

when we take the relation b/w velocity ~~and~~  $\sqrt{\frac{2}{m}} \sqrt{E - V(x)}$

$$\text{i.e. } \dot{x} = \sqrt{\frac{2}{m}} \sqrt{E - V(x)}$$

$$\dot{x} = \left( \pm \right) \sqrt{\frac{2}{m}} \sqrt{E - V(x)}$$

double

So in principle for the same <sup>Total</sup> Energy 'E' we have two possibilities of velocity one +ve and another -ve

+ two average momentum (P)

i.e. Two opposite value of Average momentum correspond to same energy and that means that Energy is even w.r to momentum.

→ So, substantially we found an important result that if we ~~for~~ consider the Average Momentum we find constant of motion like in the case of Free particle.

Average Momentum is Related to Energy only.

'Energy is Even w.r to not only momentum (P) but also Average Momentum (P)'

The only thing that changes is that the relation b/w "Avg. Momentum & Energy" is not Quadratic anymore.

Q What we analyzed till now is it sufficient?

When we consider a semiconductor crystal, which is obviously periodic, so the reasoning of "Periodic potential energy" applies to that. But the device has contacts and we also apply voltages to the contacts. So the issue is that potential energy that acts on the electrons in the crystal is not periodic any more.

### The New Potential Energy

It is the superposition of the P.E imposed by the crystal and the external non-periodic energy imposed by external voltage applied to the semiconductor crystal.

बैरोन, रेड्डी, एडिता, Pexarith, EBIT

However, we can still consider the Average Momentum because the total P.E that exists in a crystal when we apply external voltages to the contacts is made of two contributions. One is periodic energy of atoms and that is very strong and rapidly varying function (i.e. it is the function which is same order as lattice constant)

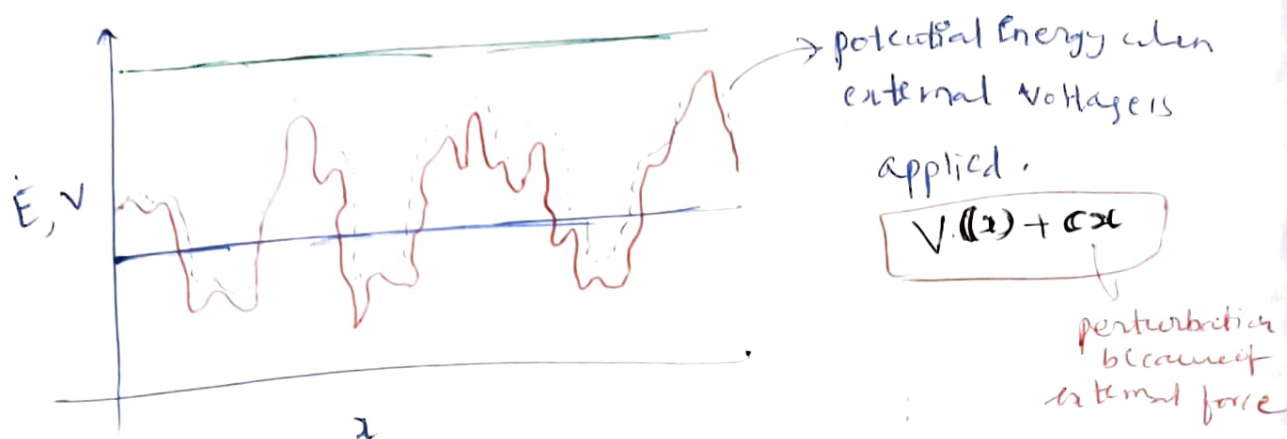
That means forces due to that are enormous.

Forces due to external voltages are small and they are non-periodic.

So we can try to continue on the same line as before that the external forces can be considered as small perturbation.

to the existing Periodic Potential Energy due to crystal.

And we can see it in the figure



→ we assume that we superimpose to the periodic P.E  $V(x)$  a small non periodic potential  $cx$  because of external force

→ And external force produced by  $(cx)$  is a derivative with negative sign, it is like we are adding a constant force due to a linear potential energy. So we consider this as small perturbation.

Then we repeat the calculation by calculating again the average momentum incorporating into the calculation the small perturbation.

Small perturbation is called  $cx$  and the equation it is written as

$$\tau(s) = \sqrt{\frac{M}{2}} \int_{s-a}^{s+a} \frac{dx}{\sqrt{E - V(x) - \delta V(x)}}$$

$$\hat{p}(s) = \sqrt{\frac{2M}{a}} \int_s^{s+a} \frac{\cancel{dx}}{\sqrt{E - V(x) - \delta V(x)}} dx$$



→  $\delta V$  is small wrt  $V$  (i.e.  $\delta V$  is almost constant over a period) and  $\delta V$  has small dependence on  $x$  and  $V(x)$  has strong dependence on  $x$ .

∴ we can consider

$$\sqrt{E - V - \delta V} \approx \sqrt{E - V} \left( 1 - \frac{1}{2} \frac{\delta V}{E - V} \right)$$

Taylor expansion  
~~inside integral~~

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

It is dependent on  $s$  now because  $V(x)$  is not periodic anymore

If  $\delta V$  is almost constant over a period

Then we can replace  ~~$\delta V(x)$~~   $\delta V(x)$  with  $\delta V(s)$ .

Then what we do is calculate the integral.

then we find

$$\hat{P}(s) = P - \frac{1}{a} \delta V(s)$$

perturbed  
average momentum

average  
momentum

~~cancel  $\partial \mathcal{L}$  w.r.t  $\partial x$~~   
Rexanth, EBIT

$$\frac{\hat{P}(s+a) - \hat{P}(s)}{1} = \frac{-\delta V(s+a) + \delta V(s)}{a}$$

The variation of Average Momentum in Time necessary for particle to cross one period

Variation of the external potential energy divided by the Period  $a$ .

→ The relation tells us that in cases where internal force is much weaker than the periodic force and also the external force changes little over a period

→ we can find that change in Average momentum is only due to external perturbation  $(\delta V(x))$

∴ we can say that the average force acting on a particle is external force. This is a very fundamental result because it gives us the possibility to describe the dynamics of a particle inside a crystal by considering only the external forces.

The conclusions we draw are:

Average momentum in place of real momentum  
External Forces instead of Total Forces

provided external forces are constant and not too strong which is the case for the typical operating conditions of semiconductor devices.

Essentially when we use Avg. Momentum ~~in a~~ Crystal (or) Periodic structure

It's like we are considering a particle in free space with an external force.

It's like crystal has disappeared.

→ we also deducted that the energy <sup>Relation b/w</sup> and Average momentum is not Quadratic anymore this is the price we have to pay to eliminate the action of the lattice that acts on the particle. ~~The periodic po.~~

$$P_1 = \frac{1}{a} \int_s^{s+a} p dx = \frac{\sqrt{2m}}{a} \int_s^{s+a} \sqrt{E - V(x)} dx$$

→ all the above analysis is done using ~~Quantum~~ Classical Mechanics.

→ But to obtain appropriate results we should use Quantum Mechanics.

~~\*\*\*~~ Now we jump back to Volume di Elettronica Book

The difference b/w using QM & CM and the interpretation of the results.

→ we shall still use in QM case Average momentum this Average should be considered in time it is a

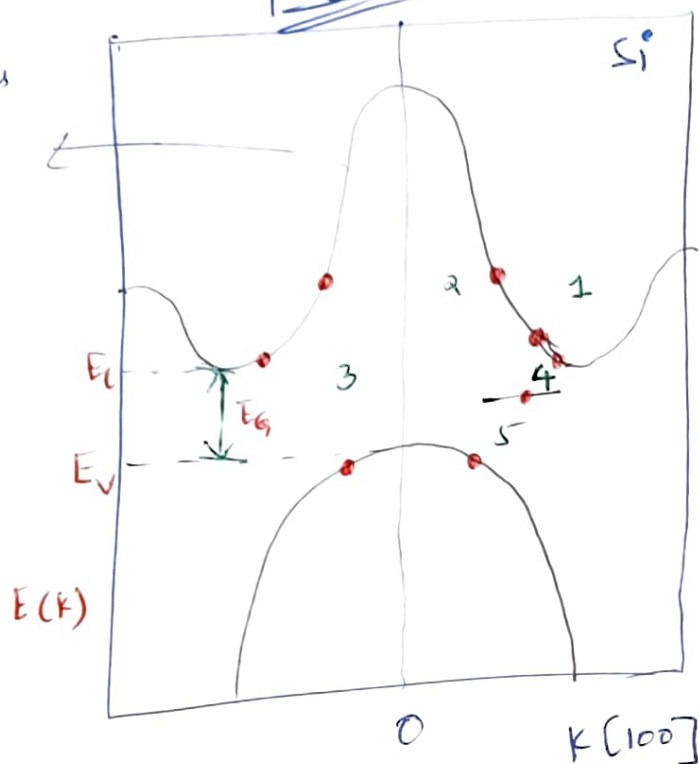
Statistical Average.

→ The Average momentum of a particle in a crystal according to QM is proportional to the vector belonging to the 'scaled reciprocal lattice' that we call  $\mathbf{k}$



Fig. 3

These curves represent energies electrons can have



### Transitions

- 1: Intra-valley
- 2: Inter-valley
- 3: Inter-band
- 4: Intra-band
- 4+5: Trap-assisted

There are several <sup>difference</sup> in the results we obtain using QM. on a crystal w.r.to to the case of a treatment based on classical mechanics.

→ The most important results are:

we shall use Average-Momentum, this (Avg.  $\vec{p}$ ) is not calculated in time, it is a statistical average

→ The Average momentum of a particle in a crystal is proportional to the vector belonging to the scaled Reciprocal Lattice. That we call ' $\vec{k}$ ',

The vector ' $\vec{k}$ ' we studied earlier had only ~~Geometrical~~ Geometrical meaning of a Scaled Reciprocal Lattice.

$\vec{k} \propto$  Avg. momentum of Quantum mechanical treatment of the particle.

→ Because of this then we can expect Energy when we take averages, Energy depends on Avg. Momentum that means  $E$  is expected to depend on  $K$

i.e.  $E = P(x)$  [Energy as a function of ' $P$ ' in classical mechanics]

↓  
This is Replaced by

$E = K(x)$  [Energy as a function of ' $K$ ' in QM treatment]

(This relation is not quadratic).

when we learned SPL (scaled Reciprocal lattice) we also observed periodicity in that case.

So, one of the outcomes of the QM treatment that eventually gives the form of the Relation b/w Energy and Momentum i.e.  $E = K(x)$  shows us that This relation is periodic.

~~So~~ <sup>ee</sup> So Energy is a periodic function of Momentum. <sup>in QM</sup> very different from

"Quadratic term we observed in Classical Mechanics".



→ When we have a periodic function it's sufficient to consider one period. and one period is as we remember

### Brillouin Zone

" $E$  vs  $\vec{k}$  Momentum" from now will be considered in one period (Brillouin zone)

Fig. 3 looks strange but it's one of the results using QM for a crystal lattice

Relation btw

$E$  vs  $\vec{k}$  in QM interpretation is a many valued function.

To each ' $\vec{k}$ ' there correspond many possible energies.

So, we find that it's made of several or infinite branches. ~~can~~ Platz QM for You?

Hahaha.

If we consider one branch at a time it gonna take forever.

∴ The standard method is to select one specific element in space and remember that in cubic lattice

' $k_1$ ' component is aligned with (100) direction

$$k_2 = (010)$$

$$k_3 = (001)$$

→ We simply consider the (100) direction i.e.  $K_1$  and show  
the total energy in vertical direction w.r.to  $K_1$  as shown  
in Fig-3 (Energy as function of  $k$   
&  $K$  is a function of energy/momentum)