Quantum Superposition and Optical Transitions

Outline

Generating EM Fields

Time-Varying Wavefunctions

Superposition of Energy States

Maxwell and Schrödinger

Maxwell's Equations

$$\oint_C \vec{E} \cdot d\vec{l} = -\frac{d}{dt}\left(\int_S \vec{B} \cdot d\vec{l}\right)$$

$$\oint_C \vec{H} \cdot d\vec{l} = \int \vec{J} \cdot d\vec{A} + \frac{d}{dt}\int_S \epsilon\vec{E} \cdot d\vec{A}$$

The Wave Equation

$$\frac{\partial^2 E_y}{\partial z^2} = \epsilon\mu\frac{\partial^2 E_y}{\partial t^2}$$

Dispersion Relation

$$\omega^2 = c^2 k^2$$

$$\omega = ck$$

Energy-Momentum

$$E = \hbar\omega = \hbar ck = cp$$

Quantum Field Theory

... is thought to be the unique and correct outcome of combining the rules of quantum mechanics with the principles of the theory of relativity.

The Schrodinger Equation

$$-j\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

(free-particle)

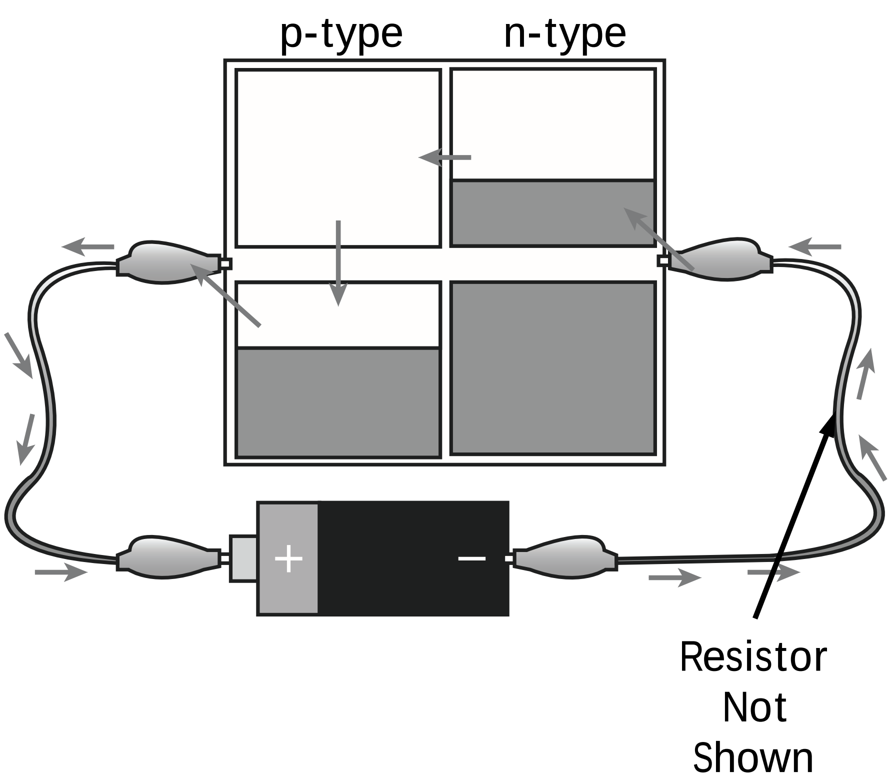
Dispersion Relation

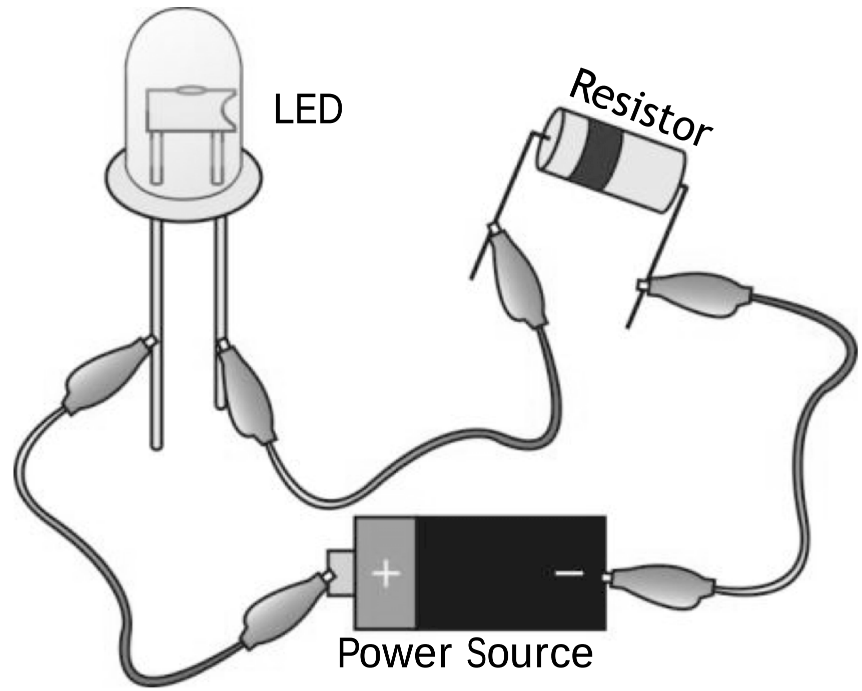
$$\hbar\omega = \frac{\hbar^2 k^2}{2m}$$

Energy-Momentum

$$E = \frac{p^2}{2m}$$ (free-particle)

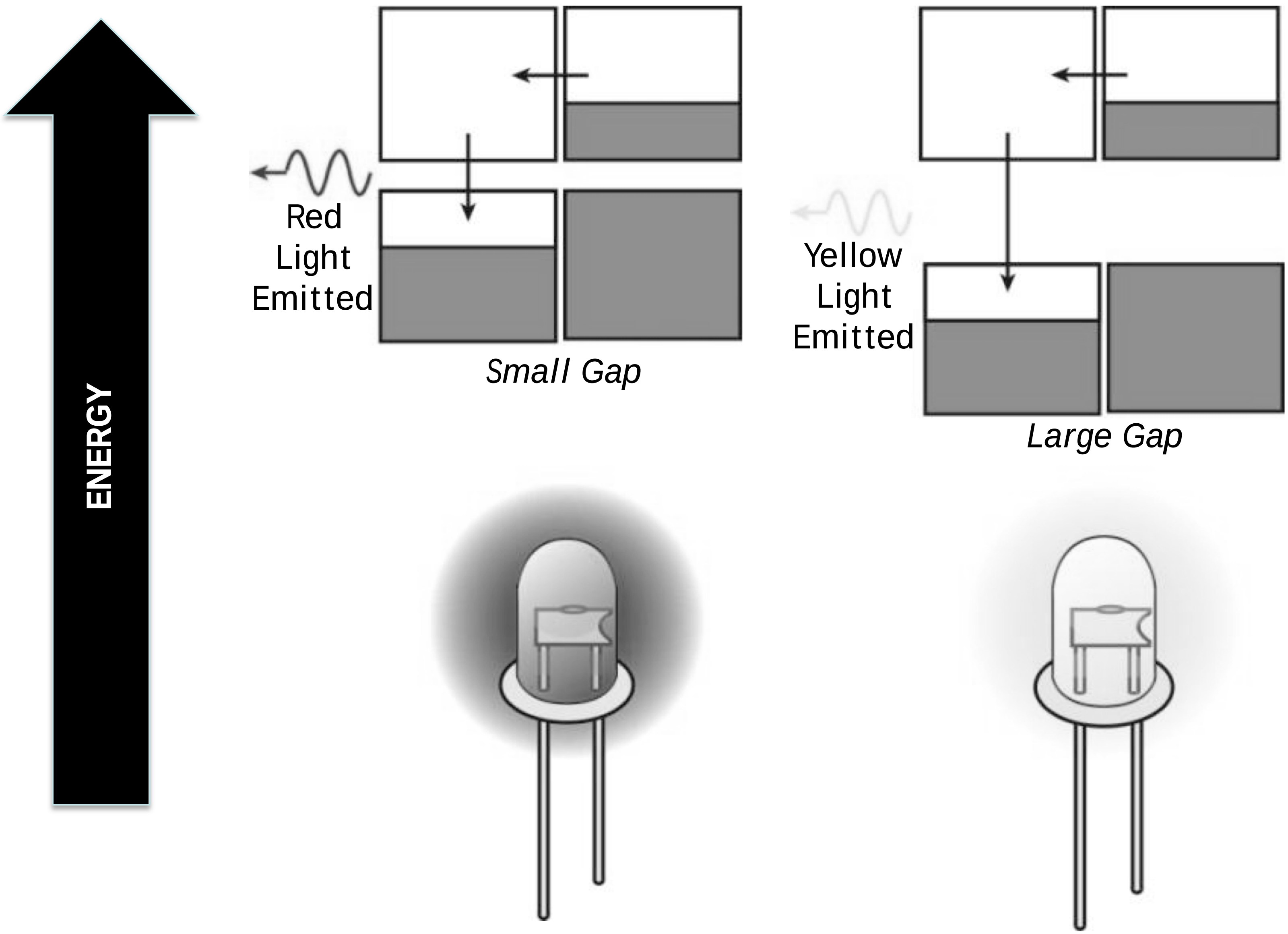
P-N Junctions and LEDs



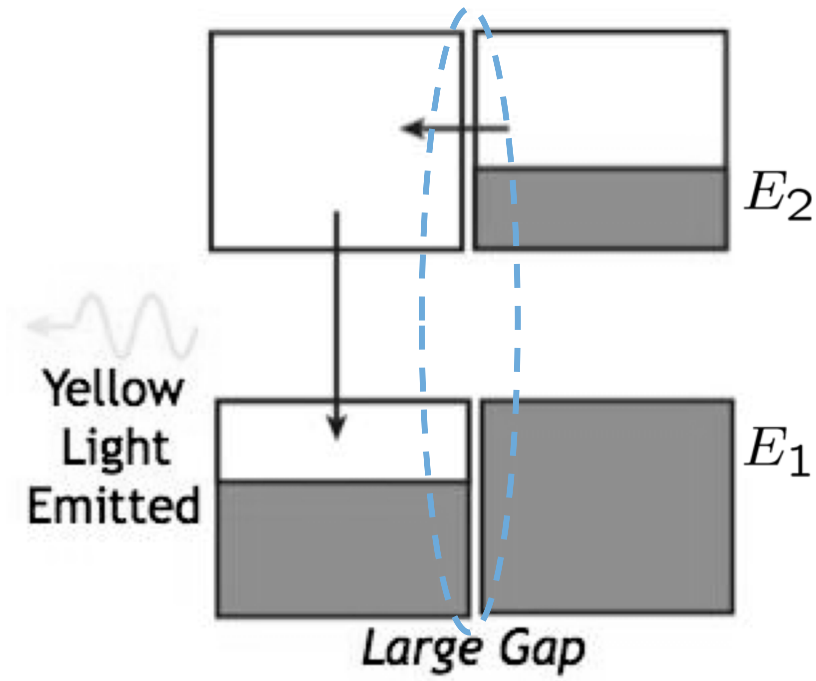


High energy electrons (n-type) fall into low energy holes (p-type)

P-N Junctions and LEDs



P-N Junctions and LEDs



Uncertain energy during transition from high energy to low energy

$$\Psi(x,t) = \psi_1(x)e^{-iE_1 t/\hbar} + \psi_2(x)e^{-iE_2 t/\hbar}$$

Coupling of Electric and Magnetic Fields

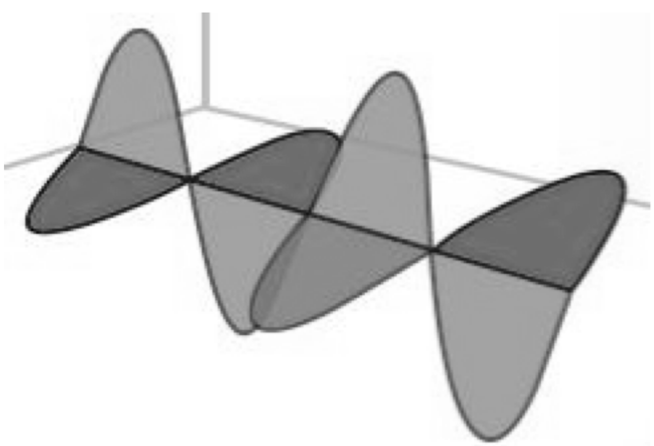
Maxwell's Equations couple H and E fields..

Oscillating B generates H...

$$\oint_C \vec{E} \cdot d\vec{l} = -\frac{d}{dt}\left(\int_S \vec{B} \cdot d\vec{A}\right)$$

Oscillating E generates H...

$$\oint_C \vec{H} \cdot d\vec{l} = \int_S \vec{J} \cdot d\vec{A} + \frac{d}{dt}\int_S \epsilon\vec{E} \cdot d\vec{A}$$



How are the oscillating fields generated ?

Time-Dependent Schrodinger Equation

For that matter, how do we get ANYTHING to move ?

states of definite energy

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

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi \quad \Longrightarrow \quad E\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

Schrodinger says that definite energy states do not move, they are stationary !

$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

Example: Superposition of Energy States

- It is possible that a particle can be in a superposition of "eigenstates" with *different* energies.

  - Such superpositions are also solutions of the time-dependent SEQ!
  - What is E of this superposition?

Let's see how these superpositions evolve with time.

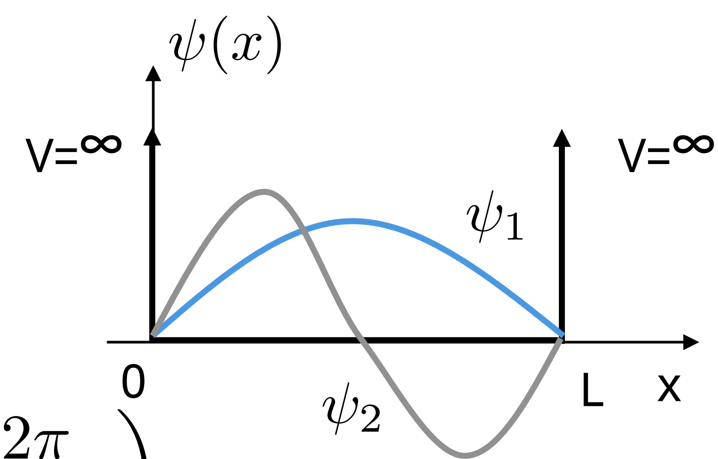
- Particle is described by a wavefunction involving a superposition of the two lowest infinite square well states (n=1 and 2)

$$\Psi(x,t) = \psi_1(x)e^{-i\omega_1 t} + \psi_2(x)e^{-i\omega_2 t}$$

$$\omega_1 = \frac{E_1}{\hbar} \qquad \omega_2 = \frac{E_2}{\hbar}$$

$$E_1 = \frac{\hbar^2}{8mL^2} \qquad E_2 = 4E_1$$

$$\psi_1(x) = A_1 \sin\left(\frac{\pi}{L}x\right) \qquad \psi_2 = A_1 \sin\left(\frac{2\pi}{L}x\right)$$



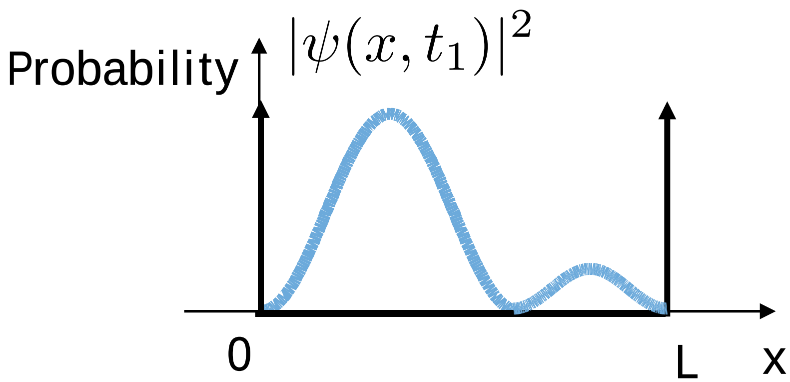
Example: Superposition of Energy States

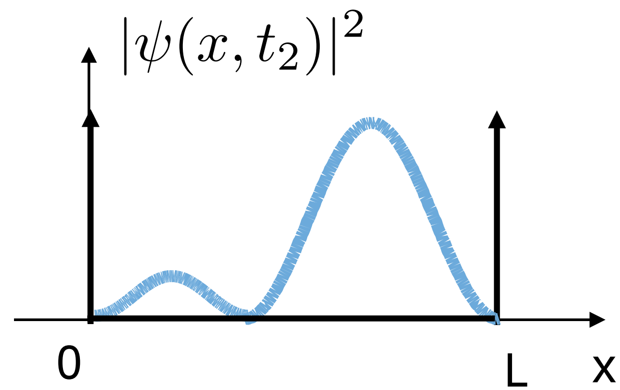
The probability density is given by: $|\Psi(x,t)|^2$:

$$|\Psi(x,t)|^2 = |\psi_1(x)|^2 + |\psi_2(x)|^2 + 2\psi_1\psi_2 \cos((\omega_1 - \omega_2)t)$$

Because the cos term oscillates between ±1, $|\Psi(x,t)|^2$ oscillates between:

$$|\Psi(x,t_1)|^2 = |\psi_1(x) + \psi_2(x)|^2 \qquad |\Psi(x,t_2)|^2 = |\psi_1(x) - \psi_2(x)|^2$$





particle localized on <u>left</u> side of well

particle localized on <u>right</u> side of well

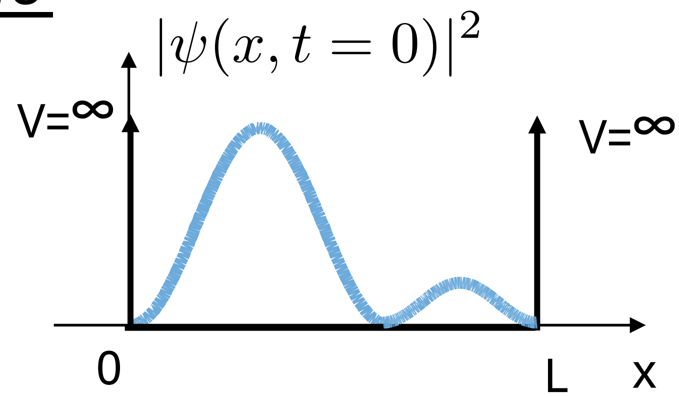
The frequency of oscillation between these two extremes is $\omega = \dfrac{E_2 - E_1}{\hbar}$

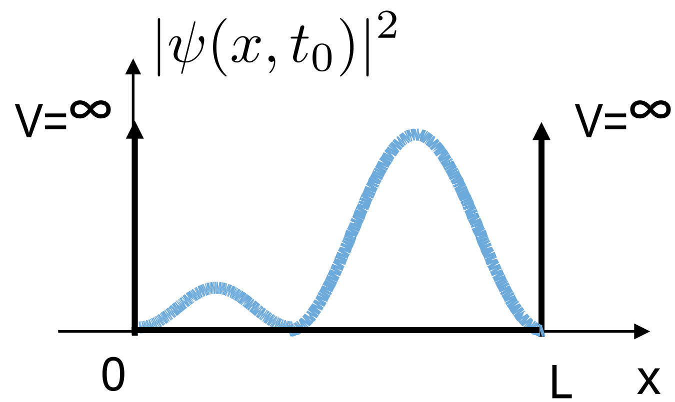
Numerical Example

- Consider the numerical example:

An electron in the infinite square well potential is initially (at t=0) confined to the left side of the well, and is described by the following wavefunction:

$$\Psi(x,t=0) = A\sqrt{\frac{2}{L}}\left(\sin\left(\frac{\pi}{L}x\right) + \sin\left(\frac{2\pi}{L}x\right)\right)$$





If the well width is L = 0.5 nm, determine the time t_o it takes for the particle to "move" to the right side of the well.

period $T = 1/f = 2t_0$ with $f = (E_2 - E_1)/h$

$$E_n = \frac{h^2}{2m_e\lambda_n^2} = \frac{1.505\text{eV}\cdot\text{nm}^2}{\lambda_n^2}$$

$$\lambda_n = 2L/n$$

$$E_n = E_1 n^2$$

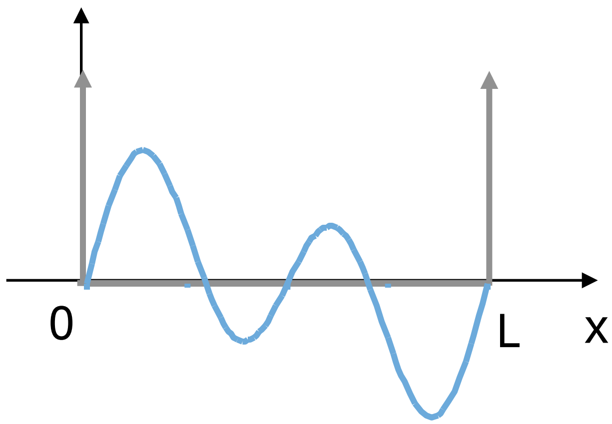
$$E_1 = \frac{1.505\text{ eV}\cdot\text{nm}^2}{4L^2} = \frac{1.505\text{ eV}\cdot\text{nm}^2}{4(0.5\text{ nm})^2} = 1.505\text{ eV}$$

$$t_o = \frac{T}{2} = \frac{h}{2(E_2 - E_1)} = \frac{h}{2(3E_1)} = \frac{4.136\times10^{-15}\text{ eV}\cdot\text{sec}}{2(3\times1.5\text{ eV})} = 4.6\times10^{-16}\text{ sec}$$

Example: Superposition of Energy States

Consider a particle in an infinite potential well, which at t= 0 is in the state:

$$\Psi(x,t) = 0.5\psi_2(x)e^{-i\omega_2 t} + 0.866\psi_4(x)e^{-i\omega_4 t}$$



with $\psi_2(x)$ and $\psi_4(x)$ both normalized.

$$\psi_2(x) = A_2 \sin\left(\frac{2\pi}{L}x\right)$$

$$\psi_4(x) = A_4 \sin\left(\frac{4\pi}{L}x\right)$$

1. If we measure the energy of the particle: What is the measured energy?

   (a) E_2 (b) E_4 (c) $0.25\ E_2 + 0.75\ E_4$
   (d) It depends on *when* we measure the energy

2. If we measure the energy of the particle: What is the expected (average) energy?

   (a) E_2 (b) E_4 (c) $0.25\ E_2 + 0.75\ E_4$
   (d) It depends on *when* we measure the energy

Normalizing Superposition States

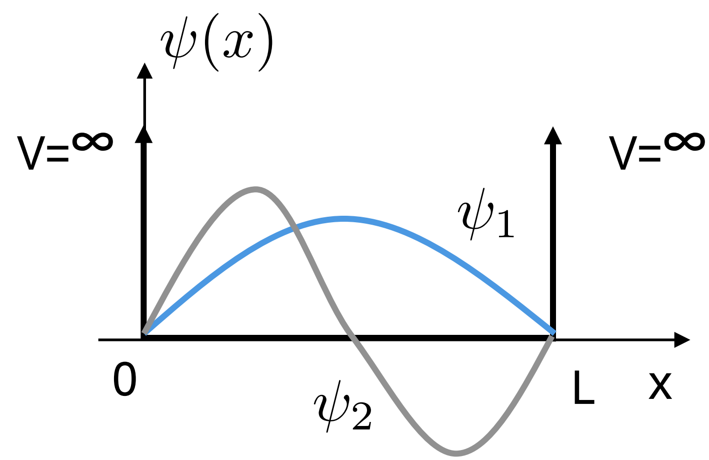
- It's a mathematical fact that any two eigenstates with different eigenvalues (of any measurable, including energy) are ORTHOGONAL
  - » Meaning:

$$\int \psi_1^*(x)\psi_2(x)dx = 0$$

So when you normalize a superposition of normalized energy eigenstates, you just have to make the sum of the absolute squares of their coefficients come out 1.

$$\psi_1(x) = A_1 \sin\left(\frac{\pi}{L}x\right)$$

$$\psi_2(x) = A_2 \sin\left(\frac{2\pi}{L}x\right)$$



Energy of Superposition States

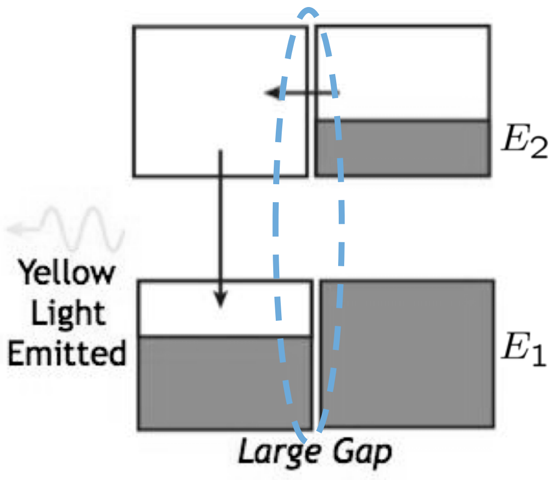
- The important new result concerning superpositions of energy eigenstates is that these superpositions represent quantum particles that are *moving*. Consider:

$$\Psi(x,t) = A_1\psi_1(x)e^{-i\omega_1 t} + A_2\psi_2(x)e^{-i\omega_2 t}$$

- But what happens if we try to measure E on a wavefunction which involves more than one energy?
  - *We can still only measure one of the allowed energies*, i.e., one of the eigenstate energies (e.g., only E_1 or E_2 in $\Psi(x,t)$ above)!

If $\Psi(x,t)$ is normalized, $|A_1|^2$ and $|A_2|^2$ give us the probabilities that energies E_1 and E_2, respectively, will be measured in an experiment!

- When do we not know the energy of an electron ?



Beautiful Consistency

- At what frequency does the charge oscillation occur ?

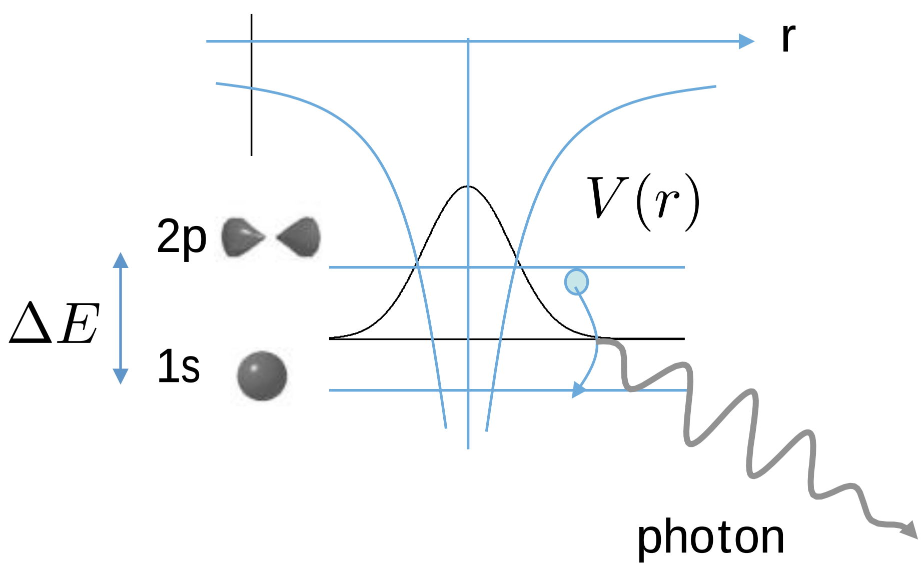
- How much energy does the field take away ?

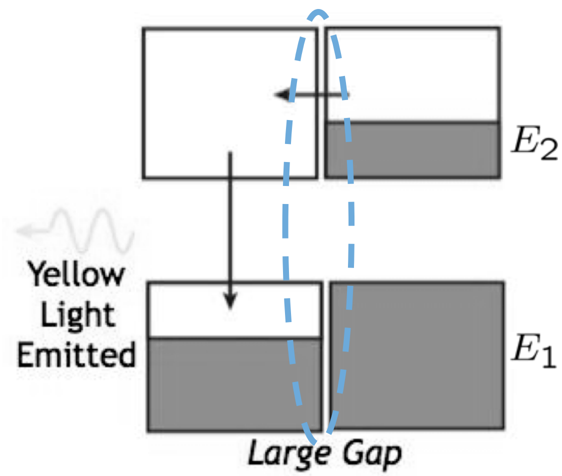
- What is the energy of the photon that is released ?

Quantum mechanics gives us the oscillating dipole,
Maxwell gives us the field !

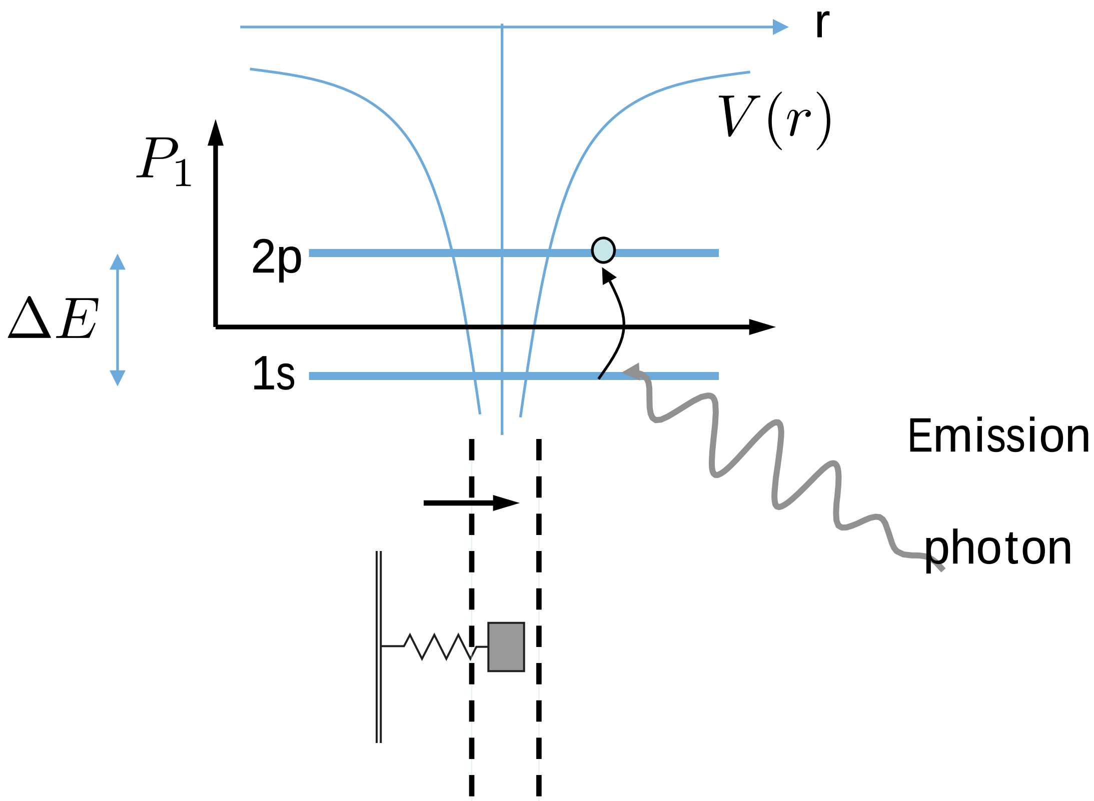
Atomic Transitions

$$\Psi = c_{1s}\phi_{1s}e^{iE_{1s}t} + c_{2p}\phi_{2p}e^{iE_{2p}t}$$





Solar Cells and Photodetectors

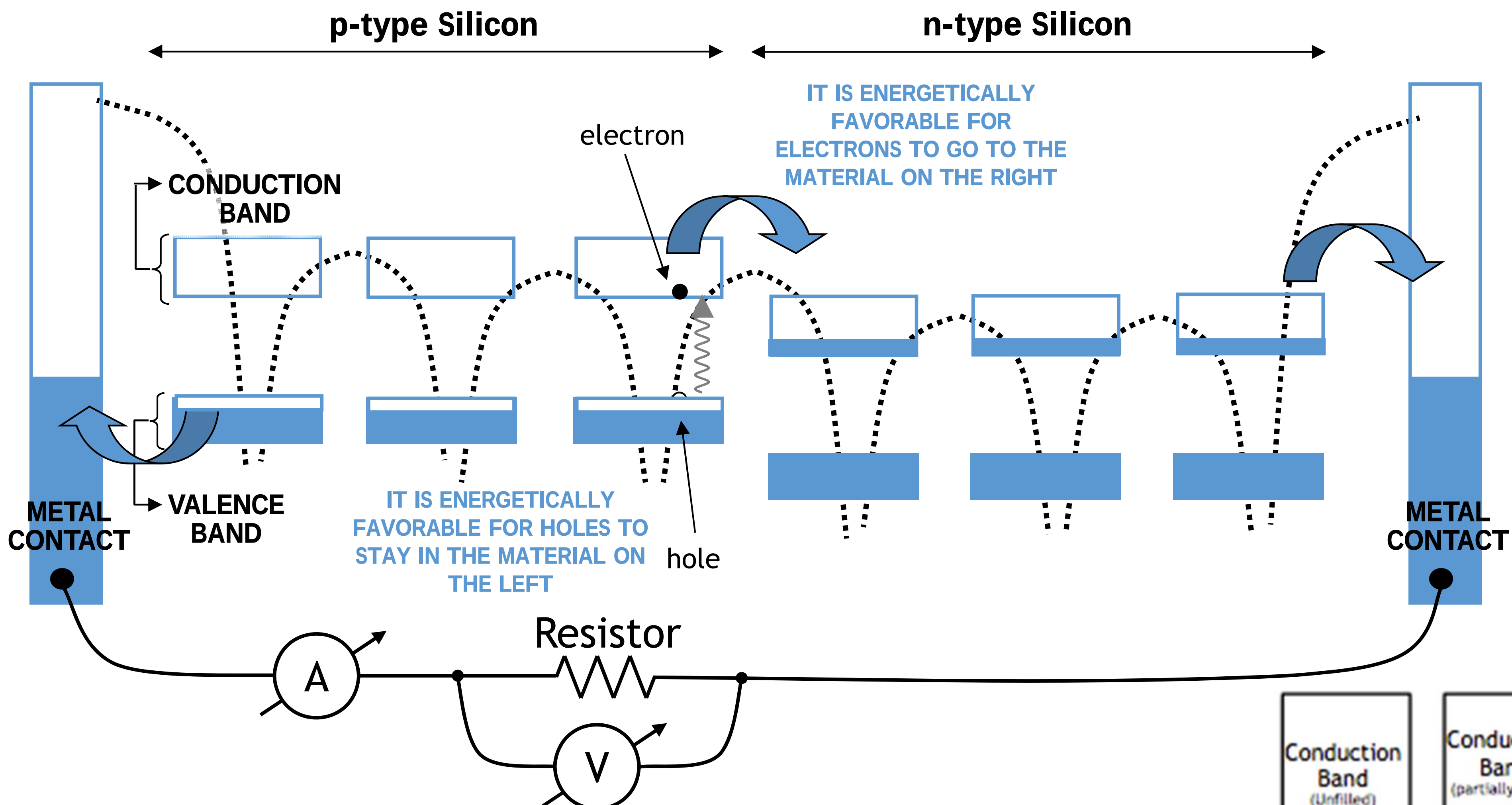


Classical: Oscillating electric field drives charge oscillation

Quantum: Electric field creates superposition of energy states
– which have an oscillating charge density

(junction of two differently doped pieces of the same semiconductors)

Semiconductor Homojunction Solar Cell



Animated Photogeneration