.529\,\text{Å}\right)$$

$$= 4.14\times10^{16}\ \text{rad/s}$$

- Much higher frequencies.
- Therefore the quantum energy is large:

$$\Delta E = \hbar\omega = 27.2\ eV$$

Correspondence Principle

$$\frac{\Delta E_n}{E_n} = \frac{E_{n+1} - E_n}{E_n} = \frac{\hbar\omega(n+\frac{3}{2}) - \hbar\omega(n+\frac{1}{2})}{\hbar\omega(n+\frac{1}{2})}$$

$$= \frac{1}{n+\frac{1}{2}}$$

$$\lim_{n\to\infty} \frac{\Delta E_n}{E_n} \to 0$$

- 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.

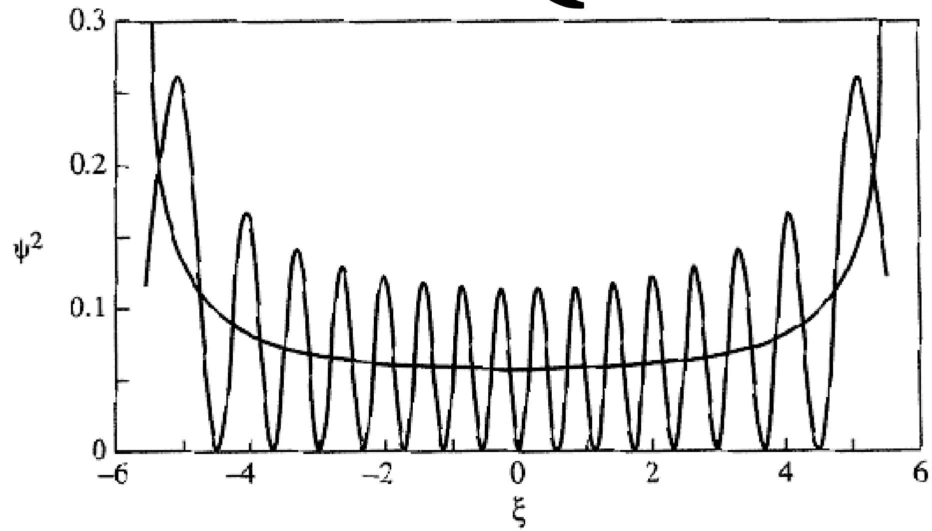


FIGURE 5.3 Probability densities for $n = 15$ classical (smooth upward-opening curve) and quantum (wiggly curve) oscillators. The classical turning points of the motion are $\xi \sim \pm 5.57$.

- Probability density for classical harmonic oscillator (see Reed section 5.5) and for QM oscillator for n=15.
- $P_{classical}$ diverges at the turning points
  - Oscillator is momentarily at rest at those points and has a high probability of being found there
- $P_{classical}$ tracks closely the running average of P_{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:

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

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

classically forbidden region $\quad V(x) > E_0$

$$\Rightarrow \frac{1}{2} k x^2 > \frac{\hbar\omega}{2}$$

$$\Rightarrow |x| > c \qquad c = \sqrt{\frac{\hbar\omega}{k}} = \frac{1}{\alpha}$$

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

$$P(\text{inside}) = \int_{-c}^{c} \psi_0^* \psi_0 \, dx = 2\int_0^c \psi_0^* \psi_0 \, dx$$

$$= \frac{2\alpha}{\sqrt{\pi}} \int_0^c e^{-\alpha^2 x^2} dx$$

- Change variables: $\xi = \alpha x \quad dx = \frac{1}{\alpha} d\xi$

$$P(\text{inside}) = \frac{2}{\sqrt{\pi}} \int_0^{\alpha \cdot c} e^{-\xi^2} d\xi$$

- This integral is known as the error function

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^{z} e^{-\xi^2} d\xi$$

$\Rightarrow$ here $z = \alpha \cdot c = \alpha \cdot \frac{1}{\alpha} = 1$

$\Rightarrow P_{inside} = \mathrm{erf}(1)$

$= 0.843$

$\Rightarrow P_{outside} = 1 - P_{inside} = 1 - 0.843 = 0.157$

$\Rightarrow \underline{P_{outside} = 15.7\%}$

Harmonic Oscillator Uncertainties

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

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

$$\langle p_n \rangle = -i\hbar \int_{-\infty}^{\infty} \psi_n^* \frac{d\psi_n}{dx} \, dx$$

- If Ψ_n has <u>even</u> parity, $d\Psi_n/dx$ has <u>odd</u> parity
- If Ψ_n has <u>odd</u> parity, $d\Psi_n/dx$ has <u>even</u> parity
- So, $\langle p_n \rangle = 0$
  - Not a surprise!

Harmonic Oscillator Uncertainties, con't

Using $\displaystyle\int_{-\infty}^{\infty} \xi^2 H_n^2(\xi) e^{-\xi^2} d\xi = \sqrt{\pi}\, 2^n\, n!\, (n+1/2)$

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

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

$$= \frac{x_{\text{turning point}}}{\sqrt{2}}$$

since $x_{\text{turning point}} = \sqrt{\frac{\hbar}{m\omega}(2n+1)}$

$$\langle p_n^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi^* \frac{d^2\psi_n}{dx^2}\, dx$$

$$= \hbar m \omega \,(n + 1/2)$$

$$(\Delta p)_n = \sqrt{\langle p_n^2 \rangle - \langle p_n \rangle^2} = \sqrt{\hbar m \omega \,(n + 1/2)}$$

$$\Delta p_n \, \Delta x_n = (n + 1/2)\hbar$$

- For n=0 it just barely satisfies uncertainty principle!

Expectation Value of KE

- For the H.O. in the ground state, let's find the expectation value of the Kinetic Energy: see this week's HW for a different method.

$$P_{op} = -i\hbar \frac{\partial}{\partial x} \Rightarrow KE_{op} = \frac{P_{op}^2}{2m} = \frac{1}{2m}\left(-\hbar^2 \frac{\partial^2}{\partial x^2}\right)$$

$$\langle KE \rangle = \int_{-\infty}^{\infty} \psi_0^* \, KE_{op} \, \psi_0 \, dx = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi_0^* \frac{\partial^2}{\partial x^2} \psi_0 \, dx$$

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

$$\frac{d^2}{dx^2} e^{-\alpha^2 x^2/2} = -\alpha^2 e^{-\alpha^2 x^2/2} + \alpha^4 x^2 e^{-\alpha^2 x^2/2}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\alpha}{\sqrt{\pi}}\right)\left[-\alpha^2 \underbrace{\int_{-\infty}^{\infty} e^{-\alpha^2 x^2}\,dx}_{\frac{\sqrt{\pi}}{\alpha}} + \alpha^4 \underbrace{\int_{-\infty}^{\infty} x^2 e^{-\alpha^2 x^2}\,dx}_{\frac{\sqrt{\pi}}{2\alpha^3}}\right]$$

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

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

So,

$$\langle KE\rangle = \frac{\hbar\omega}{4}$$

Similarly:

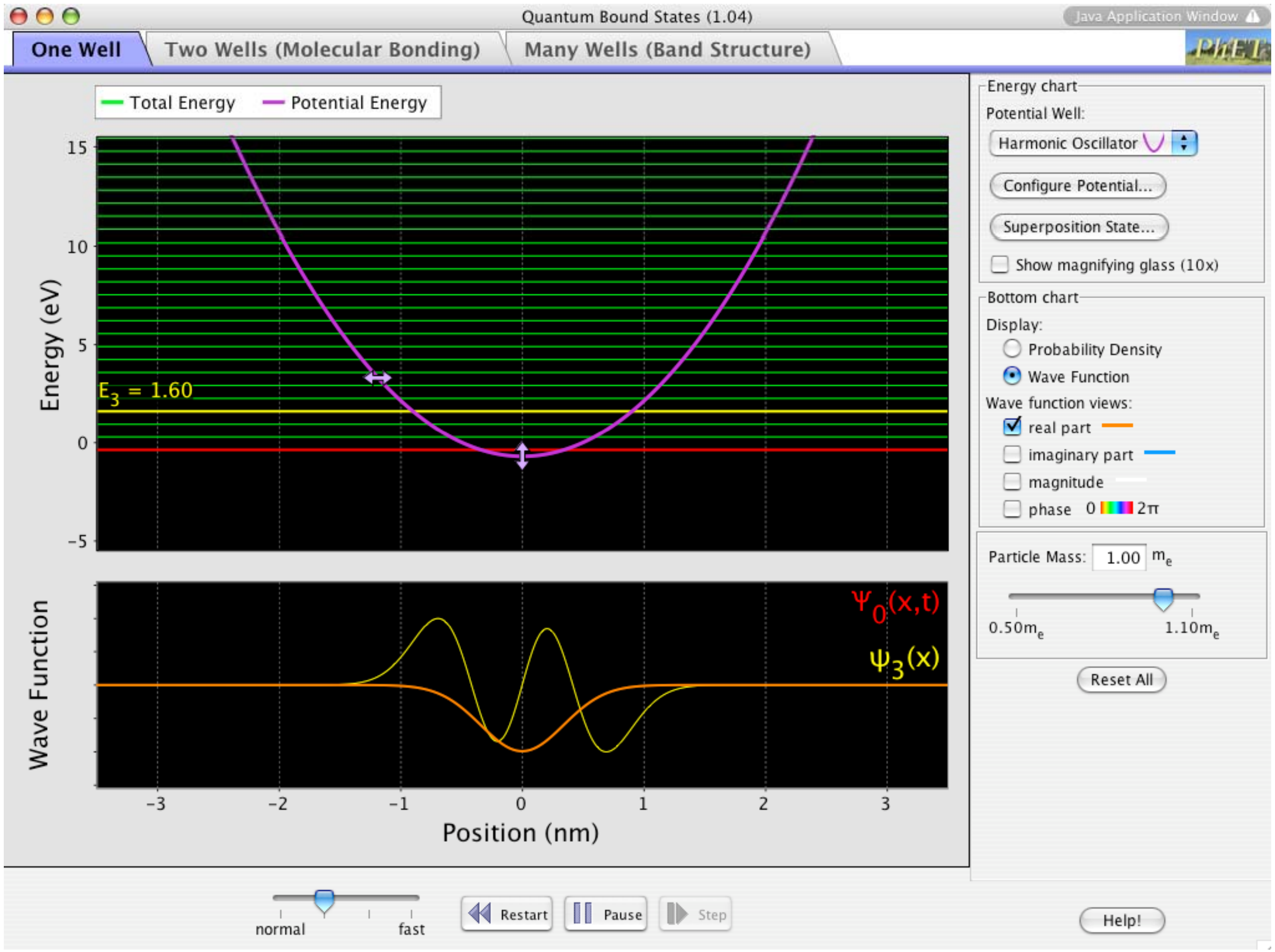
$$\langle V\rangle = \frac{1}{4}\hbar\omega$$

where $V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$

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

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

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

$$= -\frac{1}{2\alpha^2}\left(\frac{d^2\psi}{dx^2} - \alpha^2\psi - \alpha^2 x\frac{d\psi}{dx} + \alpha^2 x\frac{d\psi}{dx} - \alpha^4 x^2\psi\right)$$

$$= -\frac{1}{2\alpha^2}\left(\frac{d^2\psi}{dx^2} - \alpha^2\psi - \alpha^4 x^2\psi\right)$$

$$A^+(A^-\psi) = -\frac{1}{2\alpha^2}\left(\frac{d^2\psi}{dx^2} + \alpha^2\psi - \alpha^4 x^2\psi\right)$$

So,

$$[A^-, A^+]\psi = (A^-A^+ - A^+A^-)\psi$$
$$= \psi$$

Unity operator: $[A^-, A^+] \equiv 1$

- This is independent of the wavefunction being operated on.

Now let's apply this operator on Ψ

$$(A^-A^+ + A^+A^-)\Psi = -\frac{1}{\alpha^2}\frac{d^2\Psi}{dx^2} + \alpha^2 x^2 \Psi$$

After canceling terms

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

Look familiar?

$$H_{op} \equiv \frac{\hbar\omega}{2}(A^-A^+ + A^+A^-)$$

Hamiltonian

$$A^-A^+ - A^+A^- = 1 \Rightarrow A^-A^+ \equiv 1 + A^+A^-$$

$$\Rightarrow \quad H_{op} \equiv \hbar\omega \left(A^+A^- + \tfrac{1}{2}\right)$$

$$\Rightarrow \quad [H_{op}, A^+]\Psi \equiv (\hbar\omega A^+)\Psi$$

$$\Rightarrow \quad [H_{op}, A^-]\Psi \equiv (-\hbar\omega A^-)\Psi$$

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

$$\Rightarrow (H_{op}A^+)\Psi - A^+(E\Psi) = \hbar\omega(A^+\Psi)$$

$$\Rightarrow \quad \underline{H_{op}(A^+\Psi) = (E+\hbar\omega)(A^+\Psi)}$$

Similarly,

$$\underline{H_{op}(A^-\Psi) = (E-\hbar\omega)(A^-\Psi)}$$

Let's discuss this

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

- Similarly, when A^- acts on Ψ, it gives rise to a new function ($A^-\Psi$) whose energy eigenvalue is the same as that of Ψ but <u>less</u> 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:

$$H_{op} \psi_0 = E_0 \psi_0$$

$$\Rightarrow \hbar\omega\left(A^+A^- + \tfrac{1}{2}\right)\psi_0 = \hbar\omega\Big(\underbrace{A^+(A^-\psi_0)}_{0} + \tfrac{1}{2}\psi_0\Big)$$

$$= \frac{\hbar\omega}{2}\psi_0 = E_0\psi_0 \quad \checkmark$$

A^+ and A^- action on H.O. wavefunctions

- See proof in your book

$$A^+\psi_n = i\sqrt{n+1}\,\psi_{n+1}$$

$$A^-\psi_n = -i\sqrt{n}\,\psi_{n-1}$$

- We can also rearrange original equations to get:

$$P_{op} = -i\hbar\frac{\partial}{\partial x}$$

$$\Rightarrow \quad P_{op} = \frac{\alpha\hbar}{\sqrt{2}}\left(A^+ + A^-\right)$$

Momentum and position operators

$$\Rightarrow \quad X_{op} = \frac{-i}{\sqrt{2}\,\alpha}\left(A^+ - A^-\right)$$

Example

- Let's use this new knowledge to calculate $<x^2>$:

$$\langle x^2 \rangle = \int \psi_n^* \left(x_{op}^2 \psi_n \right) dx$$

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

$$= \frac{-1}{2\alpha^2} \int \psi_n^* \left(\underbrace{A^+ A^+ \psi_n}_{\propto \psi_{n+2}} - A^+ A^- \psi_n - A^- A^+ \psi_n + \underbrace{A^- A^- \psi_n}_{\propto \psi_{n-2}} \right) dx$$

$$= \quad \underbrace{\qquad}_{\psi_n^* \psi_{n+2}} \qquad \underbrace{\qquad}_{\psi_n^* \psi_{n-2}}$$

- Recall, orthogonality:

$$\langle \psi_k^* | \psi_n \rangle = \delta_k^n$$

So,

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

$$= \frac{1}{2\alpha^2} \frac{2}{\hbar\omega} \int \psi_n^* H_{op} \psi_n \, dx$$

$$= \frac{1}{\alpha^2 \hbar\omega} \int \psi_n^* E_n \psi_n \, dx = \frac{E_n}{\alpha^2 \hbar \omega}$$

$$\langle x^2 \rangle = \frac{1}{\alpha^2} \left(n + \tfrac{1}{2} \right) \quad \checkmark$$

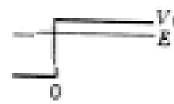
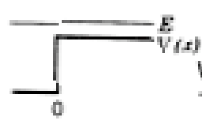
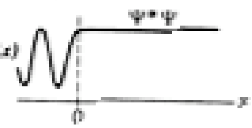
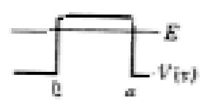
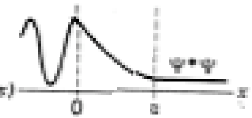
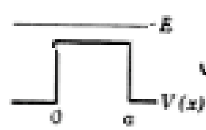
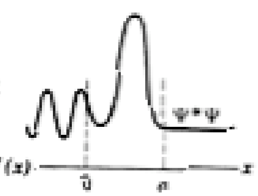
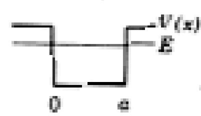
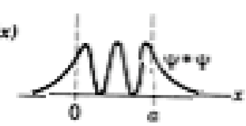
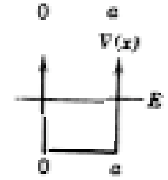
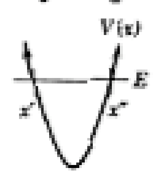
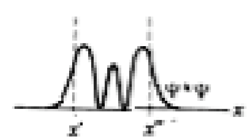
Similarly for $\langle p^2 \rangle$.

Eisberg

&

Resnick

Table 6-2. A Summary of the Systems Studied in Chapter 6

Name of System	Physical Example	Potential and Total Energies	Probability Density	Significant Feature
Zero potential	Proton in beam from cyclotron			Results used for other systems
Step potential (energy below top)	Conduction electron near surface of metal			Penetration of excluded region
Step potential (energy above top)	Neutron trying to escape nucleus			Partial reflection at potential discontinuity
Barrier potential (energy below top)	α particle trying to escape Coulomb barrier			Tunneling
Barrier potential (energy above top)	Electron scattering from negatively ionized atom			No reflection at certain energies
Finite square well potential	Neutron bound in nucleus			Energy quantization
Infinite square well potential	Molecule strictly confined to box			Approximation to finite square well
Simple harmonic oscillator potential	Atom of vibrating diatomic molecule			Zero-point energy

Summary/Announcements

- Next time: Review for exam: Bring questions!

- Midterm exam Wed. Oct. 19 in class - it will be **closed book**- One letter size formula-only sheet allowed: (for example, solution steps are not allowed) needs to be turned in together with the answer book.