

Lecture-2

"એવો રૂપ ને કરીયા હશે!"

In Lecture 1 we discussed about definition of the Reciprocal scaled lattice and we made a comparison between this construction and a relation that occurs b/w Time & Frequency in the Fourier Transform of function that depend on Time and Frequency.

So, There can be a question in our mind.

~~Q~~ when you consider a function of time and the function is periodic of some period ' T '. You simple define the frequency as $\frac{1}{T}$ (inverse of ' T ')

In the case of a crystal, that is periodic in SPACE. where the periodicity along first direction with a period equal to a_1 .

& in 2nd direction. a_2 & so on.

Q Do why don't we take ^{simply} $b_1 = \frac{1}{a_1}$ & $b_2 = \frac{1}{a_2}$?

Ans we can not do it because the characteristic vectors of the Lattice a_1, a_2, a_3 are not Mutually orthogonal only in the case where they are mutually orthogonal we can simply take the

$$|b_1| = \frac{1}{|a_1|} \text{ & so on.}$$

we shall see an example to understand it.

\therefore we must in general consider the definition of 'b' vectors as

$$b_1 = \frac{a_1 \wedge a_3}{T_L} \quad \text{as seen in Reciprocal Lattice}$$

Ex. we take any vector ℓ , which has integer coefficients in the direct lattice.

$\therefore \ell \rightarrow$ translational vector in Direct Lattice

we also take g , i.e "g" is any translational vector of Reciprocal scaled lattice

Then we take the scalar product of $\ell + g$

~~but~~ otherwise we expect the scalar product to be a number. Because ℓ has the unit of length and g has the unit of inverse of length.

But we just use the definition. i.e

$$\ell = m_1 a_1 + m_2 a_2 + m_3 a_3$$

ℓ is linear combination of vectors a_1, a_2, a_3 with integer coefficients $m_1, m_2 + m_3$

$$g = n_1 2\pi b_1 + n_2 2\pi b_2 + n_3 2\pi b_3$$

g is linear combination of the vectors $2\pi b_1, 2\pi b_2, 2\pi b_3$ with integer coefficients n_1, n_2, n_3

If we take scalar product of $\ell + g$

$$l \cdot g = \sum_{i,s=1}^3 m_i a_i \cdot n_s 2\pi b_s = 2\pi \sum_{i,s=1}^3 m_i n_s s_i$$

$$= \boxed{2\pi \sum_{i=1}^3 m_i}$$

Because $s_i = a_1 \cdot b_i \rightarrow a_1 \cdot \frac{(a_2 \wedge a_3)}{\tau_L} = \frac{T_L}{\tau_L} = 1$

$$\begin{cases} a_1 \cdot b_2 \\ a_1 \cdot b_3 \end{cases} = 0$$

$$\therefore l \cdot g = 2\pi \left(\sum_{i=1}^3 m_i n_i \right) = \boxed{2\pi M}$$

where M is an Integer. $\because m_i, n_i$ are integers.

→ Let takes exponential of an Argument

$$\exp[jg \cdot (r+l)] = e^{[jg \cdot (r+l)]}$$

$$\text{i.e. } e^{[jg \cdot (r+l)]} = \cancel{e^{jg}} \cdot e$$

$$\Rightarrow e^{jgr + jgl} \quad \because gl = 2\pi M$$

$$\Rightarrow e^{jgr} \cdot e^{j2\pi M} \quad e^{j0} = \cos 0 + i \sin 0$$

$\therefore M$ is an integer.

This part equals to '1'

$\therefore e^{jg \cdot r} \rightarrow$ we can see that this function is periodical in r .

~~Note~~ $r = \mu_1 a_1 + \mu_2 a_2 + \mu_3 a_3$ with $0 \leq \mu_i \leq 1$

where r belongs to the cell of the side a_1, a_2, a_3

in \mathbb{R} in direct lattice

$e^{jg \cdot r}$ is periodic for any value of (l) chosen in $[jg(r+1)]_e$

Then we have the possibility of using $e^{jg \cdot r}$ to obtain a Fourier expansion of some other function that is periodic.

∴ for any function F i.e periodic in the lattice i.e ' F ' calculated at $(r+l)$

$$\Rightarrow F \rightarrow F(r+l)$$

$$\boxed{F(r+l) = F(r)}$$

We should remember that ' F ' is a periodic function in non-orthogonal space. But it is still periodic

The following holds

$$\therefore \boxed{F(r) = \sum_g F_g \exp(jg \cdot r)} \rightarrow \text{Fourier expansion in non-orthogonal space}$$

Q What is ' g '?

We remember, we must sum over the vector ' g

' g ' is a vector is a linear combination with integer coefficients of the characteristic vectors of the Reciprocal scaled Lattice

$$\boxed{g = n_1 2\pi b_1 + n_2 2\pi b_2 + n_3 2\pi b_3}$$

of ' g '

So we have to sum over the coefficients and the coefficients are integers. n_1, n_2, n_3

$$\therefore \sum_g = \sum_{n_1, n_2, n_3} \quad (\text{A triple sum})$$

where (n_1, n_2, n_3) are Integers which go from $\pm \infty$ to $\pm \infty$

Q What is the form of F_g ?

$$(F_g) = \frac{1}{V_L} \int_{T_L} F(r) \exp(-ig \cdot r) d^3r$$

Fourier This typical form of Fourier coefficient
coefficient

Fourier transform of original

function over a

period of V

period of V

2 Here the period of V is an elementary

cell so the Integral should be carried over
volume (V_L) of the elementary cell. It doesn't really
matter of which ~~particular~~ cell. Because of the
periodicity of original function $F(r)$.

$$\text{i.e } F(r+l) = F(r) \rightarrow \text{Periodic function}$$

* we may do the same process of finding
Fourier coefficients in reverse. It may happen
that we may have to deal with functions that are
periodic in scaled Reciprocal lattice.

and they are periodic with respect to (k)

Reciprocal scaled Lattice:

$$K = v_1 2\pi b_1 + v_2 2\pi b_2 + v_3 2\pi b_3 \quad \text{with}$$

$$0 \leq v_i \leq 1$$

From

$$\text{Similarly } \exp[jl \cdot (k+g)] = \exp[jl \cdot k]$$

i.e $\boxed{\phi(k+g) = \phi(k)}$

ϕ is periodic in 'k'

ϕ Reciprocal scaled lattice wave function

'k' is periodic π^3 & so does.

$$\phi(k) = \sum_l \phi_l \exp(jl \cdot k)$$

$$\phi_l = \frac{1}{V_g} \int_{V_g} \phi(k) \exp(-jl \cdot k) d^3k$$

* This explains why we need this type of construction in a lattice

* Now, we start examining an important type of lattice it is important because typical semiconductors which are used in manufacturing electronic devices are based on materials like for instance Silicon, Germanium & Gallium Arsenide whose lattice is of this type.

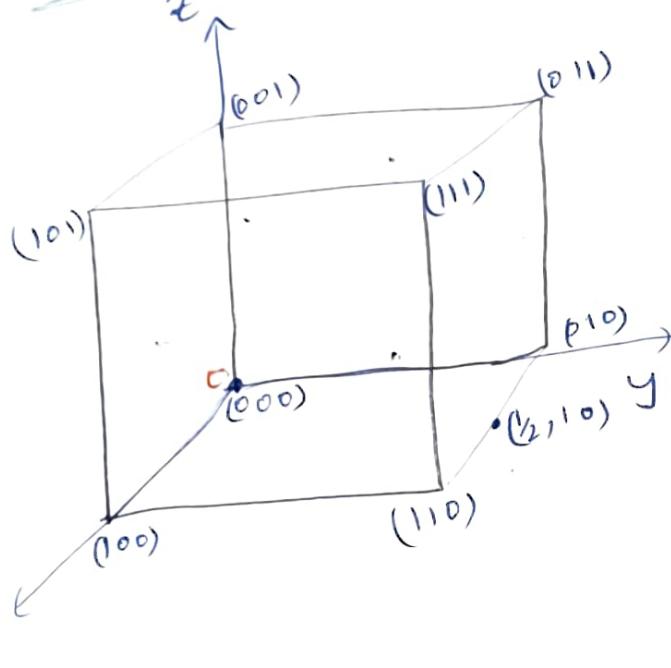
* Now we will explore some properties of so called cubic lattice.

→ In cubic lattice the characteristic vectors are mutually orthogonal and they are also of equal length

→ Now we have to learn to describe Nodes, crystal directions & crystal planes in general but in now this special case of Cubic lattice

Describing Crystal Lattice

(i)



In this cube

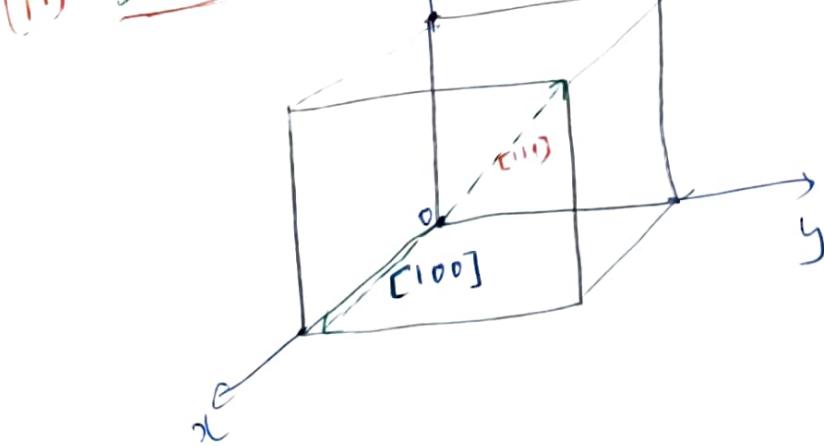
vector a_1 is aligned along x-axis

vector a_2 is aligned along y-axis

vector a_3 is aligned along z-axis

We have chosen that the length of the vectors a_1, a_2, a_3 is equal to one. Then we fix arbitrarily one node as Origin(0) & we define the coordinate points with respect to the origin. Nodes may be negative also.

Describing Crystal Directions



[100]: Crystal Direction from [000] to [100]

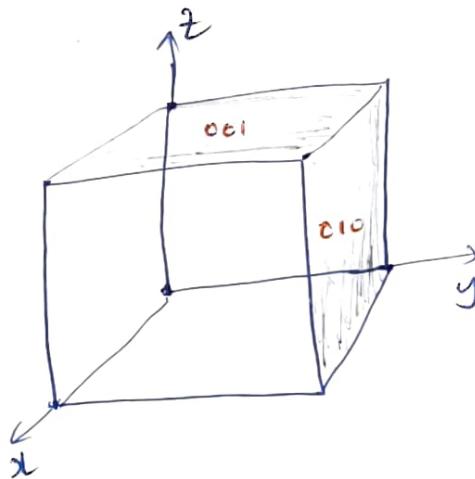
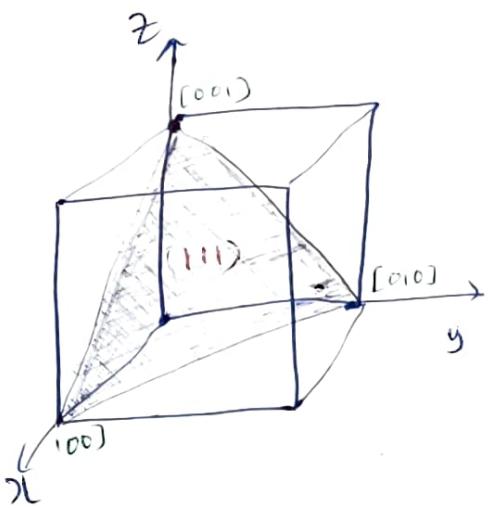
Crystal direction \mathbf{u} obtained by subtracting origin point from end point:

Note: when we find Crystal direction vector which turn out to be fractional then we have to multiple all the coordinates of the vector with an Integer so that they become integer.

Ex:- $[-\frac{1}{2}, -1, 1]$ multiply by 2

$$2 \left[-\frac{1}{2}, -1, 1 \right] \Rightarrow \boxed{(-1, -2, 2)}$$

Crystal planes



→ Good & wise
Reinhardt, EBIT

Here the ~~dar~~ crystal plane has (111)

if we increase the value of 'z' then the inclination of the plane changes and if we keep on increasing then the value of $z \rightarrow \infty$ then the plane may not even touch the z -axis. and it is ^(i.e. infinity & Non integers) not encouraged in crystallography

* So we must find a complicated construction in order to avoid at the same time Non-integers and infinity when we describe crystal planes.

Miller Indices

A crystallographic plane ' Π' ' is identified by the triplet of integers (m_1, m_2, m_3) indicating the intercepts of ' Π ' with the directions of the characteristic vectors. The triplet (rm_1, rm_2, rm_3) with $r \neq 0$ an integer, spans a set of planes parallel to ' Π '.

If M is the largest divisor of m_1, m_2, m_3 then

$$(m'_1, m'_2, m'_3) = \left(\frac{m_1}{M}, \frac{m_2}{M}, \frac{m_3}{M} \right)$$

identifies the plane Π' parallel to Π , and closest to the origin.

If $\underline{\underline{\Pi}}$ ^{here a plane} is parallel to a_i , then m_i and m'_i become infinite. To avoid this the inverse of the triplet's elements are taken: $(\frac{1}{m'_1}, \frac{1}{m'_2}, \frac{1}{m'_3})$

Finally, to avoid fractional numbers the new elements

$(\frac{1}{m'_1}, \frac{1}{m'_2}, \frac{1}{m'_3})$ are multiplied by the least multiple ' N '

of the m'_i that are not infinite:

$$(m''_1, m''_2, m''_3) = \left(\frac{N}{m'_1}, \frac{N}{m'_2}, \frac{N}{m'_3} \right)$$

The elements (m''_i) are the Miller Indices of

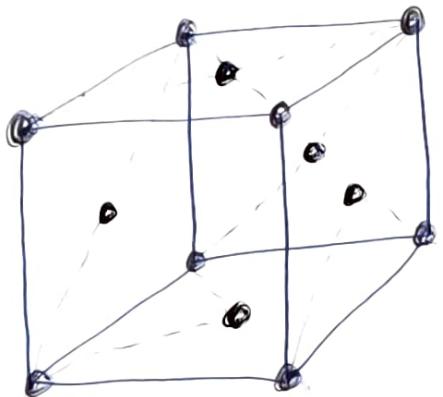
e.g. $(\infty, 2, 4) \rightarrow (\cancel{\infty}, \cancel{2}, \cancel{4}) \rightarrow (0, 1, \frac{1}{2}) \rightarrow (0, 1, 1)$
 Miller Indices

* Now, we have to investigate a more realistic type of crystal.

Q How is silicon made?

Now we discuss FCC lattice

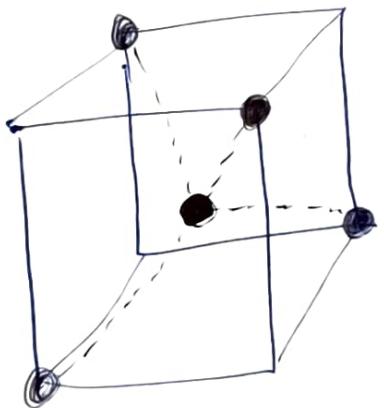
Face centered cubic lattice



we have atoms at each of the vertex of the cube and at the centre of each phase.

$$\therefore 8 + 6 = 14 \text{ atoms}$$

For structure of silicon look into the
Havale Electronics Book.



Face centered cubic structure.

page
(351-353)

Silicon crystal has Face centered cubic structure with

* Now let's try and obtain Wigner-Seitz cell of the silicon atom.

→ In 2D if we take two atoms connected by a line segment then we take a perpendicular axis to the line segment connecting two atoms and passing through centre.

when we go from 2D to 3D

we take a plane i.e. normal to the segment connecting two atoms at the centre of segment itself in this way we form Wigner and Seitz cell of the lattice in 3D.

We can do this also for scaled reciprocal lattice and the Wigner-Seitz cell of reciprocal lattice centered in the origin is called First Brillouin zone.

Brillouin zone is what
Wigner-Seitz cell of the
Reciprocal scaled lattice

L01_fetcoli.pdf
on crystal lattice,
section pdf

Q Why is Brillouin zone very important?

The Brillouin zone is important because it is the interval of periodicity of Reciprocal scaled lattice we have sort of Duality w.r.t. Direct lattice

Weigner Seitz cell

Direct lattice

Brillouin zone

dual

Reciprocal scaled lattice



From PDF

Periodic Potential Energy (in Virtual)

Cartesian coordinates

Follow this PDF for
this part of the lecture

Conservative Forces

Follow by angle
Feynman, EBIT

considering again the case where the cartesian co-ordinates are used. If $F_i = -\frac{\partial V}{\partial x_i}$, where V (potential energy) is a scalar function that depends on the x_1, \dots, x_N co-ordinates only.

Follow the PDF (Periodic potential Energy)

for conservative forces

$$T + V = E$$

T = Kinetic Energy
 V = Potential energy

$$H = \frac{P^2}{2m} + V(r)$$

Hamiltonian function,

The notes are written from the PDF in virtual

Periodic Potential Energy

We will be studying a bit of Analytical Mechanics
For conservative forces

- If we consider a particle or system of particles
For simplicity consider a set of cartesian co-ordinates.
And these particles are subjected to external forces and
interact with each other.
- we have an important case where the Forces
acting on the particles are conservative.
- Remember, the meaning of conservative is this.
There exists a function V that we call Potential energy
this function is a scalar function that depends
only on coordinates, and it has property that if
we take a derivative of this function w.r.t the
coordinate we find a Force (i.e component of force)
that acts along the coordinate.

$$F_i = \frac{\partial V(x)}{\partial x_i}$$

The definition can be extended to the systems
made of many particles, but in our case ~~the~~ we
need only to consider a single particle.

If we have a conservative Force then we have
"conservation of Total Energy".

Conservative forces have energy conservation this is Elementary physics.

T : Kinetic Energy of particle = $\frac{1}{2}mv^2$

V : Potential Energy of particle

In conservative case

$$T + V = E$$

T & V in conservative force depend on time
but their sum is ^{Total Energy is} _{Independent of Time.}

An other issue is for the conservative case we can define momentum of particle as simply

momentum $P = m\dot{x}$

$$V = \dot{x} = \frac{dx}{dt}$$

→ If we are in one dimensional situation the velocity \dot{x}

Remember $P = m\dot{x}$ to hold we need to be in conservative case and we cartesian coordinate system.

→ If we consider a Non conservative Force i.e. the case when particle is subjected to electromagnetic field the momentum (P) is not equal to $(m\dot{x})$

Kinetic Energy instead of $\frac{1}{2}m\dot{x}^2$ in conservative case can be written as $\frac{P^2}{2m}$

→ So this is a one dimensional situation and we have an Hamiltonian function defined in a one dimensional case as

$$H = \frac{P^2}{2m} + V(x) = \dot{x}P - L$$

where
 $L = T - V$
 $= KE - PE$

Here 'H' is also the sum of $KE + PE$

∴ as E Total Energy H Hamiltonian Function also remain constant even though KE (T) PE (V) Separately dependent on Time.

→ When we have one dimensional situation we can relatively express these functions in terms of Graphs.

and we know that

$$KE = \frac{1}{2}m(\dot{x})^2$$

is a Parabola

The PE can be a complicated function.

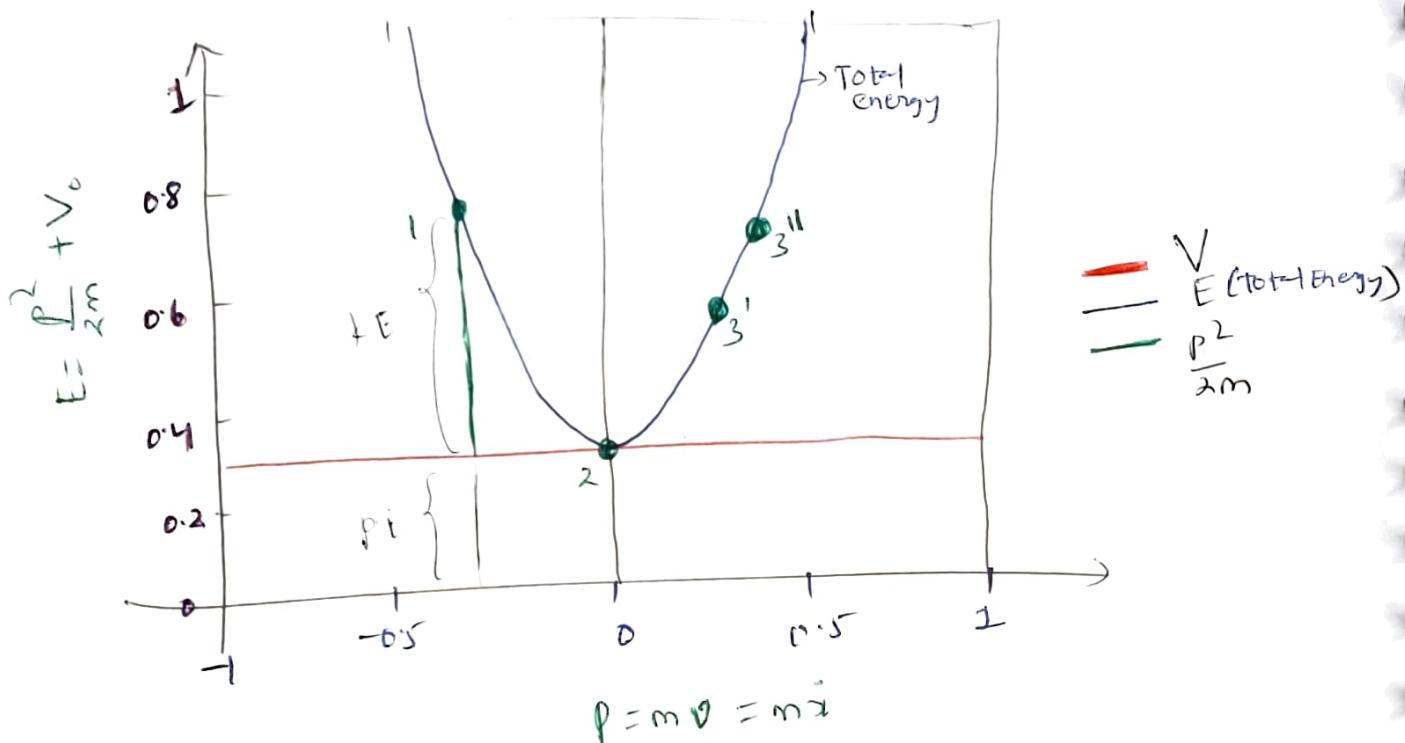
→ when we consider a crystal. We must consider the PE acting on one of the Electron that is inside a Crystal.

Crystal has many electrons in it, those that belong to external shell of the Atoms can move relatively easily those that are in the interior of the Atom don't move much they are attached to the atoms.

∴ we consider only External Electrons and from which we take One Electron and try to represent the type of PE that the Electron is subjected to.

→ It is Intuitive that this P-E is periodic because we know that the Crystal is periodic.

→ So there is a Figure in which we consider a simple case of Free particle and the particle is not subjected to any External Force.



Here the P-E is a straight line i.e. in conservative forces we have

$$F = -\frac{\partial V}{\partial x}$$

if there is no Force in this example. That means derivative of potential Energy is equal to zero.

∴ the potential Energy for a particle not subjected to a Force can be any constant, so we can assume that

$$P-E = V = V_0$$

Case 1

→ At point 1 The momentum of particle is non zero. ∴ we can say that the particle is moving

and we can say that "Total Energy = $K \cdot E + P \cdot E$

↓
green
verticle
Line

distance from
horizontal
axis to
 $P \cdot E$ Line

→ "Remember, if a particle subjected to No Force the velocity of the particle does not change."

So, the Green Dot • represents the Dynamicality of particle until it is subjected an external perturbation that will change its motion.

case 2 ~~BBB~~ energy ~~in atse~~

It is the case where the Momentum of the particle is zero. i.e. Velocity of particle zero

case 3

It is the case of the particle which has some momentum i.e. the if particle is left unperturbed then the velocity of the particle will not change.

So, Again

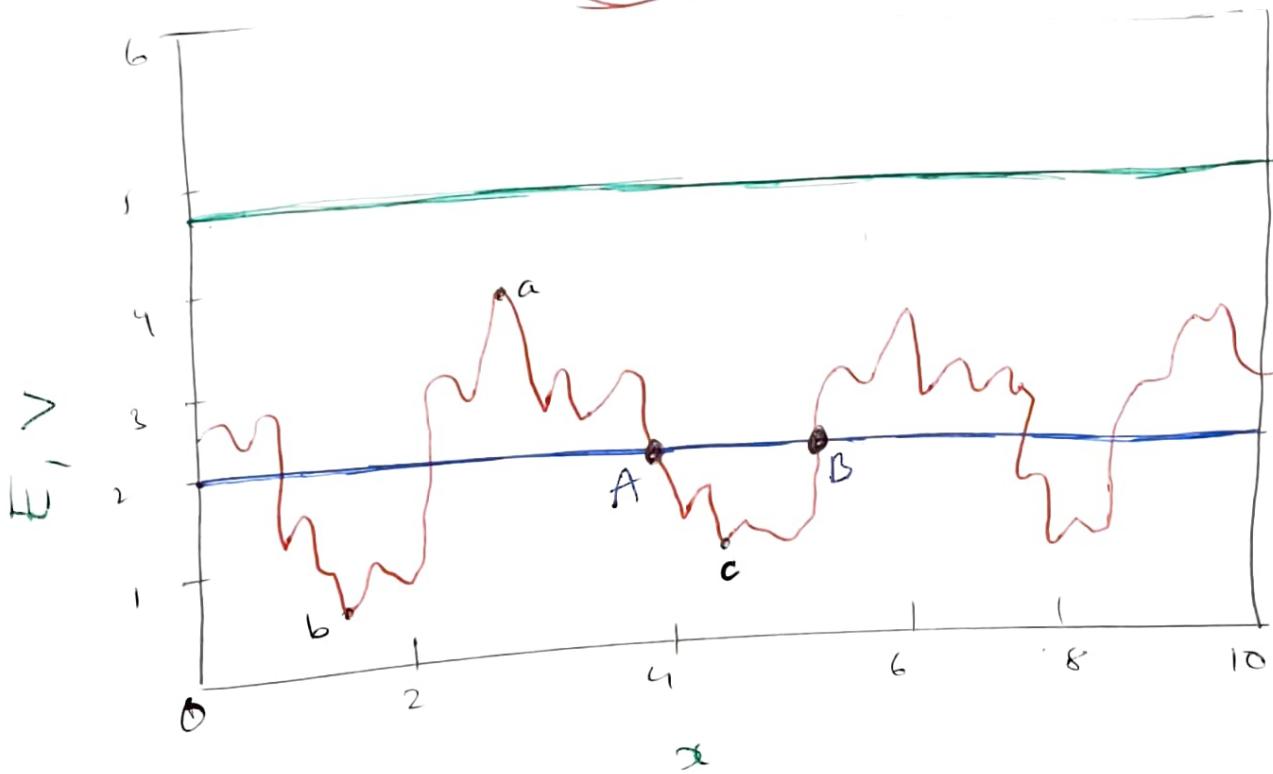
~~Case 3~~ ~~in atse~~
Revanth, EBIT

case 3"

A case where some external perturbation is applied to the particle and it changes its motion and increase its velocity.

Now we go to next figure where we consider a different situation the particle is subjected to Forces and these Forces derive from a periodic potential Energy.

Fig 2



$V(x)$: A periodic Potential Energy

- $V(x)$
- $E > V_{\text{max}}$
- $E < V_{\text{max}}$

\therefore we have a P.E the motion of particle is conservative that means Total Energy is independent of time conserved in Time, i.e. it is constant.

And we have two possibilities in this case we see that that P.E curve has Minima + Maxima

In which the constant representing total energy is larger than the maximum P.E

The constant representing the what does it mean?

It means that $T \cdot E = K \cdot E + P \cdot E$ If $T \cdot E > V_{max}$ then

$K \cdot E$ will be strictly positive never equal to zero.

If $K \cdot E > 0$ then particle will have velocity i.e. always positive

(either always to the right or always to the left)

Who decides whether the particle moves to the Right or the left?

It is decided by the initial conditions of the particle.

The motion of particle, you remember is described by second order differential Equation in Time. So we need two initial conditions one for position & one for velocity.

If the velocity is initially positive and we are considering a situation with Gravitational then velocity will always be +ve. Because $K \cdot E$ in this case can never become zero.

→ 2nd possibility which is not shown in the figure is that the Total Energy is smaller than minimum of Potential Energy. This case is physically impossible at least in classical mechanics.

If $T \cdot E < V$

That means $K \cdot E$ is -ve but this physically impossible because

$$K \cdot E = \frac{1}{2} p v^2$$

as mass should be -ve which is never possible

Intermediate case Blue line

i.e T-E is in between Absolute Maxima & Absolute minima of the Potential Energy which is indicated using Blue line.

If we see two (Black Dots) in the Picture

which represent a segment.

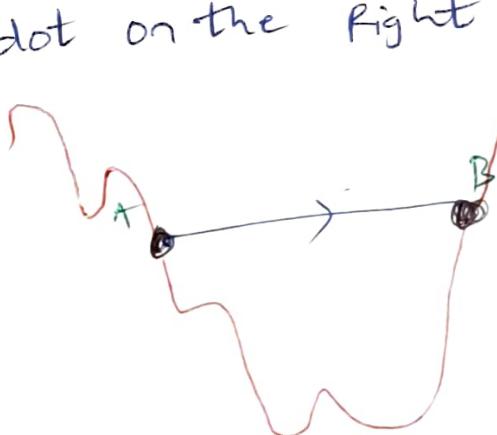
→ Assume that initial conditions of the motion are such the particle is in that segment at time = 0 is going to the right.

As long as the particle is inside the segment

T-E > P.E so we can say that the

particle has some ~~P.E~~ KE & it will continue move to the right.

And at some point the particle will reach the Black dot on the right



At 'B'
The particle has $T-E = P.E$
and at this point the particle cannot proceed to the right.

Because if does move the $T-E < P.E$ and

$K.E$ has to become negative which is

Impossible!

The only possibility of the particle to have a K.E is that it Bounces back to the left and goes to the left.

Here, we have an Inversion of Motion.
and after reaching the Black dot on the Left the particle again Bounces to the ~~left~~ Right.

∴ If the T.E is the Blue line the particle can only stay only in one of the two intervals one i.e marked by two Black dots

∴ The particle will be Oscillatory Motion.

The point is :- Assume if we want to describe the motion of a particle inside a crystal i.e inside a crystal i.e inside a periodic energy using classical mechanics.

It is a very difficult task because form of P.E to which particle is subjected is very complicated.

* Consider the particle is on Green Line of Fig 2
in which particle keeps moving always to the Right (or) always to the Left depending on the initial conditions

→ If the particle is at \textcircled{a} Then the P.E of the particle is the highest. So we have a minimum K.E and the particle is slow and if it moves right the P.E decreases and K.E keeps increasing.

∴ we can say that the velocity of particle changes periodically if it has initial ^{Total Energy} of particle is higher than the Maximum P.E

$$T.E > \cancel{V_{\max}}$$

$$V = P.E$$

Q Now what is the typical Period of P.E in a crystal?

The period is determined by the distances between the atoms. So the typical period is Lattice constant (5 \AA)

Q Do we really need to consider the details of motion of one electron over a distance of 5 \AA ?

Probably not, it would be a waste of time to ~~be~~ describe the details of motion of electrons over one period of the P.E.

∴ The Idea is why don't we take the average of Velocity or Momentum of Electron over a period of lattice.

This is very important and we will try to do calculate Average motion of Electron in a

PERIODIC POTENTIAL and we shall find very very interesting conclusion.

using Classical Mechanics

Atom $\frac{1}{2}m\dot{x}^2$
Period, EBIT



periodic Potential Energy

we consider at

$$V(x+a) = V(x)$$

Here 'a' is the period

and the T.E is strictly large than Maximum of Potential Energy.

$$T.E > V_{max}$$

i.e. $T.E = T = \frac{1}{2}m\dot{x}^2$ then this is also strictly positive and never vanishes.

We also assume that the particle has initial Velocity oriented from Left to Right.

and then it is easy to integrate equation of Motion

In this case because if $K.E + P.E = T.E$, we can rearrange the expression.

$$T + V = E$$

$$K.E + P.E = T.E$$

$$T = E - V$$

$$\frac{1}{2}m\dot{x}^2 = E - V(x)$$

$$\dot{x}^2 = \frac{2}{m} [E - V(x)]$$

$$\dot{x} = \sqrt{\frac{2}{m} [E - V(x)]}$$

$$\frac{dx}{dt} = \sqrt{\frac{2}{m} [E - V(x)]}$$

$$dt = \sqrt{\frac{m}{2}} \frac{1}{\sqrt{E - V(x)}} dx$$

Generally

$$\dot{x} = \frac{dx}{dt}$$

Here we take the motion in x do space

This equation can be used to find the time T taken by the particle to move by one period.

If initial position is s_0

$$T = \sqrt{\frac{m}{2}} \int_{s_0}^{s_{\text{final}}} \frac{dx}{\sqrt{E - V(x)}}$$

$\because V$ is periodic $\frac{dt}{ds} = 0$ that means the time $V(x+a) = V(x)$ necessary for the particle to cross a period of $P.E$ does not depend on the initial position of the particle.

\therefore why don't we calculate the Average Momentum of a particle over period?

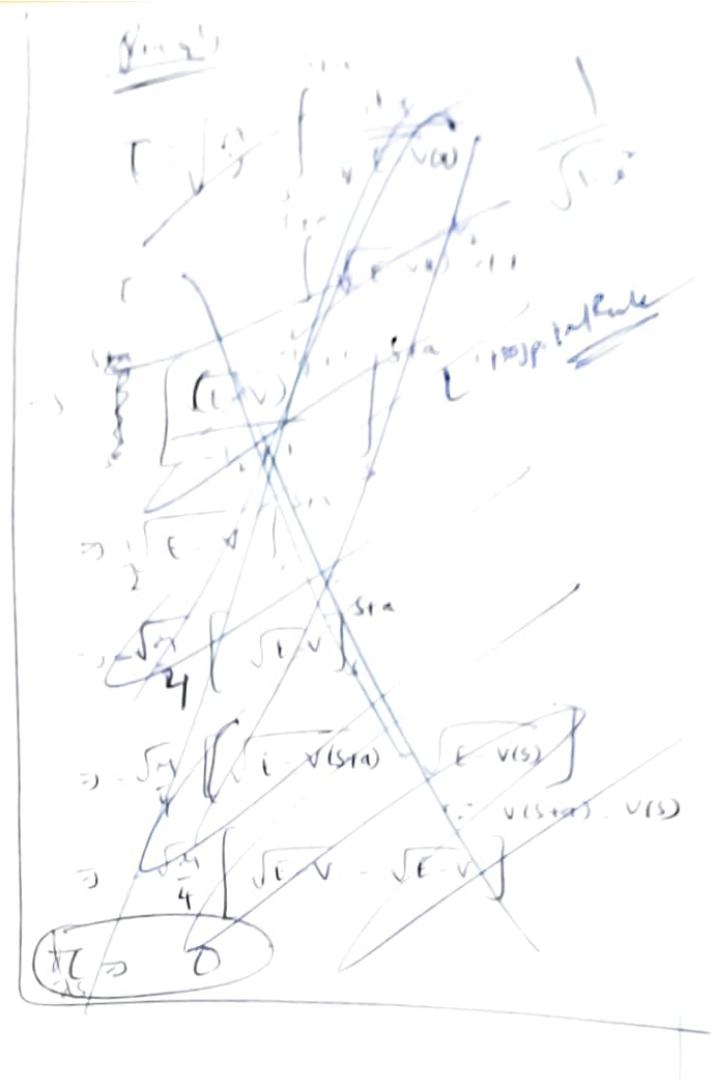
$$p = m\dot{x}$$

P : average momentum

$$P = \frac{1}{a} \int_s^{s+a} p dx$$

$$\Rightarrow \frac{1}{a} \int_s^{s+a} \sqrt{m} \sqrt{E - V(x)} dx$$

$$P = \frac{\sqrt{2m}}{a} \int_s^{s+a} \sqrt{E - V(x)} dx$$



After computing this integral we can see that the

fundamental parameter that P depends on is

Total Energy E which is independent of time.

\therefore we can say P also does not depend on Time

If you consider Average momentum like having free particle. \because for free particle momentum is constant.

Small P $p = m\dot{x}$ → does depend on Time

Capital P $P = \text{average momentum}$ → does not depend on Time because P mostly depends on it which is constant and is independent of Time