Sequence (1)

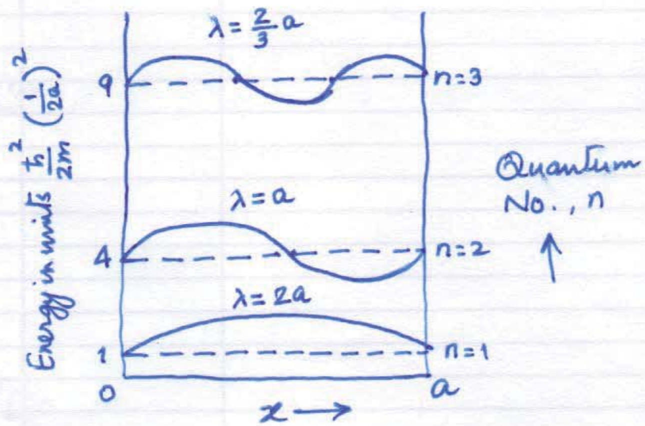
# Energy lev's in 1-dim

Starting from

$$H\psi_n = E\psi_n$$

and converting that to Schrödinger's eqn

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = E_n\psi_n$$




The B.C. of such potential well case insists that

$$\psi_n(0) = 0 = \psi_n(a)$$

This is satisfied only if $\psi$ is a sinusoidal fn with an integral multiple of $\lambda/2$ in the extent of a, i.e.,

$$a = n\frac{\lambda_n}{2} \quad \& \quad \psi_n = A\sin\left(\frac{2\pi}{\lambda_n}x\right)$$

From this form of $\psi_n = A \sin\left(\frac{n\pi}{a}x\right)$ by substituting $\frac{\lambda}{2} = \frac{a}{n}$

$$\frac{d\psi_n}{dx} = A\left(\frac{n\pi}{a}\right)\cos\left(\frac{n\pi}{a}x\right)$$

$$\frac{d^2\psi_n}{dx^2} = -A\left(\frac{n\pi}{a}\right)^2 \sin\left(\frac{n\pi}{a}x\right) = -\left(\frac{n\pi}{a}\right)^2 \psi_n$$

From the Schrodinger's eq.$^{n}$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = E_n\psi_n$$

$$\Rightarrow -\frac{\hbar^2}{2m}\cdot -\left(\frac{n\pi}{a}\right)^2\psi_n = E_n\psi_n$$

$$\Rightarrow \quad E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

Considering a 3-dim cubic cell,
Schrödinger's equ.$^n$ becomes

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2 \psi_k(\vec{r}) = E_k \psi_k(\vec{r})$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_k(\vec{r}) = E_k \psi_k(\vec{r})$$

where $$\psi_n(\vec{r}) = A \sin\left(\frac{\pi n_x}{a} x\right) \sin\left(\frac{\pi n_y}{a} y\right) \sin\left(\frac{\pi n_z}{a} z\right)$$

where $n_x, n_y, n_z$ are integers, +ve

B.C. are

$$\psi(x+a, y, z) = \psi(x, y, z)$$
$$\psi(x, y+a, z) = \psi(x, y, z)$$
$$\psi(x, y, z+a) = \psi(x, y, z)$$

and the 3-dim wavefn takes the form

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$$

where,

$$k_x = 0, \pm \frac{2\pi}{a}, \pm \frac{4\pi}{a}, \dots$$

$$k_y = 0, \pm \frac{2\pi}{a}, \pm \frac{4\pi}{a}, \dots$$

$$k_z = \dots$$

meaning any component of $\vec{k}$ is of the form $\frac{2n\pi}{a}$ where $n$ is +ve or -ve

Let's check if it satisfies the BC

$$\psi(x+a, y, z) = \psi(x, y, z)$$

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} = e^{i(k_x x + k_y y + k_z z)}$$

$\Rightarrow \quad e^{i[k_x(x+a)]}$ has to be $e^{ik_x x}$

Now, $\quad e^{i[k_x(x+a)]} = e^{i\frac{2\pi n}{a}(x+a)}$

$$= e^{i\frac{2n\pi}{a}x} \; e^{i\frac{2\pi n}{a}a}$$

$$= e^{i\frac{2n\pi}{a}x} \; e^{i2n\pi}$$

$$= e^{i\frac{2n\pi}{a}x}$$

$$= e^{ik_x x}$$

On substituting

$$\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$$

in the Schrödinger eq$^n$, we get

$$E_k = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

From the [illegible] we have

$$k_x = \frac{2\pi n_x}{a}$$

$$k_y = \frac{2\pi n_y}{a}$$

$$k_z = \frac{2\pi n_z}{a}$$

where $n_x, n_y, n_z$ are integers.

Since there is one $\vec{k}$-state for every distinct choice of integer quantum numbers, $n_x, n_y, n_z$, the volume per $\vec{k}$ state would be

$$\frac{2\pi}{a} \times \frac{2\pi}{a} \times \frac{2\pi}{a} = \frac{(2\pi)^3}{a^3} = \frac{(2\pi)^3}{V}$$

where $V = a^3$ is the 3-D vol. of the crystal of side $a$.

⇒ The numbers of levels/ states for 3-D in a $\vec{k}$ - space of $\Delta\vec{k}$ elemental width

$$= \frac{a^3}{(2\pi)^3} \Delta\vec{k}$$

From Pauli Exclusion Principle each such level may be occupied by 2 electrons of opposite spins, hence # states

$$= \left( \frac{a^3}{(2\pi)^3} \Delta\vec{k} \right) \times (2) \text{ spin}$$

⇒ The number of states per unit vol. in 3-D

$$= \frac{2}{(2\pi)^3} (\Delta\vec{k})$$

In general, for p-dimension, the generalized expression is

$$\text{Number of states per unit vol.} = \frac{2}{(2\pi)^p}(\Delta\vec{k})$$

Here we are mainly interested in energy states so we need to transform from $\vec{k}$-space to E-space and for that the following relation comes handy that:

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}$$

$$\text{Energy} = \frac{p^2}{2m} = \frac{1}{2}mv^2$$

$p$ is $\hbar k$

$$\Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

and we can express

$$N(E)\,dE = \frac{2}{(2\pi)^p}(\Delta\vec{k})$$

To find it out we need to calculate $\Delta\vec{k}$ in 1,2,3-D space in terms of E-space.

From the relation for p-dimensional # states per unit vol. $= \frac{2}{(2\pi)^p}(\Delta\vec{k})$

In 3-D case

$\Delta\vec{k}$ (The 3-D infinitesimal vol. element) is in fact vol. of a spherical shell

$$\Rightarrow \Delta\vec{k} = 4\pi k^2 dk \qquad \text{(ref. fig IV-1a-c)}$$

In 2D- case

$\Delta\vec{k} = (2\pi k)dk$ area element of ring of radii k and k+dk

and in 1-D case (The line element having +ve and -ve sides on the line)

$$\Delta\vec{k} = 2dk$$

Hence from $E(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}$

$$\Rightarrow \quad k = \sqrt{\frac{2m^* E}{\hbar^2}}$$

and therefore

$$dk = \sqrt{\frac{m^*}{2}}\,\frac{1}{\hbar}\,\frac{1}{\sqrt{E}}\,dE$$