Photons & Atoms

13.11.2012
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photons are interacting with electrons

generation of
- laser
- thermal
- luminescence

} light

Quantum mechanical particles (electrons of free mass m_0) subject to a potential $V(\bar{r},t)$ is governed by a complex wavefunction $\Psi(\bar{r},t)$ that satisfies the Schröedinger's equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\bar{r},t)+V(\bar{r},t)\Psi(\bar{r},t)=-j\hbar\frac{\partial\Psi(\bar{r},t)}{\partial t}$$

Born Postulate: probability of finding the particle in a volume dV, surrounding the position of $\bar{r}$, within the time interval between t and $t+dt$ is

$$p(\bar{r},t)\,dV\,dt = |\Psi(\bar{r},t)|^2\,dV\,dt$$

If the potential is not time varying, i.e., $V(\bar{r})$ the energy levels of the particle is determined by the separation of variables:

$$\Psi(\vec{r},t) = \underline{\underline{\psi(\vec{r})}}\exp\left[j(E/\hbar)t\right],$$ where

$\psi(\vec{r})$ satisfies the time-independent Schroedinger's eqn.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\bar{r})+V(\bar{r})\,\psi(\bar{r})=E\,\psi(\bar{r})$$

similar to Helmholtz Equation

E's are eigenvalues

$\psi(\bar{r})$ are the eigenfunctions

Example:

lets solve the Schrödinger's Eqn. by using the separation of variables: (1-D)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V\,\psi(x,t)=-j\hbar\frac{\partial\psi(x,t)}{\partial t}$$

$$\psi_{(x,t)}=\varphi(x)\cdot\phi(t)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}\cdot\phi(t)+V\,\varphi(x)\cdot\phi(t)=-j\hbar\frac{\partial\phi(t)}{\partial t}\cdot\varphi(x)$$

divide both sides by $\varphi(x)\phi(t)$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}\cdot\frac{1}{\varphi(x)}+V}_{\text{is a function of } x \text{ only}} = \underbrace{-j\hbar\frac{\partial\phi(t)}{\partial t}\frac{1}{\phi(t)}}_{\text{a function of } t \text{ only}}$$

This is only possible when both sides are equal to a constant.

Take the constant as E

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2}\cdot\frac{1}{\varphi(x)}+V=E \qquad -j\hbar\frac{\partial\phi(t)}{\partial t}\frac{1}{\phi(t)}=E$$

$$\frac{\partial^2\varphi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(E-V)\varphi(x)=0 \qquad \frac{\partial\phi(t)}{\partial t}+\frac{1}{j\hbar}E\phi(t)=0$$

$$\frac{\partial^2\varphi(x)}{\partial x^2}-\frac{2m}{\hbar^2}(V-E)\varphi(x)=0$$

$$\left(D^2 - \frac{2m}{\hbar^2}(V-E)\right)\varphi(x) = 0$$

$$D = \mp\sqrt{\frac{2m}{\hbar}(V-E)}$$

$$K = \pm\sqrt{\frac{2m}{\hbar}(V-E)}$$

$$\varphi(x) = B e^{kx} + C e^{-kx}$$

$$\frac{\partial \phi(t)}{\partial t} - j\frac{E}{\hbar}\phi(t) = 0$$

$$\left(D - j\frac{E}{\hbar}\right)\cdot\phi(t) = 0$$

$$D = j\frac{E}{\hbar}$$

$$\phi(t) = A\, e^{j\frac{E}{\hbar}t}$$

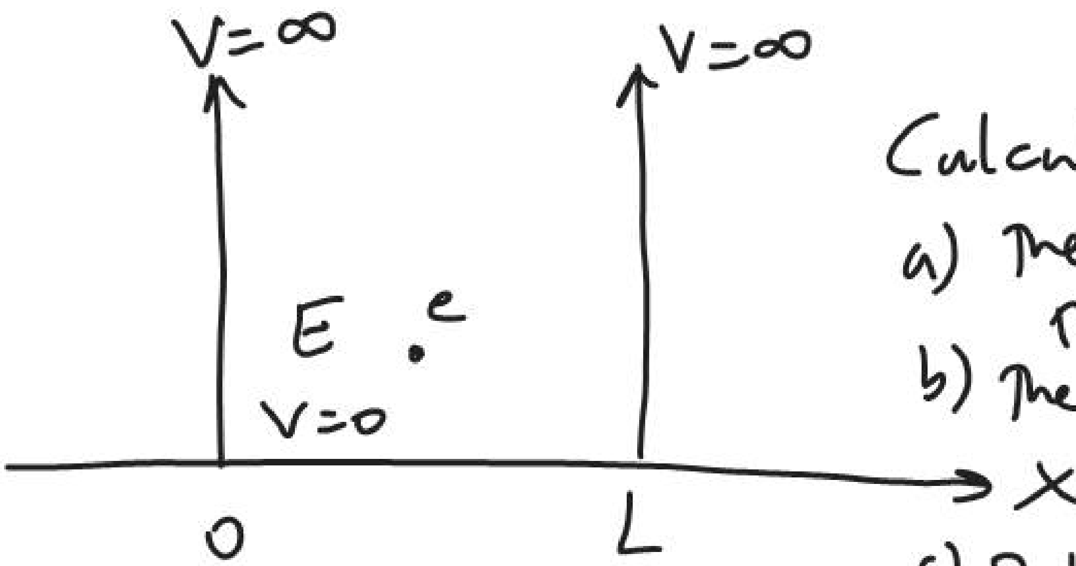
$$\Psi(x,t) = \varphi(x)\cdot\phi(t)$$

$$\Psi(x,t) = \left(Be^{kx} + Ce^{-kx}\right)A\cdot e^{j\frac{E}{\hbar}t}$$

$$\frac{E}{\hbar} = w \Rightarrow E = \hbar w = \frac{h}{\cancel{2\pi}}\cdot\cancel{2\pi}\nu$$

$$\boxed{E = h\nu}$$

Example a 1-D quantum well (no time dependence)



Calculate

a) The wavefunction of the electron

b) The energy states that electron can take

c) Determine where the electron is

$V=\infty$ at $x=0, L$

$V=0$ at $0<x<L$

$$\frac{\partial^2 \psi(x)}{\partial x^2} - \frac{2m}{\hbar^2}(V-E)\,\psi(x) = 0$$ time independent part

in the well $V=0$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2} E \, \psi(x) = 0$$

$$\left(D^2 + \frac{2m}{\hbar^2} E\right) \psi(x) = 0$$

$$D^2 = -\frac{2m}{\hbar^2} E$$

$$\sqrt{\frac{2m}{\hbar} E} = k$$

one of the solutions that satisfy is :

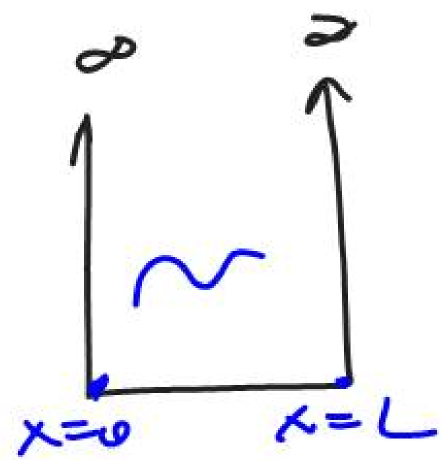
$$\psi(x) = A \sin kx + B \cos kx$$

we know that at $x = 0$ and L ψ should be zero.

(electron cannot be outside of the infinite well

$$B = 0$$

$\psi(x) = A \sin kx$



$\psi(L) = 0$

$\psi(L) = 0 = A \sin kL$

$\sin kL = 0$

$\underline{kL = n\pi}$ — $k = \frac{n\pi}{L}$

$n = 0, 1, 2, \ldots$

n: quantum number

$$\frac{\sqrt{2mE}}{\hbar} = k \qquad \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}$$

$$2mE = \frac{\hbar^2\pi^2}{L^2} n^2$$

$$\boxed{E = \frac{\hbar^2\pi^2}{2mL^2} n^2}$$

energy is quantized

$n=1 \quad E_1 = \frac{\hbar^2\pi^2}{2mL^2}$

$n=2 \quad E_2 = \frac{2\hbar^2\pi^2}{mL^2}$

$\vdots$

$$\psi(x) = A \sin kx = A \sin \frac{n\pi}{L} x$$

since electron is somewhere in the well:

$$\boxed{\int_0^L \psi_{(x)}^* \cdot \psi_{(x)} \cdot dx = 1}$$

$$p(x) = |\psi|^2$$

normalization

$$\int_0^L A^2 \sin^2 \frac{n\pi}{L} x \, dx = 1$$

$$\int_0^L A^2 \left(\frac{1 - \cos \frac{2n\pi}{L} x}{2} \right) \cdot dx = 1$$

$$\sin^2 x = \frac{1 - \cos 2x}{2}$$

$$\int_0^L \frac{A^2}{2} dx - \frac{1}{2} \cancel{\int_0^L A^2 \cos \frac{2n\pi}{L} x \, dx} = 1$$

$$\sin^2 x + \cancel{\cos^2 x} = 1$$

$$- \quad \cancel{\cos^2 x} - \sin^2 x = \cos 2x$$

$$\sin^2 x = \frac{1 - \cos 2x}{2}$$

$$\frac{A^2}{2} L = 1 \qquad A^2 = \frac{2}{L} \qquad A = \sqrt{\frac{2}{L}}$$

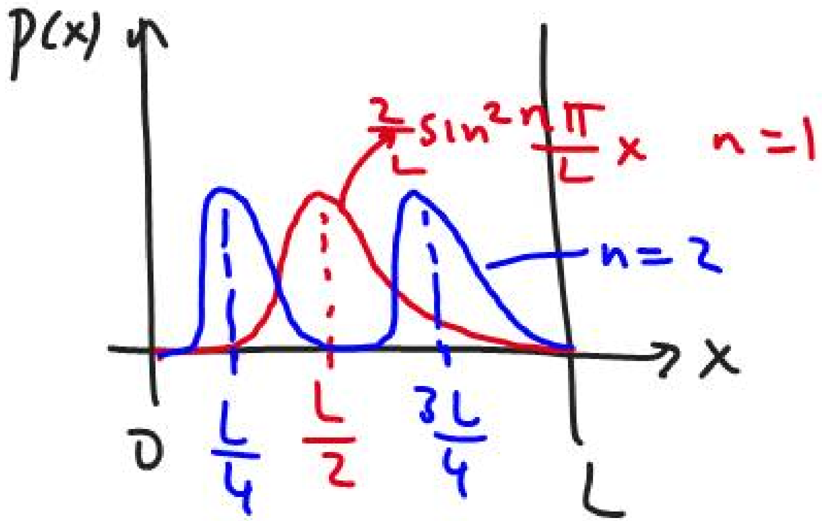
$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$ wavefunction (eigenfunction)

$P = \psi^*_{(x)} \cdot \psi_{(x)}$ The Probability Distribution Function (PDF)

$\psi^2(x) = \frac{2}{L} \sin^2 \frac{n\pi}{L} x$

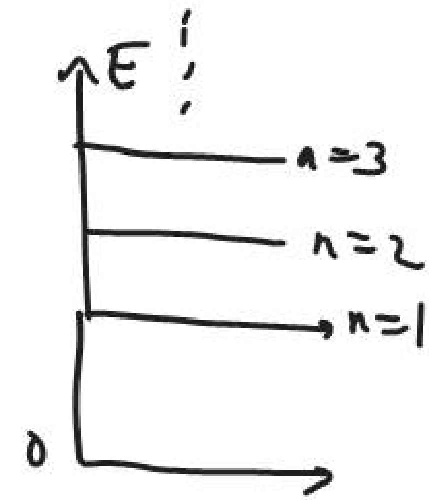
$n=1 \propto \sin^2 \frac{\pi}{L} x$

at $x=0, x=L \Rightarrow 0$

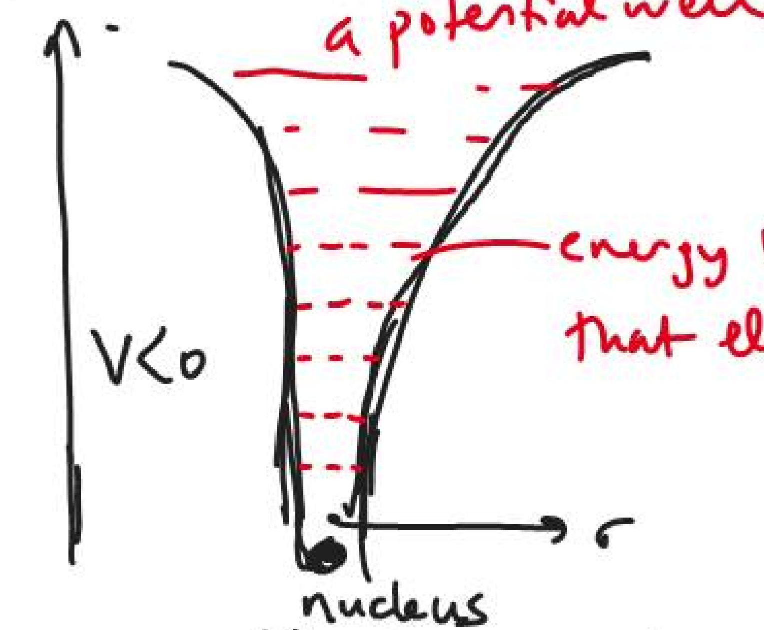


$n=2 \propto \sin^2 \frac{2\pi}{L} x$

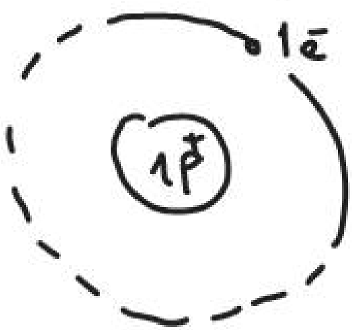
$x=L$



an Atom



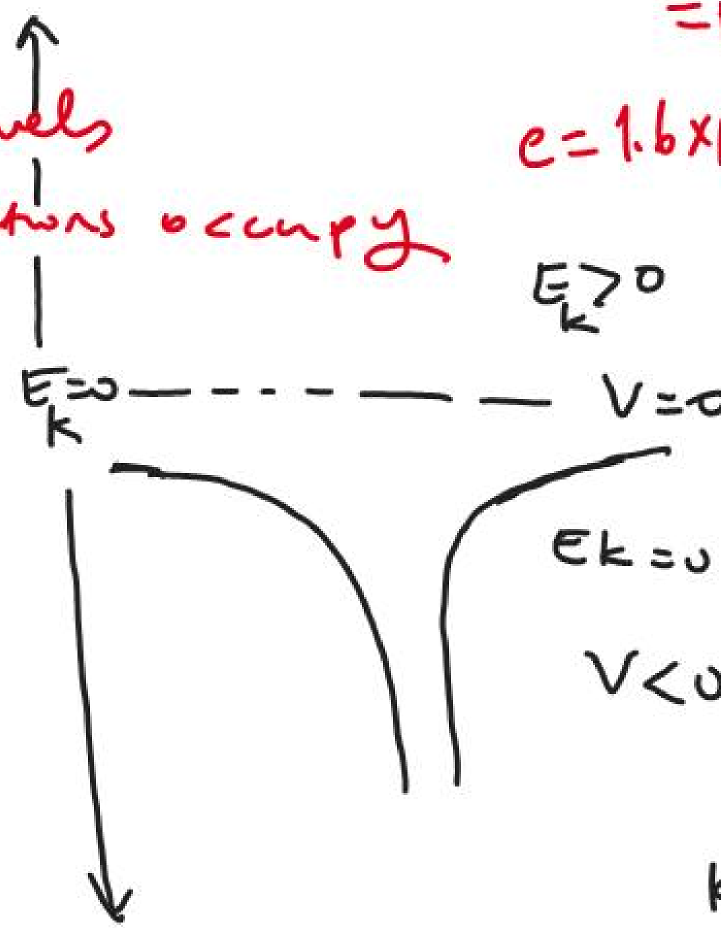
a Hydrogen atom



$$V(\bar{r}) = -\frac{Ze^2}{r}$$

Z = atomic number = # of protons

$e = 1.6 \times 10^{-19}\,C$



$E_k + V = $ Energy Total

E_k: Kinetic energy

V: potential energy

A hydrogen atom's wavefunction can be calculated using the Schroedinger's eqn.

$$\Psi_{n\ell m}(r,\theta,\phi) = \underbrace{R_{n\ell}(r)}_{\text{Laguerre's functions}} \underbrace{\Theta_{\ell m}(\theta)}_{\text{Legendre's functions}} \underbrace{\Phi_{m}(\phi)}_{\text{phase function}}$$

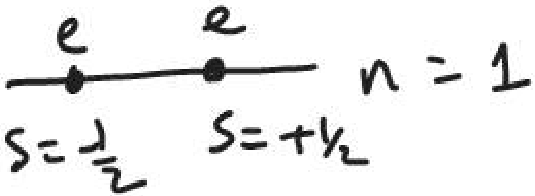
$n = 1, 2, 3, \ldots$ principal quantum number

$\ell = 0, 1, 2, \ldots (n-1)$ azimuthal quantum number

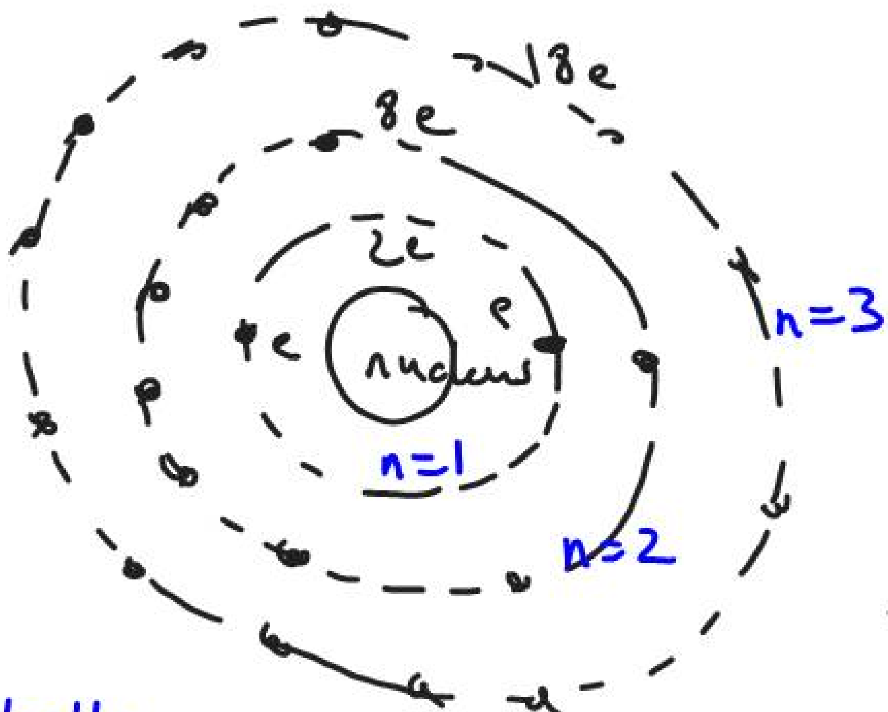
$m = 0, \mp 1, \mp 2, \ldots \mp \ell$ magnetic quantum number

Pauli exclusion Principle: no two electrons have the same quantum numbers

s = spin quantum number $= \mp \frac{1}{2}$



An energy level can be occupied by <u>at most</u> 2 electrons of opposite spin numbers.



Shells, $\underline{n}$

$n = 1$

$l = 0, 1, 2, \ldots (n-1)$

$n = 1$, $l = 0$

$m = 0, \mp 1, \mp 2, \ldots \mp l$, $m = 0$

$n=1$	$l=0$	$m=0$	$= 2e \rightarrow 1s^2$	
$n=2$	0	0	2e	$8e^{2s^2 2p^6}$
	1	-1	2e	
		0	2e	
		1	2e	

$1s^2 2s^2$

$1s^2 2s^2 2p^6$

$1s^2 \underbrace{2s^2 2p^2}_{\text{valence electrons are 4}} \Rightarrow$ Group $\boxed{IV}$ in Periodic Table

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} - -$

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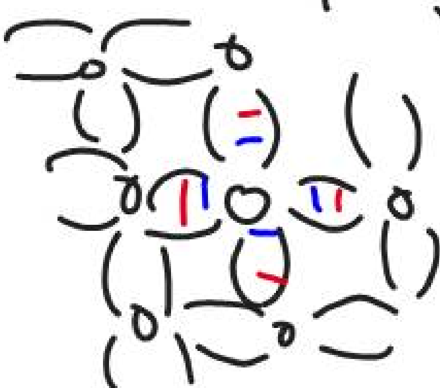
ex Si has $Z = 14$

$1s^2 2s^2 2p^6 \underbrace{3s^2 3p^2}_{\text{4 valence electrons}}$



- $\overset{+2}{Na}\,\overset{-1}{Cl_2}$

  Ionic bond
- Metallic bond
- covalent bond