PHY293 Lecture #16

November 28, 2017

1. Wave Equations

- Waves on a String
  - Transverse waves on a string governed by: $\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2}$
  - v depends on the mass density and string tensions and y is the amplitude of the transverse wave
  - Derived by applying $F = ma$ to a small segment of the string
  - Has the solution $y(x,t) = A\sin(kx - \omega t)$ with $v = \omega/k$
- Electromagnetic Waves
  - In the absence of charges or currents Maxwell's equations are

$$\vec{\nabla}\cdot\vec{E} = 0 \qquad \vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t} \qquad \vec{\nabla}\cdot\vec{B} = 0 \qquad \vec{\nabla}\times\vec{B} = \frac{1}{c^2}\frac{\partial\vec{E}}{\partial t}$$

  - These can be 'promoted' to wave equations by considering the quantities:

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{E}) = \vec{\nabla}(\vec{\nabla}\cdot\vec{E}) - \nabla^2\vec{E} = \vec{\nabla}\times\frac{-\partial\vec{B}}{\partial t} = -\frac{\partial}{\partial t}(\vec{\nabla}\times\vec{B}) = \frac{-1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2}$$

  - And similarly for B

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{B}) = \vec{\nabla}(\vec{\nabla}\cdot\vec{B}) - \nabla^2\vec{B} = \vec{\nabla}\times\frac{1}{c^2}\frac{\partial\vec{E}}{\partial t} = \frac{1}{c^2}\frac{\partial}{\partial t}(\vec{\nabla}\times\vec{E}) = \frac{-1}{c^2}\frac{\partial^2\vec{B}}{\partial t^2}$$

  - Given that $\vec{\nabla}\cdot\vec{E} = 0$ (and same for $\vec{B}$) these reduce to:

$$\nabla^2\vec{E} = \frac{1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2} \qquad \nabla^2\vec{B} = \frac{1}{c^2}\frac{\partial^2\vec{B}}{\partial t^2}$$

  - The equations of waves for $\vec{E}$ and $\vec{B}$ travelling with velocity c
  - The solutions for these are $\vec{E}(x,t) = A\sin(kx - \omega t)\hat{y}$ and $\vec{B}(x,t) = \frac{A}{c}\sin(kx - \omega t)\hat{z}$ with $c = \frac{\omega}{k}$
  - These are similar in form to the waves on a string, but there is no medium of propagation (ie. no ether)
  - The presence of c in these equations, with no reference to any specific reference frame was one of the things that led Einstein to formulate special relativity with c the same for all inertial frames.
- Matter Waves
  - We have a slightly different wave equation for our "matter waves"
  - The **Schrodinger equation**, in the absence of external particles is (in one dimension)

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

  - We won't derive this from first principles (didn't really do that for EM waves either...)
  - Will see these two terms represent the particle's kinetic energy, and total energy when we see first solutions for $\Psi(x,t)$
  - Note that the equation is explicitly complex (with i on the RHS).
  - Solutions ($\Psi(x,t)$) are also complex, so we need to interpret the probability of finding a particle was $|\Psi(x,t)|^2 = \Psi^*\Psi$
  - The probability to find a particle at x and t is given by $|\Psi(x,t)|^2 = \Psi^*\Psi$

2. Solutions to the Schrodinger equation

- The explicit presence of an i in the partial differential equation means that $\sin$ or $\cos$ wave solutions won't work:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[A\sin(kx - \omega t)] = \frac{\hbar^2 k^2}{2m}[A\sin(kx - \omega t)]$$

- While

$$i\hbar\frac{\partial}{\partial t}[A\sin(kx - \omega t)] = -i\hbar\omega[A\cos(kx - \omega t)]$$

- No way to 'align' spatial/time dependence of $\sin$ (LHS) with $\cos$ (RHS) – let alone LHS is real and RHS is imaginary
- Could try $A\sin(kx-\omega t)+A\cos(kx-\omega t)$ as a solution instead:
- Still LHS real and RHS imaginary (not to mention the first/single time derivatives of $\sin$ and $\cos$ have opposite sign)
- In fact the only way out is to consider $\Psi(x,t)=A\cos(kx-\omega t)+B\sin(kx-\omega t)$
- In fact find $B=iA$ will work, and in fact this solution can also be written as $Ae^{i(kx-\omega t)}$
- Need a complex mix of sinusoidal components (out of phase by 90^o) to solve the Schrodinger equation
- Convince yourselves that

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[Ae^{i(kx-\omega t)}]=i\hbar\frac{\partial}{\partial t}[Ae^{i(kx-\omega t)}]$$
$$\Rightarrow -\frac{\hbar^2}{2m}(ik)^2[Ae^{i(kx-\omega t)}]=i\hbar(-i\omega)[Ae^{i(kx-\omega t)}]$$

- This will be a solution iff $-\frac{\hbar^2}{2m}(ik)^2=i\hbar(-i\omega)$ or $\frac{\hbar^2k^2}{2m}=\hbar\omega$
- Recall that we had $p=h/\lambda=\hbar k$ and $E=h\nu=\hbar\omega$
- From these two expressions we can see that the solution to the Schrodinger equation is just another way of stating (classical/non-relativistic) energy conservation for a free particle: $\frac{\hbar^2k^2}{2m}=\hbar\omega$ is another way of saying $p^2/2m=E$
- Non-relativistically a free particle's total energy (its kinetic energy) is just $p^2/2m$
- Wave function itself not directly detectable, have said $|\Psi(x,t)|^2$ should represent the probability to find particle at x and t
- What is the probability then for this solution?

$$|\Psi(x,t)|^2=Ae^{i(kx-\omega t)}\cdot Ae^{-i(kx-\omega t)}=A^2$$

- The probability to find a particle at some point in space is constant (A^2)
- This is a plane wave, not localised any where is space, the same probability everywhere
- Here momentum of the particle precisely known: $\hbar k$, but no information about where in space – it has equal probability to show up anywhere/everywhere.

3. Ch 4, Problem 36:
   - A electron, with well defined momentum: 5×10^{-25} kg m/s moving along the x axis.
   - Write an expression for the matter wave associated with this electron with all numerical values:
   - This is a plane wave solution (well defined momentum $\Rightarrow$ no information about x position)

$$\Psi(x,t)=Ae^{i(kx-\omega t)}$$

   - Determine k from momentum: $\hbar k=1.05\times10^{-34}k=5\times10^{-25}\Rightarrow k=4.76\times10^{9}$ wavelengths/m or 4.76 wavelengths/nm.
   - Determine ω from Schrodinger constraint: $\hbar\omega=p^2/2m\Rightarrow\omega=(5\times10^{-25})^2/[2(9.1\times10^{-31})(1.05\times10^{-34})]=1.30\times10^{15}$ radians/s or 1.30 radians/ps.
   - So the full solution with numerical values is:

$$\Psi(x,t)=Ae^{i(4.76x-1.30t)}\qquad x\text{ in nm}, t\text{ in fs}$$

   - Note that units for x and t make sense for a single electron (wavelengths in nm and oscillations in fs), not m or s.

4. Ch 4, Problem 27:
   - A free particle is represented by a plane wave by:

$$\Psi(x,t)=Ae^{i(1.58x-79.1t)}\qquad x\text{ in pm}, t\text{ in fs}$$

   - Note I've already done the conversion to appropriate units for atomic particles
   - Find the particle's momentum, kinetic energy and mass
   - Again this is the solution to the 'free particle' Schrodinger equation so $p=\hbar k$ and $E=\hbar\omega$

- We can just read these off the wavefunction: $p = 1.05 \times 10^{-34} \cdot 1.58 \times 10^{12} = 1.66 \times 10^{-22}$ kg m/s
- $E = \hbar\omega = 1.05 \times 10^{-34} \cdot 79.1 \times 10^{15} = 8.31 \times 10^{-18}$ J
- And $m = p^2/2E = (1.66 \times 10^{-22})^2/2(8.31 \times 10^{-18}) = 1.66 \times 10^{-27}$ kg
- This is the mass of the proton... as if by accident.

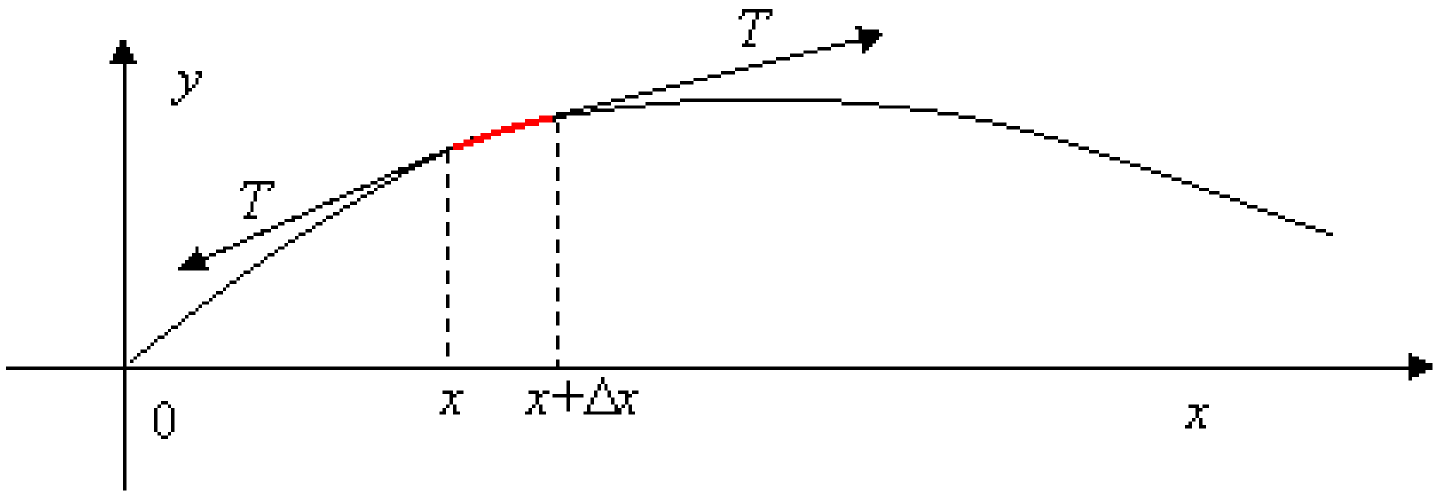
5. Introducing Potential Energy to the Schrodinger Equation

- So far we've only looked at free particle solutions to the Schrodinger equation
- Not the most interesting physics – to understand the Hydrogen atom (or how things interact) need to also consider the potential energy
- Suppose we have a simple mechanical example – higher energy barrier between two regions of constant (and equal) potential
  - Start with free particle: $E_{tot} = 1/2mv^2$
  - In the region of the barrier: $E_{tot} = 1/2m(v')^2 + U(x)$
  - On the right side we have free particle again: $E_{tot} = 1/2mv^2$
  - Whether the 'free particle' ends up on the left or the right will depend on whether $1/2mv^2 > U_{max}(x)$.
- Could also consider a bound state with two atoms that are mechanically attached by a spring
  - Such bound states interesting to show phenomena like quantisation of energy levels (ie. the H-atom yesterday)
  - Consider first the potential energy associated with a simple mass on a spring
    - Note the turning points are where the potential energy has absorbed all of the kinetic energy
    - Classically the mass is free to move anywhere between the turning points and will oscillate
  - Consider slightly more complicated case (two different masses, coupled by some unknown force)
    - Take heavy atom to define the origin of coordinate system (consider in frame where heavy atom is at rest)
    - For small x force is repulsive – creates a turning point where smaller atom cannot approach any closer to atom "1"
    - For large x force is attractive – creates a turning point beyond which atom "2" can't escape any further
    - This is similar to the potential energy we saw yesterday for the electron in a 'potential' generated by the proton
    - If kinetic energy of atom 2 is large enough, then it can overcome the attractive potential and 'escape' from Atom 1. Only one turning point at, small x where it cannot approach closer to Atom 1.
- Potentials in the Schrodinger Equation
  - We already have two terms in Schrodinger equation representing kinetic energy ($\hbar^2 k^2/2m$) and total energy $\hbar\omega$
  - It makes some sense to just add the potential energy to the LHS of the Schrodinger equation:

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

  - This is referred to at the "Time Dependent Schrodinger Equation"
    - Perhaps a bit confusing because we always had $\partial/\partial t$ in the first version
    - But without a potential we found time-independent – free particle wave solutions
    - When we introduce a potential we can find solutions that give different probabilities as a function of time
  - In classical mechanics we solve $\vec{F} = m\vec{a}$ (ie. to analyse a mass on a spring)
  - In non-relativistic quantum mechanics we solve the TDSE for a particular choice of potential ($U(x)$)

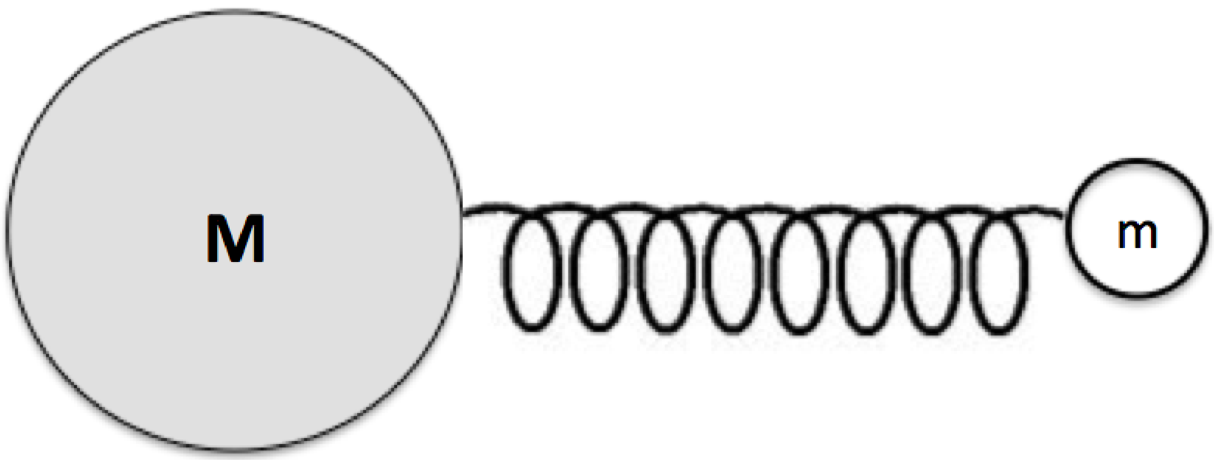
Waves on a String



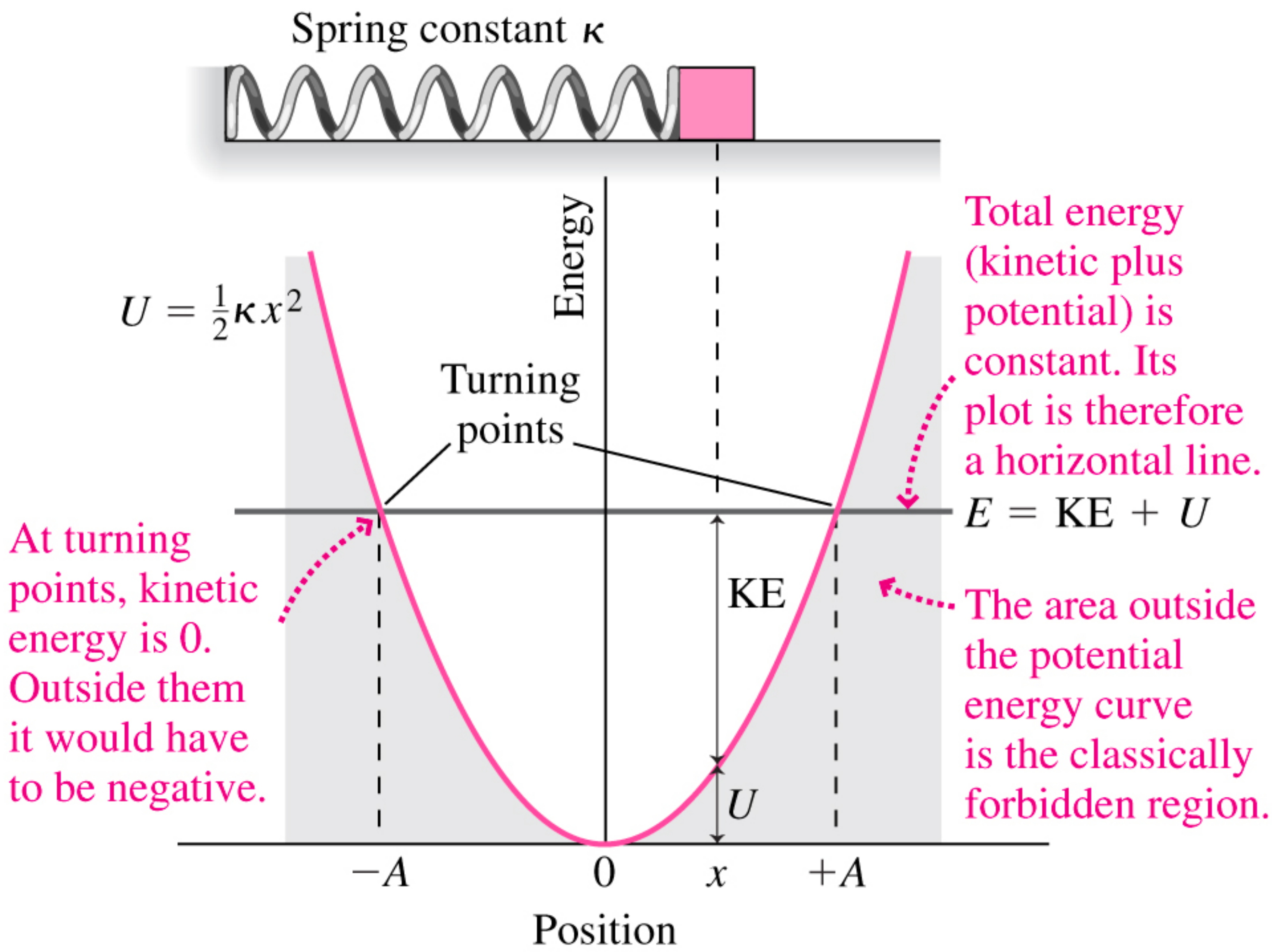
Dynamics of a short segment of string: neglecting gravity, the only forces are the tension forces T acting on the ends.

Simple Potential

Two Atom Molecule



Potential Energy of Mass on Spring



Potential Energy of Bound Atoms