PHYS-3301

Lecture 8

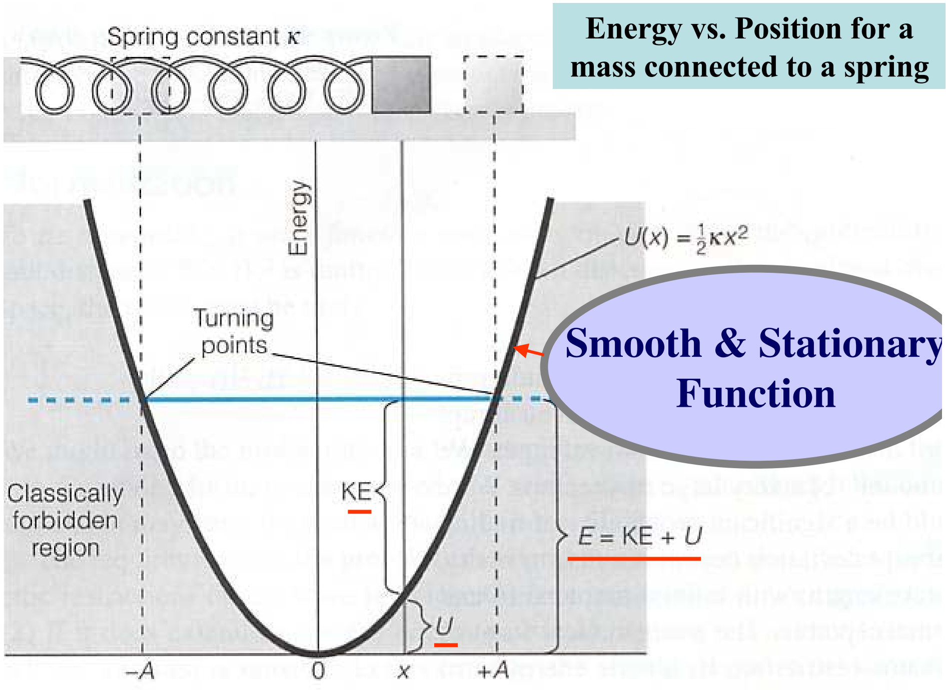
Sep. 20, 2022

Chapter. 5
Bound States: Simple Case

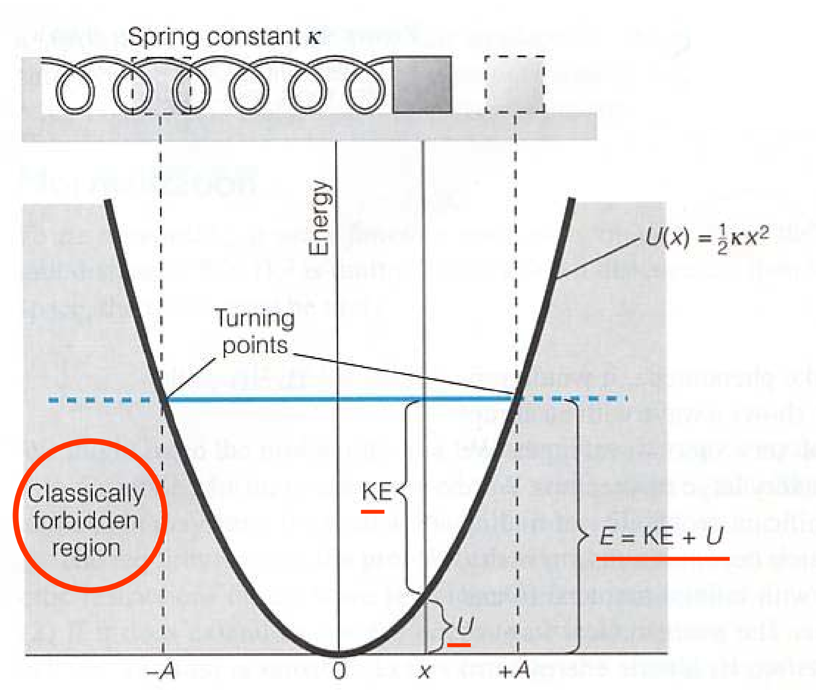
Outline:

- **The Schrödinger Equation (for interacting particles)**
- **Stationary States**
- **Physics Conditions: Well-Behaved Functions**
- **A Review of Classical Bound States**
- **Case 1: Particles in a Box – The Infinite Well**
- **Case 2: The Finite Well**
- **Case 3: The Simple Harmonic Oscillator**
- **Expectation Values, Uncertainties, and Operators**

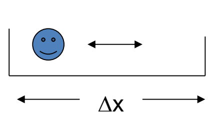
Energy vs. Position for a mass connected to a spring



Smooth & Stationary Function



Bound Systems

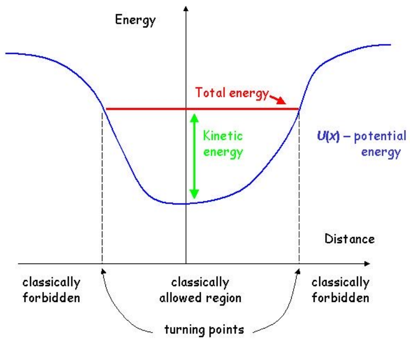


A bound system: any system of interacting particles where the nature of the interactions between the particles keeps their relative separation limited. Classical example: the solar system.

In general, the problem is very difficult.

Simplification: motion of a single particle that moves in a fixed potential energy field $U(x)$. The mass of the particle is small compared to the total mass of the system (e.g. heavy nucleus - light electron).

Classical bound system: $E(x) = K(x) + U(x)$



$E(x) = U(x)$

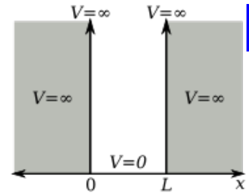
Classically allowed region:

$E(x) > U(x) \qquad K(x) > 0$

Classically forbidden region:

$E(x) < U(x)$

The Infinite Square Well



a particle in the potential is completely free, except at the two ends where an infinite force prevents it from escaping

Outside the well: $\psi(x) = 0$ - the probability of finding the particle =0

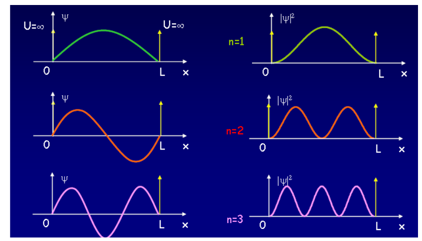
Inside the well: $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$

$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \qquad k \equiv \frac{\sqrt{2mE}}{\hbar}$ - the harmonic oscillator equation

General solution: $\psi(x) = A\sin kx + B\cos kx$ - constants A and B are fixed by boundary conditions

Continuity of the wave function: $\psi(0) = \psi(L) = 0 \qquad \psi(0) = A\sin k0 + B\cos k0 = B = 0$

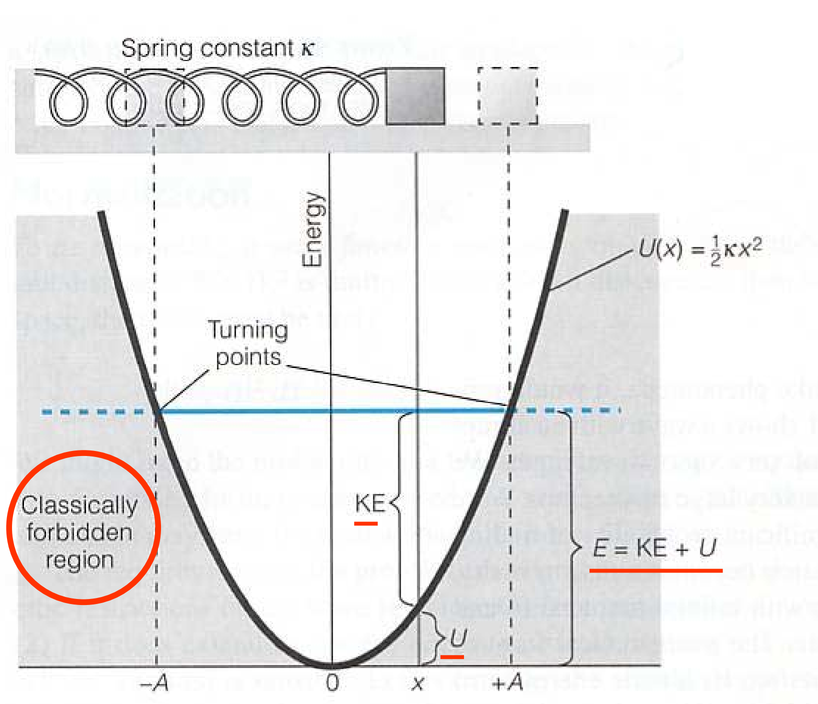
Thus, $\psi(x) = A\sin kx \qquad \psi(L) = A\sin kL = 0 \qquad kL = 0, \pm\pi, \pm 2\pi, \ldots$

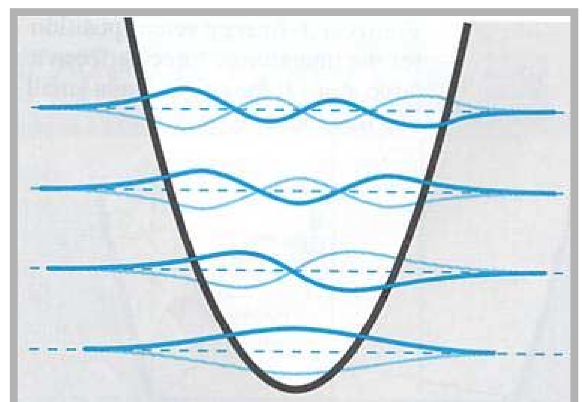


$$k_n = \frac{n\pi}{L},\ n = 1, 2, \ldots$$

n – ***quantum number*** (1D motion is characterized by a single q.n., for 2D motion we need two quantum numbers, etc.)

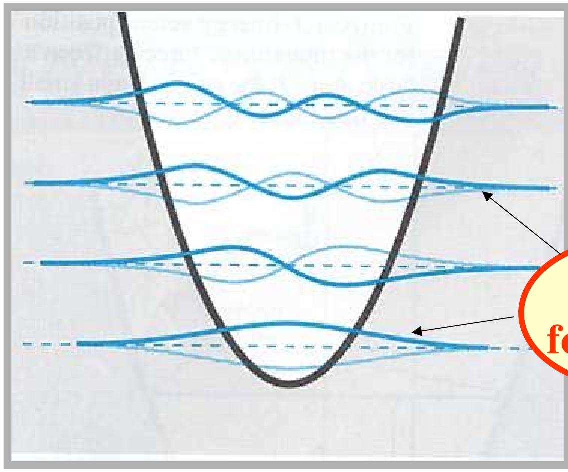
See later for details



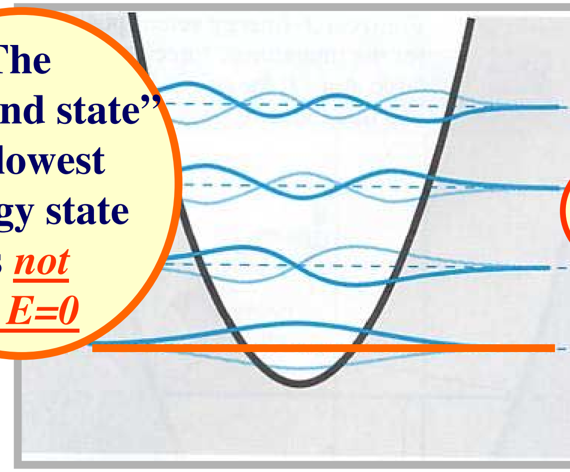


Bound states is one in which a particle's motion is restricted by an external force to finite region of space

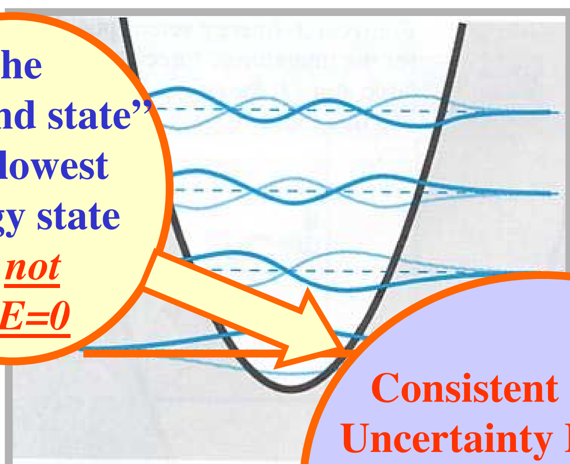
In Quantum Mechanics – Bound States are Standing Waves



In Quantum Mechanics – Bound States are Standing Waves



In Quantum Mechanics – Bound States are Standing Waves



Consistent with the Uncertainty Relations:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

The Schrodinger Equation for Interacting Particles

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$$

For free particles

or in the absence of external forces

$Ae^{i(kx-wt)}$

$$-\frac{\hbar^2}{2m}(ik)^2 Ae^{i(kx-\omega t)} = i\hbar(-i\omega)Ae^{i(kx-\omega t)}$$

$$\frac{\hbar^2 k^2}{2m}\Psi(x,t) = \hbar\omega\Psi(x,t)$$

$$\frac{p^2}{2m}\Psi(x,t) = E\Psi(x,t) \quad \rightarrow \quad \text{KE}\ \Psi(x,t) = E\Psi(x,t)$$

Schrödinger eq. is based on E accounting - w/o external interactions

Try to add potential energy U(x)

Adding P.E.

$$(\mathrm{KE} + U(x))\Psi(x,t) = E\Psi(x,t)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

→ Time-dependent Schrödinger Eq.

→ To determine the behavior of particle

in (1) CM: solve F = m(d^2r/dt^2) for r, given knowledge of Net external F on particle

in (2) QM: solve the Schrödinger eq. for $\psi(x,t)$, given knowledge of P.E., U(x)

The Schrodinger Equation for Interacting Particles and for Stationary Potentials

$$U = U(x)$$

$$U \neq U(t)$$

Key Assumption:

Factorization of the wave function

$$\Psi(x,t) = \psi(x)\phi(t)$$

Standard Math. Technique; "Separation of variables"

Wave function may be express as a product of …

Spatial Part **Temporal Part**

Q: Why?, **A:** allows us to break a differential eq. with 2 independent variables (x,t) into simpler eqs. For position & time, separately!!

What happens with the Schrodinger equation?

$$\Psi(x,t) = \psi(x)\phi(t)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

… and factoring out terms constant w.r.t. the partial derivatives …

$$-\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x)\phi(t) = i\hbar\psi(x)\frac{\partial\phi(t)}{\partial t}$$

Divide both sides by $\psi(x)\phi(t)$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

Variables are separate now!!

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

t and x are independent

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = C$$

Consider only case in which P.E. is time-independent

Separation Constant

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = C \rightarrow \frac{d\phi(t)}{dt} = -\frac{iC}{\hbar}\phi(t)$$

The Temporal Part, ϕ(t)

$$\phi(t) = Ae^{-i(C/\hbar)t}$$

$$E = \hbar\omega = C$$

Solution (see Appendix K)

$Ae^{i(kx-\omega t)} \sim Ae^{-i\omega t}$, $\omega = C/\hbar$

$$\phi(t) = e^{-i(E/\hbar)t}$$

Temporal part

$$\Psi(x, t) = \psi(x)\phi(t)$$

$$\Psi(x, t) = \psi(x)e^{-i(E/\hbar)t}$$

Total wave function

$$\phi(t) = e^{-i(E/\hbar)t}$$

Temporal part

$$\Psi(x, t) = \psi(x)\phi(t)$$

$$\Psi(x, t) = \psi(x)e^{-i(E/\hbar)t}$$

Total wave function

$$\Psi^*(x, t)\Psi(x, t) = [\psi^*(x)e^{+i(E/\hbar)t}][\psi(x)e^{-i(E/\hbar)t}]$$
$$= \psi^*(x)\psi(x)$$

Oops!! Its time dependence disappears!!

The probability density is time-independent

Stationary States

i.e. the whereabouts of the particle don't change with time in any observable way

---

$$\phi(t) = e^{-i(E/\hbar)t}$$

Temporal part

$$\Psi(x, t) = \psi(x)\phi(t)$$

$$\Psi(x, t) = \psi(x)e^{-i(E/\hbar)t}$$

Total wave function

$$\Psi^*(x, t)\Psi(x, t) = [\psi^*(x)e^{+i(E/\hbar)t}][\psi(x)e^{-i(E/\hbar)t}]$$
$$= \psi^*(x)\psi(x)$$

Oops!! Its time dependence disappears!!

The probability density is time-independent

Stationary States

Quantum Mechanically, electron is not an accelerating charged particles, but rather a stationary "cloud"

The spatial part of $\psi(x,t)$

Replace C by E, multiply both sides by ψ(x);

The time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

Spatial part

NOTE: ***$\psi(x)$ is Real,***

but $\psi(x,t)$ is Complex, because

$$\phi(t)=e^{-i\omega t}$$