

LECTURE 16 (11/03/2024)

{ NOTE: Some portion of nanophotonic remarks, but will be covered later, perhaps after nanomechanics }

52]

Nanomechanics

deals with "motion" \rightarrow based on Newton's laws

NOTE: One of the earliest documented use of "gears"

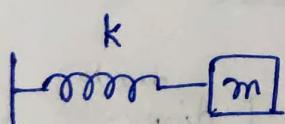
was in the form of
 'Antikythera mechanism' \rightarrow like a gearbox
 to capture motion
 of celestial objects
 (discovered in 1901;
 but first created
 perhaps by ancient Greeks (?)
 in some era
 (in BC))

Nanomechanics

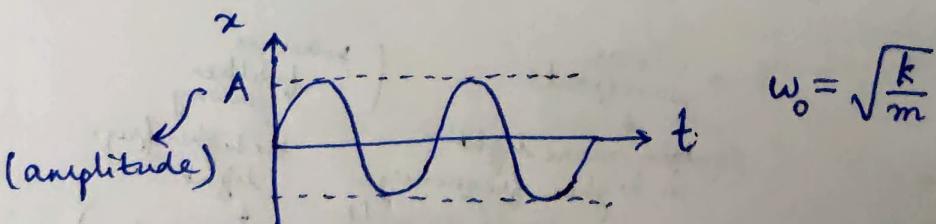
+
 deals with
 nanomaterials
 that help \leftarrow exert
 control } forces
 measure

(usually here, force
 is a springy-like
 oscillatory kind)

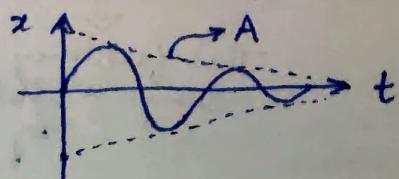
53]



$$\vec{F} = -k\vec{x} \quad (\text{undamped})$$



But for case of damped oscillator: $\vec{F} = -b\vec{v}$



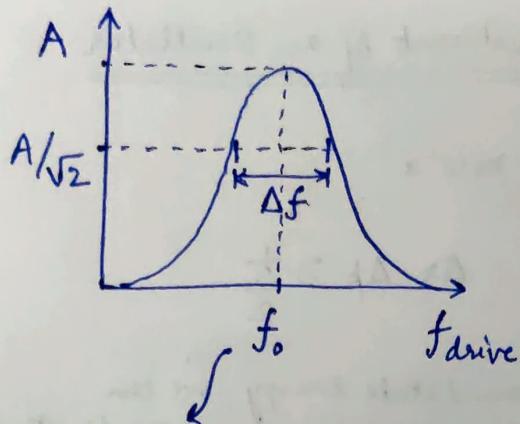
here, amplitude decreases with time

Also freq. is lower than f_0 or w_0

For forced damped oscillation

↓
there is some
driving force
↓

leads to some drive
frequency (f_{drive} or f_d)



$$Q = \frac{km}{b} \quad (\text{called the } Q\text{-factor or "Quality factor"})$$

$$Q = \frac{f_d / \Delta f}{\max A}$$

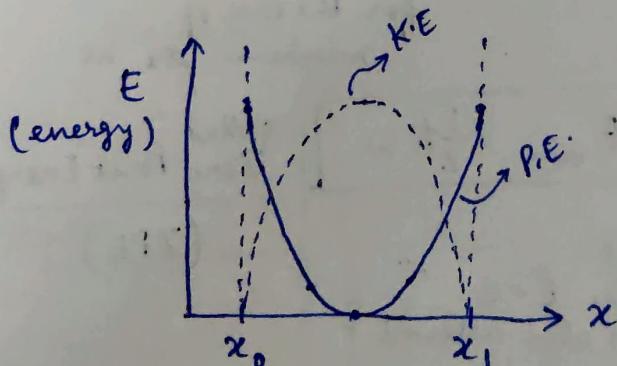
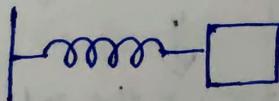
$$= \frac{f_0}{\Delta f}$$

When
drive freq.
matches the
freq. of oscillation

↓
then the amplitude
will be the highest
(i.e. A)

(Δf is defined as the width
of the region at amplitude $\frac{A}{\sqrt{2}}$)

54]

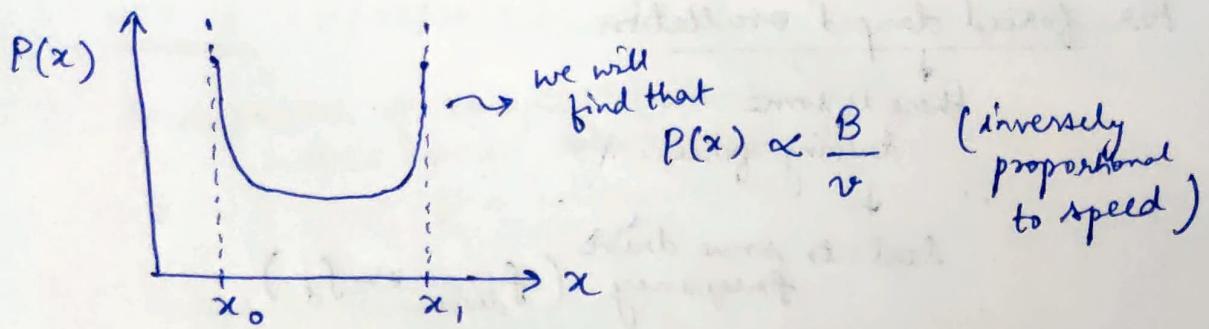


x_0 : Position when
spring is completely
compressed

x_1 : Position when
spring is completely
stretched/expanded

If we consider that we have
an oscillating system like this
and we random measure the x
↓ at arbitrary times

What will be the probability density distribution
of finding some x ?



55] Quantum Mechanical treatment of an oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$$

Now, we know, $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$

If we want to only know the ground state energy, we can approximate it by considering the smallest allowed x and p being Δx and Δp

\therefore Ground state energy, $E = \frac{\Delta p^2}{2m} + \frac{1}{2} m \omega^2 \Delta x^2$

Considering $\Delta x \Delta p \sim \hbar$, and solving $\frac{dE}{d\Delta x} = 0$
(i.e. $\Delta p \sim \frac{\hbar}{\Delta x}$)

We get the value of E for the case of minimum Δx , as:

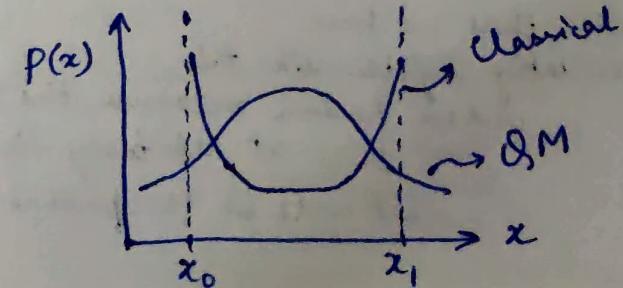
$$E_{\min} = \frac{1}{2} \hbar \omega$$

called
Zero Point Energy

(ZPE)

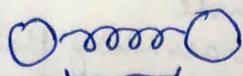
{ which differs from the classical picture, where $E=0$ was also allowed }

Here, it turns out that the probability density distribution is different
(here, $P(x) \sim 1/x^2$)



For example:

Considering an atomic system
two atoms
attached with a bond



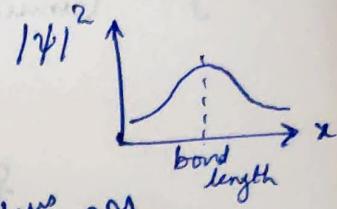
bond length

the bond length is the expected distance between the two atoms

(i.e. the 2 atoms are

unlikely to be closer

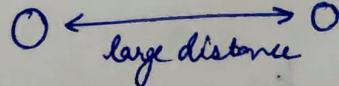
and also unlikely to be farther)



LECTURE 17 (13/03/2024)

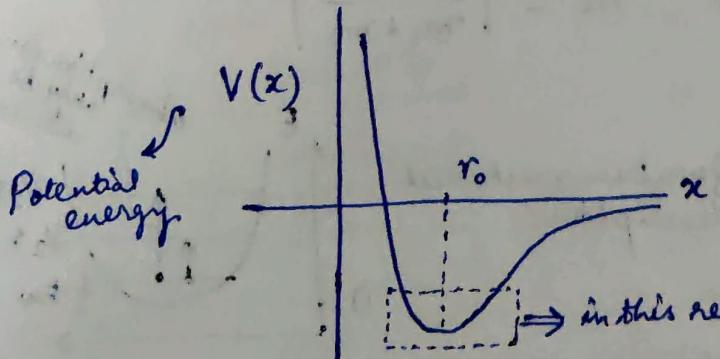
58] Why can we model the bond b/w atoms with a spring?

If the atoms are too far apart
then they CANNOT be modelled with springs



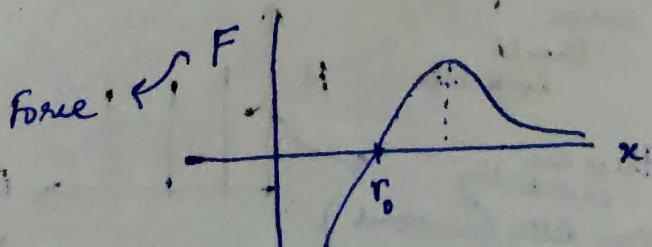
Thus, the force approximation of $\vec{F} = -k\vec{x}$
works only when they come closer

We know:



in this region the potential energy is roughly parabolic *

{ thus, the force can be linear }

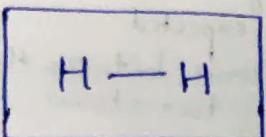


57]

Consider a H_2 molecule

+
What are the ways
in which motion could occur?

{ we can ignore
translation of the whole
system, by assuming that
we are moving the
origin along with it }

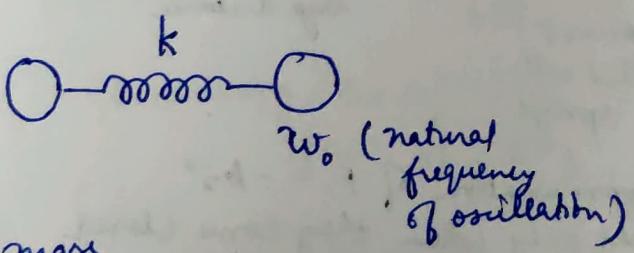


Types of motion
Bond length change Orientation change

It turns out that we
can use the classical description
for nanoscale objects (like atoms attached
with a bond)

↓
it is only that
some results obtained from
this cannot be correct.

(as they need to be
explained,
quantum mechanically
only)



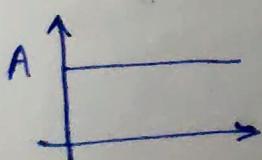
mass taken will be

$$\text{"Reduced mass", } m = \left| \frac{m_1 m_2}{m_1 + m_2} \right|$$

58]

The energy, should
behave as per quantum mechanical
description:

{ A though
classically
we would expect:

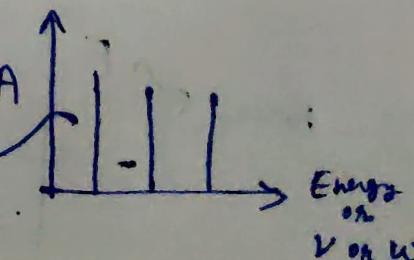
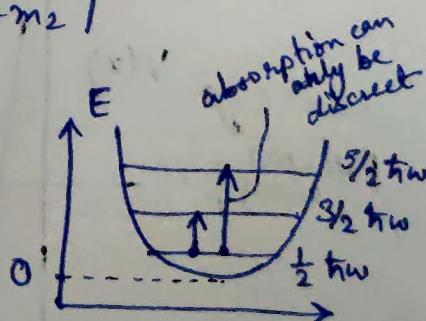


So the absorption
curve

should

look like:

(these are
essentially
delta functions)



59]

LECTURE 18 (14/03/2024)

Nanomechanics

Sensors

Memory

{ In electrical system,
voltage is used for representing 1 and 0
But here 1 and 0 is represented
through the freq. of oscillation

* NOTE: Slides uploaded
on moodle (related
to Nanomechanics)

LECTURE 19 (20/03/2024)

60]

SPM

(Scanning Probe Microscopy)

STM

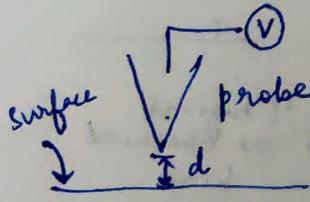
(Scanning Tunneling
Microscopy)

- i) involves tunneling current
- ii) can only work with conducting.

AFM

(Atomic Force
Microscopy)

- i) involves forces b/w tip and surface
- ii) Tip is usually a cantilever



$$\{d: 1-10 \text{ nm}\}$$

The probe is not supposed to touch the surface (else, it would damage the surface being imaged)

iii) Temp. of operation $< 4\text{ K}$
(so that STM can take images stably)

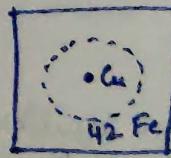
(current is measured)

this current exponentially decreases with distance:

$$I \propto e^{-d}$$

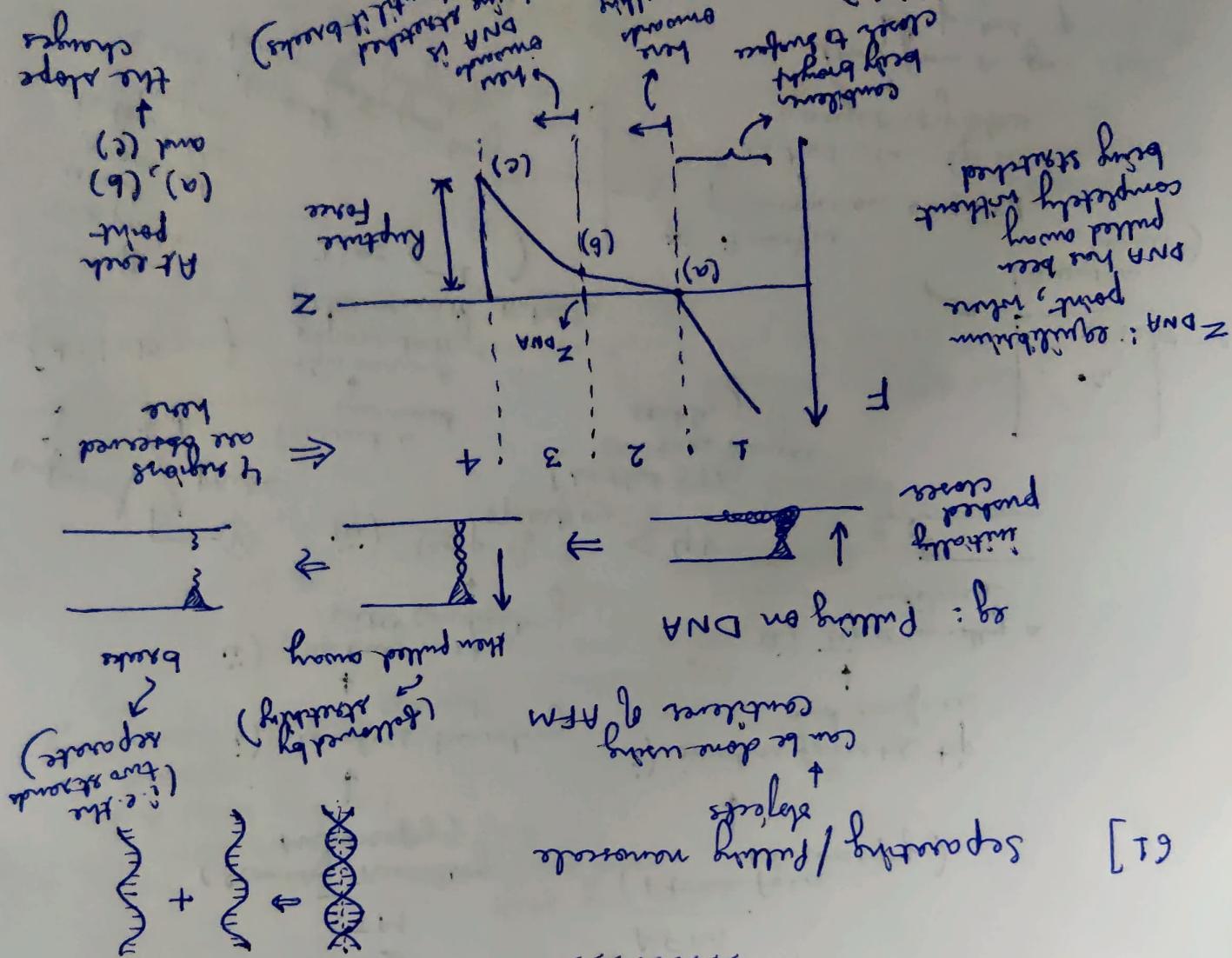


eg:



(Quantum Corral)

* A unique phenomenon observed is that when tip is brought very close atoms from surface can be picked up and moved to other places



more surface
area exposed
when pulled apart
less work
being pulled
done by
cellular life

less energy
to displace
longer bond
lengths

so less work

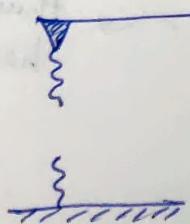
done by cellular life

less work

being pulled

done by cellular life

NOTE! If we try to braid them back close
 ↓
 they won't really
 join back easily

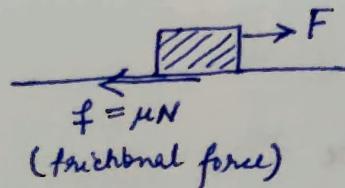


(it is
 not so easy to
 align the two strands
 back so that
 they combine
 completely)

LECTURE 20 (21/03/2024)

62]

Friction



$$f = \mu N$$

(frictional force)

We know that:

$$\mu = \frac{F_{\text{friction}}}{F_{\text{normal}}}$$

Coefficient
 of friction for
 surface

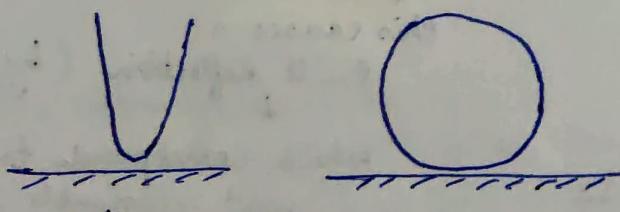
μ is independent of

the forces

contact area

type of
 interaction
 b/w surface
 and mass

However at the
 nanoscale this
 behavior changes:



$$(\mu_1 \approx 0.006, \\ \mu_2 \approx 0.1)$$

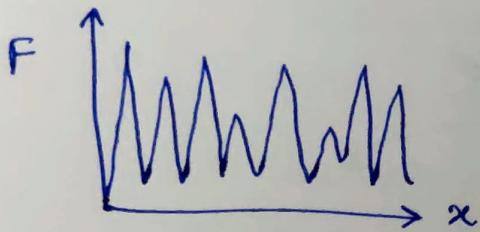
NOTE: At the nanoscale, since point of contact is very small thus, $\mu \downarrow$

↑
the probability of encountering a defect ↓ → thus, hardness ↑

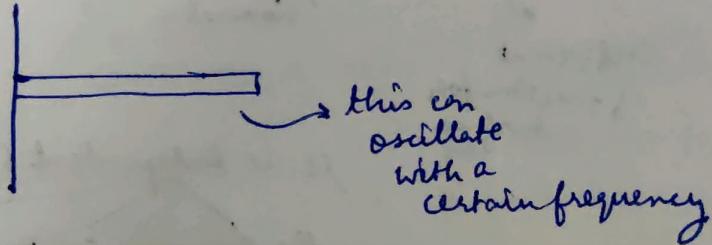
63] When moving along a surface (at nanoscale)

↓
due to surface irregularities ↓

we observe a plot like:



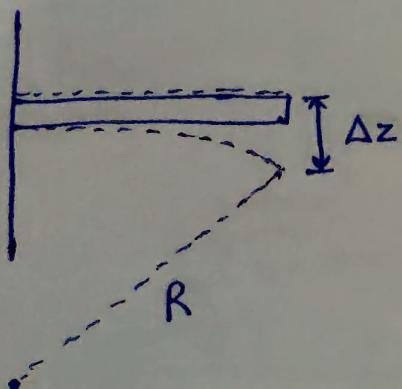
64] We can have a mechanical oscillator



Now, to detect the mass (usually in ppm) { in order to measure concentration } of chemical substances

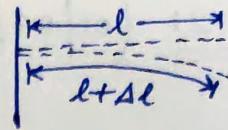
↓
we add it to the "beam"

↓
this causes a small deflection (by some Δz)

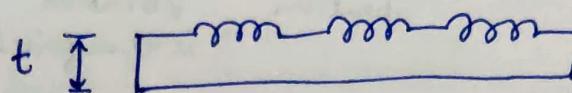


↓
which corresponds to a measurable radius of curvature (some very large R)

Due to the deflection
the upper surface
"stretches" by a small
amount
called "Surface strain"



can be modelled as:



upper surfaces
modelled
with springs

Using this we get:

$$\Delta z = \frac{C L^2 (1-\nu) \Delta \sigma}{E_M t^2}$$

Poisson ratio of
original beam

differential
stress

Young's
modulus of
the original
beam

C is a
constant

and also,

$$R = \frac{E_M t^2}{6(1-\nu) \Delta \sigma}$$

$\Delta \sigma$ tells the
difference in stresses
felt b/w the top
surface and bottom
surface

To take into account the effects of the
amount of mass added, we use
the following eqⁿ:

$$\sigma = \gamma + \frac{d\gamma}{d\varepsilon}$$

, where γ is
the amount
of energy (per unit
area)

SHUTTLEWORTH
EQUATION

spent in assembling
all the atoms added
on top of the beam

NOTE! The advantage of using this
deflection method (rather than direct frequency-amplitude
based method) is that this method
also works for small masses.

65] Nanoscale heat transfer

As temperature is increased we increase the amplitude of vibration \rightarrow this vibration is transferred



↓
How long will it take to reach the same temperature?

Consider that at T_0 they have the same amplitude of vibration

Now let's say one end is heated

$$T_0 < T_1$$

↓ Then

$$\text{amplitude of vibration } A_0 < A_1$$

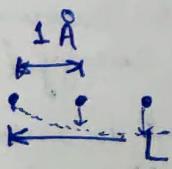
The frequency can also be determined from the relation:

$$k_B T \sim h \omega = h\nu$$

66]

Our system will have some sort of harmonic oscillator type behavior at room temp.

Now, typically atoms have a separation of $\sim 1\text{\AA}$



\Rightarrow whatever wavelengths are encountered by thermal energy are of the form of a long wave

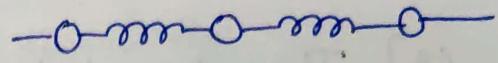
We will have standing waves, with a boundary condition at the terminals

Longest wavelength will be:
 $\lambda_{\max} = \frac{L}{2}$

Smallest one will be:
 $\lambda_{\min} = 2 \times \text{Interatomic distance}$

67] Energy of each phonon
is given by $\hbar \omega$
+ that
it is these phonons carry the
heat/thermal energy

We now have a system of
masses and springs:

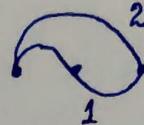


* NOTE: Phonons are a purely
Quantum mechanical concept

* NOTE: Heat transfer is done through e^- s and phonons
In metals, most of

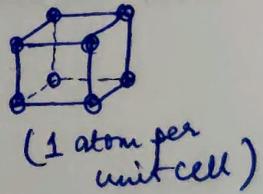
the heat transfer (heat current) is carried
through e^- s, and phonons are neglected

68] For a material with
only 3 atoms
+
there are only 2 phonon
modes



Considering p atoms

In 3D crystal, we have:
phonon modes $\approx 3p$



However, for our case there is
only 1 dimension $\Rightarrow \therefore$ it is p

and in 2D it will be $2p$

Also, there is another mode \rightarrow translation

(But since the final state is the same
+ it is a zero energy phonon)

so there are actually
3 phonon modes

(which is an allowed phonon)

NOTE: Zero frequency & Infinite wavelength
is possessed by —

+ and it is used to calibrate —

NOTE: Diamond (8) \Rightarrow 24 phonon modes

Graphite (2) \Rightarrow 6 phonon modes

69] Thermal conductivity

This is given by the following expression:

$$K_{th} = K_e + K_{ph}$$

(NOTE: When free e's exist,
K_e is generally dominating)

Now, we know that:

$$\sigma = \frac{e^2}{h}$$

or
(equivalently)

$$R = \frac{h}{e^2}$$

] for quantized case

Thus, for quantum materials
we see the relation:

$$\frac{K}{\sigma T} = \text{constant}$$

↓
(this value is called
the Lorentz Number) *

Also, another expression is:

$$k_0 = \frac{\pi^2 k_B^2 T}{3h}$$

where, k_0 is the quanta of thermal conductivity

* NOTE: Nanomaterials in the Ballistic regime show quantum thermal conductivity.

LECTURE 22 (03/04/2024)

7.0] Thermo-electric

word comes from a combination (interplay) of "thermo" & "electric"
such materials have property that

if voltage gradient applied
heat is produced
(temperature gradient is produced)

if heated (i.e., if temp. gradient applied)
voltage gradient is produced

called Seebek effect

Here there is a useful quantity called

$$ZT \quad (\text{this is } Z \cdot T) \Rightarrow ZT = \frac{S^2 \sigma}{K}$$

Z is the thermo-electric figure of merit

the overall quantity is dimensionless

S : Seabek coefficient

σ : electrical conducting

K : thermal conductivity

71] Metals

typically have low
+ value of S

also both σ and K are high

(and increasing σ , also increases K)

thus the Seebek effect

is not significant for metals

72] Insulators

here, σ is small

K is usually small, but may be high for some
↓ materials

thus these
are also generally not
significant for showing Seebek effect

NOTE: Most thermoelectric materials are thus Semiconductors.

73] Semiconductors

they have a significantly high enough
+ value of σ

thus
these
have the
most potential
to work as
thermoelectrics

K is somewhat small

(it comes from phonons mainly,
so we can call it
 K_{phonon})

74] Nanomaterials

↓ { Here, still we
have an emphasis on semiconductor type }

We want to compare $(ZT)_{\text{bulk}}$ and $(ZT)_{\text{nano}}$

Now, when band gap \uparrow

\Rightarrow then Seebeck coefficient \uparrow

Also, the thermal conductivity of nanomaterials decreases, since surface defects are large

{ doping can increase it }

+ but usually it does not

+ have much effect

i.e. the more scattering centers there are

+ the lower will be the conductivity

* NOTE: Shrinking of size of material never is made to go below the ballistic regime

electrical conductivity
* increases by
+ doping

the linear relation b/w σ and K breaks, and we get high ZT value

We want to create a size where boundary scattering is dominant

(which depends on doping, conductivity, etc.)

75] Nano-magnetism

we will largely focus on Ferro / Antiferromagnetic materials

* NOTE: Characteristic length scales

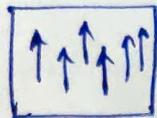
Electric \rightarrow ballistic regime (mean free path)

Quantum \rightarrow deBroglie wavelength

Thermoelectric \rightarrow Boundary scattering

Similarly, we should expect a certain length scale where nanomagnetism is shown.

For larger materials,
separate domain will form



for nanosize

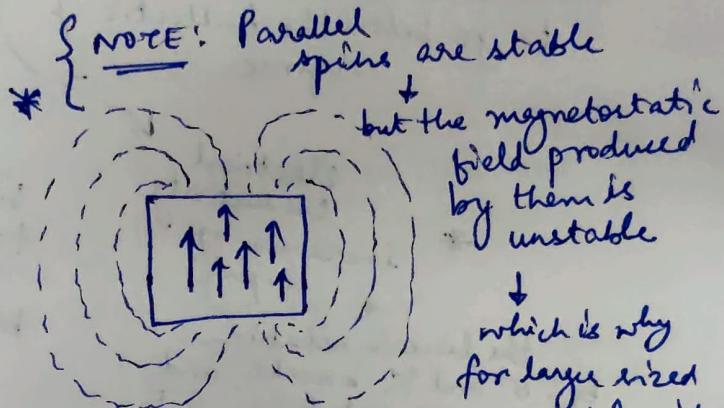
+
it is possible
to have these spins
parallel
without splitting
into different
domains



domain wall

(here a transition
from one
spin to the
other
takes place)

This occurs
for sizes smaller
than the
domain wall *



{ which cancels out much of the field }

LECTURE 23

76] Two aspects that are to be considered with regards to Nanomagnetism :

(i) Reduction in size

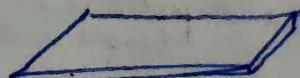


Spherical geometry

(ii) Simultaneous reduction & modification of shape

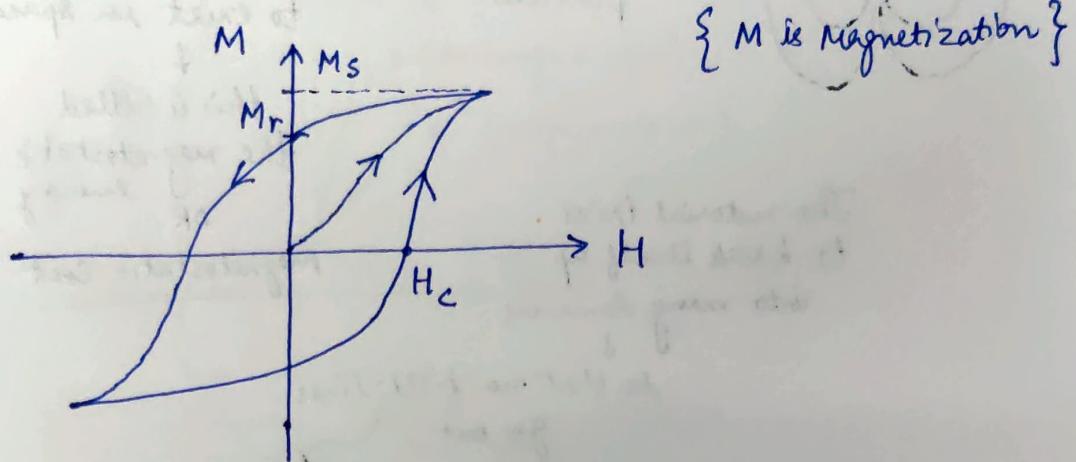


needle



thin/ultrathin films

77] We will now discuss the case for Ferromagnetic materials



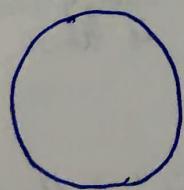
M_s : Saturation field

M_r : Remnant field

H_c : Coercive field

* NOTE: We can change the features of this field if we change the shape of the particle.

78] Case I : Spherical Particle



If it is in bulk size
then, it would like to break down

The energy can be described as :

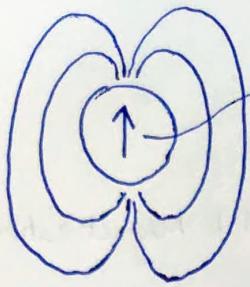
(i) Exchange energy

wants all the spins to align parallel

$\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$

(ii) Magnetostatic Energy

favours the formation of multidomains



Net magnetization
of all atoms
in the
particle

\Rightarrow There is an energy
cost for the field
to exist in space

\downarrow
this is called
the magnetostatic

OR energy

Magnetostatic Cost

The material tries
to break itself up
into many domains

\downarrow
so that no field lines
go out

\curvearrowright
this "tug of war"
between the two competing
effects ((i) & (ii))
gives rise to domains .

(iii) Magneto-crystalline Anisotropy

\downarrow
This is an anisotropic effect

Every material has a crystal structure

\downarrow
& there is a certain

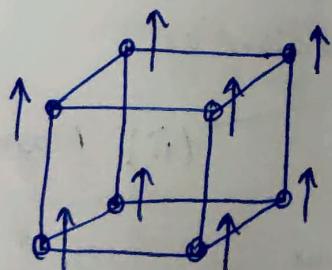
direction we can map out

where the energy cost [i.e.
is low] ease of magnetization
is good

\swarrow
Based on this we

can assume that there is

a "hard" and "easy axis" in the material



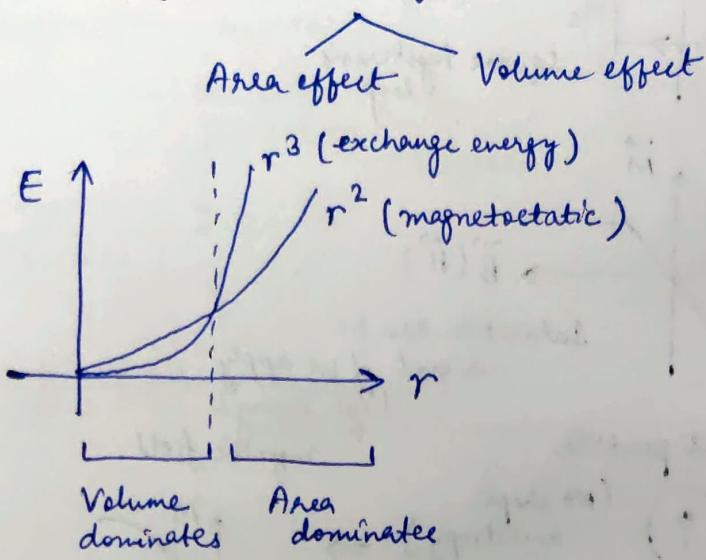
(Crystalline
anisotropy)

{ NOTE: Every material has
different spin directions
& different dependences }

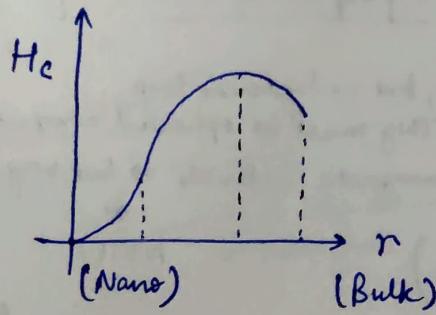
\downarrow
There is an easy axis of
magnetization }

*
NOTE: This 3rd term
becomes much more
important at nano scales

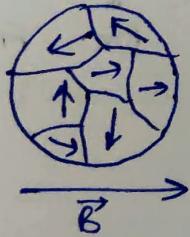
79] For a spherical particle
there are two effects



Also, the following curve is observed :

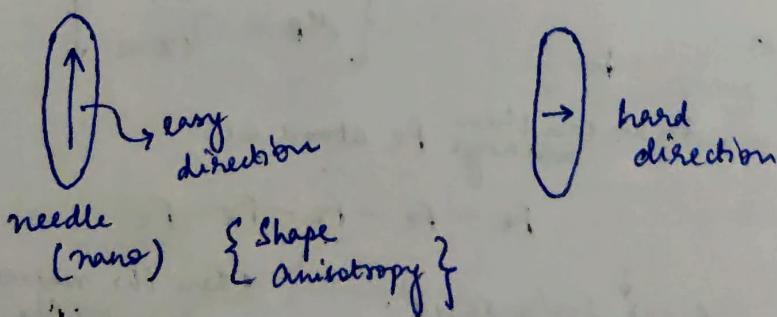


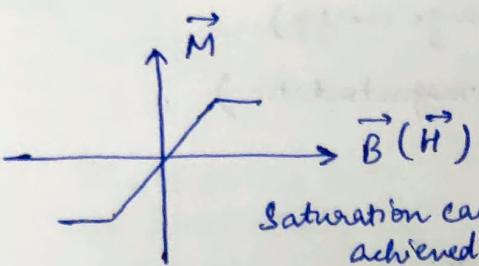
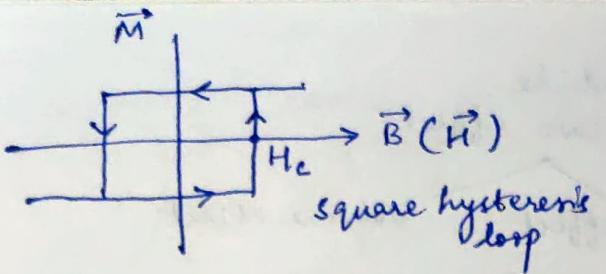
NOTE:



→ domains in the direction of \vec{B} will increase in size & the opposite domains start to rotate

80]

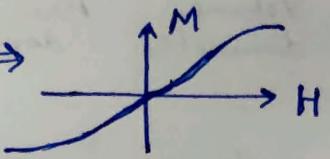




Saturation can be achieved if we apply high enough magnetic field

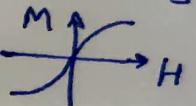
81] For spherical particle

$\vec{H} \downarrow$ (NO shape anisotropy) \Rightarrow



* NOTE: Ferromagnetic nanoparticles below certain size show superparamagnetism { * Ferromagnetism is required for this }

↓
There will be saturation, but no hysteresis loop
(They must be spherical nanoparticles)



* { It is a similar curve to paramagnetic materials \Rightarrow but very high value of magnetization is there }

LECTURE 24 (10/04/2024)

82] For an isolated Fe atom

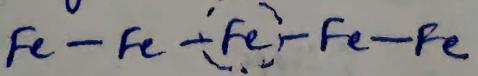
+
it will have a magnetic moment

given by: $\sim 4\mu_B$

where, μ_B is Bohr magneton

$$\left\{ \mu_B = \frac{e\hbar}{4\pi m} \right\}$$

so we can then arrange Fe atoms as:



the reason for this drop is associated with greater coordination of Fe atoms

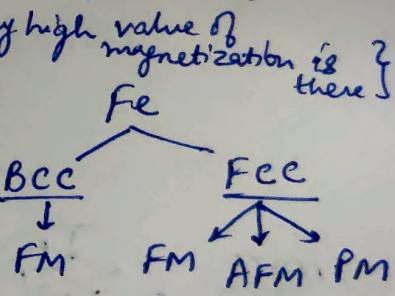
Next, for a sheet:

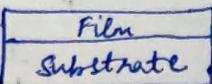


And in bulk this becomes $\sim 2\mu_B$

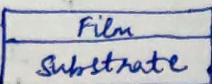
here the magnetic moment per Fe atom is $\sim 3.3\mu_B$

magnetic moment per Fe atom is $\sim 3\mu_B$



83] Thin Films  some features of these are

↓
involve some substrate
+
and the film is
present on top of that
substrate

 $\perp t$

Shape anisotropy
Surface anisotropy
Strain anisotropy
* this is due to lattice mismatch at interface
magnetic moment depends on these

{ NOTE: If film is crystalline & substrate is amorphous \rightarrow then at interface, the atoms will be slightly irregular
 ↓
 the way to solve this is by using a crystalline substrate as well, and employing epitaxial growth }

mismatch is chosen to be some (roughly within 5% of each other)
 here lattice constant for seamless transition at interface

84] Shape anisotropy
 + will prefer magnetization to be along the plane

* (NOTE: Here we are assuming uniform magnetization without domains)

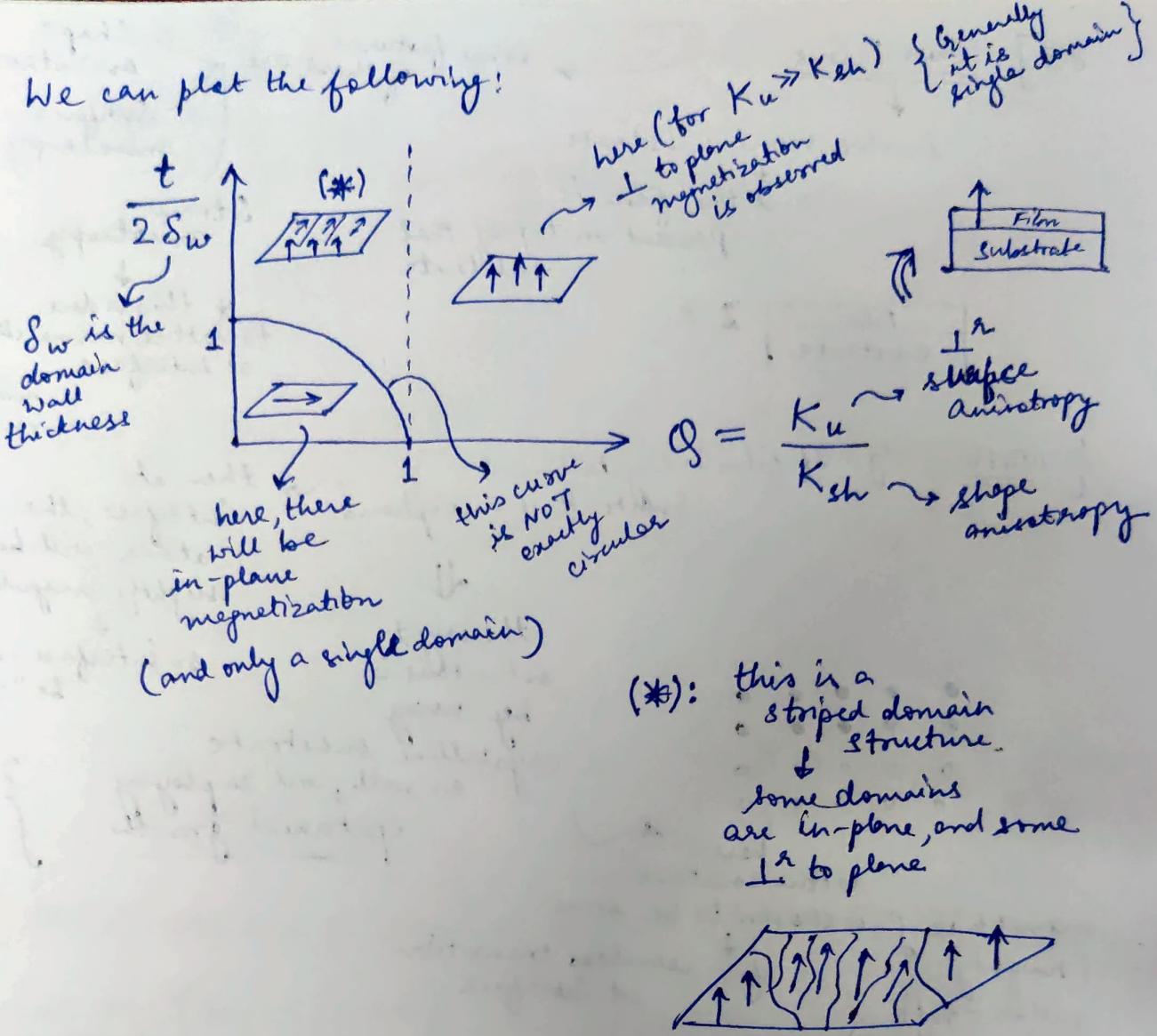


However, the other two features of surface and strain anisotropy lead to greater preference for magnetization perpendicular to the surface

* But, for a thin sheet
 + magnet
 the stray fields outside are zero ($i.e. B = 0$ outside)

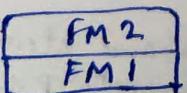
(this can be proven using Maxwell's laws)

We can plot the following:

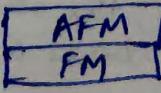


LECTURE 25 (13/04/2024)

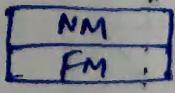
85] We want to see what happens when we couple different layers.



Case 1



Case 2



Case 3

FM: Ferromagnetic

AFM: Anti-ferromagnetic

NM: Non magnetic

In Case 1 → since both are FM

an overall ferromagnetic behaviour is going to be expected.

