

(2) 04/25

Lecture-19

30/10/20

- In the last lecture we examined the method of exploiting Magnetic field to detect & measure some internal properties of the semiconductor and we have been able to show that if a Semiconductor is doped so that we could distinguish b/w the Minority & majority carriers using a simple experiment we can measure:
 - The concentration of Majority carriers
 - The Mobility of Majority carriers
- Another possibility is exploiting the Semiconductor to measure the Magnetic field
Typical forms of the devices are relatively flat & thin . so that lateral dimensions are much larger than the other dimension.
- If you have a Device as described above and you apply voltage to the lateral contacts we have some current flowing through the device at this point if you apply Magnetic field . we will deflect the flow lines of the

Current Density.

- For this reason the current will take a different path inside the device this may be shorter or longer w.r.t the case in which the Magnetic field is absent. So we expect that given the applied voltage the current will change. If The path is longer remembering that material has Resistivity then it's like increasing Resistivity of the material.
- For a given voltage we expect the decrease in the current, if we increase the resistivity if we Bias the device with a current generator we expect an increase in the Measured voltage. This way we can detect the presence of the magnetic field.
- We assume the device is a 2D object and the Magnetic field is oriented Normal on one of the faces of the sensor.
- We also assume the Magnetic field is Normal to the plane over which the current flows
- Therefore Current density vector \vec{J}_{far}

to Magnetic Induction.

→ We have to find relationship b/w Current Density (CD) & MF

We start with a Uniform Semiconductor so that we can exclude the Diffusive part of the CD

- Importantly in the last lecture the Analysis was carried out by External Electric field now we have both Electric & Magnetic fields
- Analysis can be carried out for Electrons & Holes here we do it for e^-s .
 - we should be aware that this kind of analysis starts with the Dynamics of a single particle i.e one electron inside crystal. Then we take Average of all e^-s at a given instant of Time.

16.7 Magnetoresistive Effect

This section illustrates how the current density in a semiconductor is influenced by the application of a magnetic field.²³ The analysis is carried out considering a

Table 16.5 Applications of magnetic field sensors

Measuring the magnetic field of earth (geomagnetics)
Data storage (reading magnetic tapes and disks)
Recognizing magnetic ink patterns in banknotes
Reading credit cards
Contactless switching
Detecting a current through the magnetic field
Detecting linear/angular displacements through the displacement of a magnet

Table 16.6 Typical ranges of interest of the magnetic induction

Geomagnetic field	30–60 μT
Data storage ^a	10 μT –10 mT
Recognizing magnetic ink patterns in banknotes	10 μT –10 mT
Reading credit cards	10 μT –10 mT
Permanent magnets used in switches and sensors	5–100 mT
Permanent magnets used in measure instrumentation	4–5 T

^a Hard disks, floppy disks, video tapes.

uniformly-doped, *n*-type semiconductor; the treatment of the *p*-type case is similar. An electric field **E** and a magnetic-induction field **B** are applied to the semiconductor; it is assumed that the fields are weak enough not to perturb the uniformity of the electron concentration *n*, so that the diffusive contribution to the current density is absent.

The starting point is the description of the dynamics of a single electron; then, the current density is obtained by averaging over the momentum space. Letting **F** be the force acting on a single electron, the dynamics of the latter is described by

$$\mathbf{F} = m_n \mathbf{a}, \quad \frac{d\mathbf{u}}{dt} = -\frac{q}{m_n} (\mathbf{E} + \mathbf{u} \wedge \mathbf{B}), \quad (16.45)$$

²³ The units of the electromagnetic quantities are: electric displacement $[\mathbf{D}] = \text{C m}^{-2}$, charge density $[\rho] = \text{C m}^{-3}$, magnetic field $[\mathbf{H}] = \text{A m}^{-1}$, current density $[\mathbf{J}] = \text{C s}^{-1} \text{m}^{-2} = \text{A m}^{-2}$, magnetic induction $[\mathbf{B}] = \text{V s m}^{-2} = \text{Wb m}^{-2} = \text{T}$, electric field $[\mathbf{E}] = \text{V m}^{-1}$, electric potential $[\varphi] = \text{V}$, electric current $[\mathbf{A}] = \text{C s}^{-1} = \text{A}$, where “C”, “A”, “V”, “Wb”, and “T” stand for Coulomb, Ampère, Volt, Weber, and Tesla, respectively. It is also $1 \text{ T} = 1 \text{ W/m}^2 = 10^4 \text{ Gauss}$. In turn, the values and units of the parameters are: vacuum permittivity $\epsilon_0 = 8.85419 \times 10^{-12} \text{ C V}^{-1} \text{ m}^{-1} = \text{F m}^{-1}$, vacuum permeability $\mu_0 = 1/(c^2 \epsilon_0) = 1.256641 \times 10^{-6} \text{ s}^2 \text{ F}^{-1} \text{ m}^{-1} = \text{H m}^{-1}$, where “F” and “H” stand for Farad and Henry, respectively.

where \mathbf{u} is the group velocity of the wave packet describing the electron and \mathbf{a} the acceleration; in turn, q is the elementary charge and m_n the transport effective mass of the electron.²⁴ The motion of the electron is described as an alternation of free flights and collisions; considering an arbitrary position along a free flight, let t be the corresponding instant and τ the time elapsed from the last collision suffered by the electron. Even if the applied fields \mathbf{E} and \mathbf{B} depend on time, it can be assumed that their time variation is slow with respect to the time scale of a free flight; also, from the assumption that the fields are weak it follows that the time variation of \mathbf{u} is also slow. In these hypotheses, integrating (16.45) from $t - \tau$ to t yields

$$\mathbf{u}(t) - \mathbf{u}(t - \tau) = -\frac{q}{m_n} \int_{t-\tau}^t (\mathbf{E} + \mathbf{u} \wedge \mathbf{B}) dt' \simeq -\frac{q}{m_n} [\mathbf{E} + \mathbf{u}(t) \wedge \mathbf{B}] \tau. \quad (16.46)$$

The group velocity depends on time through the wave vector \mathbf{k} of the packet: $\mathbf{u} = \mathbf{u}(\mathbf{k})$, $\mathbf{k} = \mathbf{k}(t)$; the average velocity \mathbf{v}_n of the electrons of the conduction band is obtained as the statistical average²⁵ of \mathbf{u} using the distribution function f :

$$\mathbf{v}_n(\mathbf{r}, t) = \frac{1}{n} \iiint_{-\infty}^{+\infty} \mathbf{u} f(\mathbf{r}, \mathbf{k}, t) d^3 k. \quad (16.47)$$

The same type of average is carried out over the term $\mathbf{u}(t - \tau)$; by definition, this term is the velocity of the electron under consideration immediately after a collision. Although the duration of a collision is very short, the forces involved in it are much stronger, especially in the weak-field hypothesis, than those produced by \mathbf{E} and \mathbf{B} ; it follows that right after a collision the electron velocity “has no memory” of the orientation that was produced by the fields prior to the collision: in other terms, the collision has a randomizing effect on the electron velocities. In conclusion, the contributions to the statistical average of $\mathbf{u}(t - \tau)$ tend to cancel each other, to the point that this average can be neglected:

$$\langle \mathbf{u}(t - \tau) \rangle \simeq 0, \quad \mathbf{v}_n \simeq -\frac{q}{m_n} [\langle \tau \rangle \mathbf{E} + \langle \tau \mathbf{u}(t) \rangle \wedge \mathbf{B}]. \quad (16.48)$$

Defining the momentum-relaxation times and the mobilities with

$$\tau_{pn} = \langle \tau \rangle, \quad \tau_{pn}^* \mathbf{v}_n = \langle \tau \mathbf{u} \rangle, \quad \mu_n = \frac{q}{m_n} \tau_{pn}, \quad \mu_n^* = \frac{q}{m_n} \tau_{pn}^*, \quad (16.49)$$

yields

$$\mathbf{v}_n = -\frac{q}{m_n} \tau_{pn} \mathbf{E} - \frac{q}{m_n} \tau_{pn}^* \mathbf{v}_n \wedge \mathbf{B} = -\mu_n \mathbf{E} - \mathbf{v}_n \wedge \mu_n^* \mathbf{B}. \quad (16.50)$$

²⁴ The use of the effective mass implies the parabolic-band approximation [61, Sect. 17.6.2]. For the electrons of the conduction band of silicon it is $1/m_n = (2/m_t + 1/m_l)/3$, with m_t , m_l the transverse and longitudinal mass, respectively; compare with (16.36).

²⁵ In principle, the integral of (16.47) should be carried out over the Brillouin zone. Here the integration limits are justified by the parabolic-band approximation, combined with the observation that f becomes negligibly small away from the minima of the conduction band.

Note that $\mu_n^* \mathbf{B}$ is dimensionless. Using the definition of electron conductivity $\sigma_n = q \mu_n n$ and current density $\mathbf{J}_n = -q n \mathbf{v}_n$ provides the relation

$$\mathbf{J}_n = -q n \mathbf{v}_n = q \mu_n n \mathbf{E} + q n \mathbf{v}_n \wedge \mu_n^* \mathbf{B} = \sigma_n \mathbf{E} + \mu_n^* \mathbf{B} \wedge \mathbf{J}_n. \quad (16.51)$$

Although (16.51) relates the current density to the fields, its form is inconvenient due to the vector product involving \mathbf{J}_n at the right hand side. To proceed, one notes that $\sigma_n \mathbf{E}$ is the value of the current density when the magnetic induction is absent, namely, $\mathbf{J}_{n0} = \mathbf{J}_n(\mathbf{B} = 0) = \sigma_n \mathbf{E}$ (in passing, this is the local form of Ohm's law). Splitting (16.51) into components yields

$$\begin{bmatrix} 1 & \mu_n^* B_3 & -\mu_n^* B_2 \\ -\mu_n^* B_3 & 1 & \mu_n^* B_1 \\ \mu_n^* B_2 & -\mu_n^* B_1 & 1 \end{bmatrix} \begin{bmatrix} J_{n1} \\ J_{n2} \\ J_{n3} \end{bmatrix} = \sigma_n \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix}, \quad (16.52)$$

where the determinant of the matrix reads $1 + (\mu_n^* B)^2$. Solving for the components of \mathbf{J}_n and reverting to the vector form provides

$$[1 + (\mu_n^* B)^2] \mathbf{J}_n = \mathbf{J}_{n0} + (\mu_n^* \mathbf{B} \cdot \mathbf{J}_{n0}) \mu_n^* \mathbf{B} + \mu_n^* \mathbf{B} \wedge \mathbf{J}_{n0}. \quad (16.53)$$

This result shows that the current density is influenced by the magnetic induction. The influence is twofold: first, one notes that dividing both sides by $1 + (\mu_n^* B)^2$ makes each occurrence of $\mathbf{J}_{n0} = \sigma_n \mathbf{E}$ to be divided by the same factor, showing that the conductivity decreases with respect to the value σ_n corresponding to $\mathbf{B} = 0$. Equivalently, one may state that the resistivity increases by the factor $1 + (\mu_n^* B)^2$ with respect to the value $1/\sigma_n$ corresponding to $\mathbf{B} = 0$; the ratio $[1 + (\mu_n^* B)^2]/\sigma_n$ is called *magnetoresistivity*.

The second influence is that the flow lines of the current density are modified by the magnetic induction. To illustrate this issue, assume that the device under consideration consists of a thin layer of semiconductor, such that the component of \mathbf{J}_n normal to the layer and, similarly, the component of \mathbf{J}_{n0} normal to the layer, are equal to zero; in this case, one adjusts the reference to place the device onto the x, y plane (Fig. 16.18). The width of the device in the y direction is assumed to be infinite, so that the effect of the boundary conditions in that direction is eliminated; finally, the application of a voltage V between the two contacts shown in the figure produces an electric field along the x direction. Given these premises, if \mathbf{B} is parallel to the z axis, namely, $\mathbf{B} = B_z \mathbf{k}$, then the scalar product $\mathbf{B} \cdot \mathbf{J}_{n0}$ vanishes and (16.53) reduces to

$$J_{nx} = \frac{J_{n0x} - \mu_n^* B_z J_{n0y}}{1 + (\mu_n^* B_z)^2}, \quad J_{ny} = \frac{J_{n0y} + \mu_n^* B_z J_{n0x}}{1 + (\mu_n^* B_z)^2}. \quad (16.54)$$

On the other hand it is $J_{n0y} = \sigma_n E_y = 0$, so that (16.54) become

$$J_{nx} = \frac{1}{1 + (\mu_n^* B_z)^2} J_{n0x}, \quad J_{ny} = \frac{\mu_n^* B_z}{1 + (\mu_n^* B_z)^2} J_{n0x}. \quad (16.55)$$

The flow lines of the current density form an angle θ with respect to the x axis, such that $\tan(\theta) = \mu_n^* B_z$. In the example of Fig. 16.18 the angle is negative, corresponding to the case where the direction of \mathbf{B} is opposite to that of \mathbf{k} .

16.8 Hall Effect

The measurements based on the *Hall effect* are a powerful investigation tool that exploits the combined action of the electric and magnetic field. The Hall effect is the production of a voltage drop, transverse to the direction of the electric current, due to the application of a magnetic field. The qualitative features of the method are explained with the aid of Fig. 16.19. Consider a uniformly doped, prismatic block of semiconductor. The block is slender, and a constant voltage V is applied to it to produce an electric field \mathbf{E} aligned with the longitudinal direction. As a consequence, one can assume that the flow lines of the current density be parallel to \mathbf{E} ; due to spatial uniformity, such a current density is essentially due to the drift of

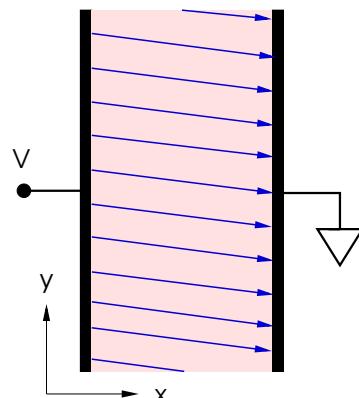


Fig. 16.18 A layer of material illustrating the deformation of the flow lines of the current density produced by the magnetoresistive effect

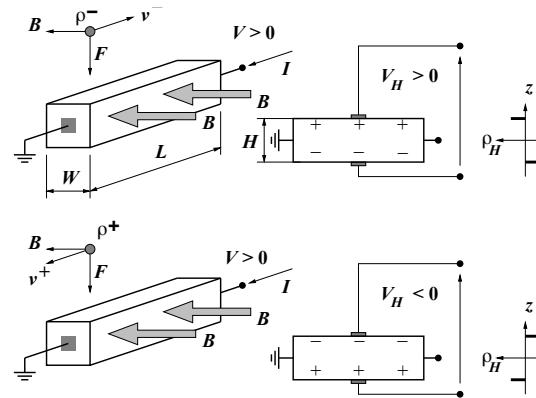


Fig. 16.19 Scheme of a Hall-voltage measurement

majority carriers. At the same time, a constant magnetic-induction field \mathbf{B} is applied, normal to one of the lateral faces. The upper part of the figure refers to an n -doped semiconductor; there, the majority carriers are electrons, whose average velocity is oriented opposite to the field; it follows that the Lorentz force $\mathbf{F} = \rho^- \mathbf{v}^- \wedge \mathbf{B}$ is oriented as shown in the figure. The negative indices in the expression of the Lorentz force remind one that the charge density and average velocity are those of negative charges. The mobile electrons are pushed by the Lorentz force towards the lower face of the device, where they form a negative charge layer. The flow lines of the current density, at least in the central part of the device, far from the contacts, are still parallel to the longitudinal direction; however, their density is not uniform any more. Due to the global charge neutrality, the negative charge layer is compensated by a positive charge layer that forms at the upper face. The two opposite layers, schematically indicated in the diagram in the upper-right part of Fig. 16.19, produce an electric field normal to the upper and lower faces; as a result, a measurable voltage drop (*Hall voltage*) between the two faces comes into existence: for the example in hand, the voltage of the upper face is larger than that of the lower face.

In a p -doped semiconductor (lower part of Fig. 16.19), the majority carriers are holes, whose average velocity is oriented in the direction of the field; the Lorentz force $\mathbf{F} = \rho^+ \mathbf{v}^+ \wedge \mathbf{B}$ is oriented as in the previous case, because both charge density and average velocity change sign with respect to the n -doped semiconductor. The consequence is that the mobile holes are pushed towards the lower face of the device, where they form a positive charge layer. In conclusion, the sign of the Hall voltage is opposite with respect to the case of the n -doped semiconductor.

The analysis of the experiment is based on the equations incorporating the magnetic terms. Due to the uniformity of the material one can neglect the diffusion term and use (16.53); the equation is simplified by assuming that \mathbf{B} is weak, so that the terms of (16.53) that are quadratic in the components of \mathbf{B} are negligible: this yields

$$\mathbf{J}_n = q \mu_n n \mathbf{E} - q a_n \mu_n^2 n \mathbf{E} \wedge \mathbf{B}, \quad a_n = \mu_n^*/\mu_n. \quad (16.56)$$

Similarly, for the hole-transport equations one finds

$$\mathbf{J}_p = q \mu_p p \mathbf{E} + q a_p \mu_p^2 p \mathbf{E} \wedge \mathbf{B}, \quad a_p = \mu_p^*/\mu_p. \quad (16.57)$$

The derivation of the general form of (16.56, 16.57) including the diffusive terms is given in [61, Sects. 19.5.2, 19.5.3], where it is shown that $a_n = \mu_t (\mu_t + 2 \mu_l) / (3 \mu_n^2)$ with

$$\mu_t = \frac{q \tau_{pn}}{m_t}, \quad \mu_l = \frac{q \tau_{pn}}{m_l}, \quad \mu_n = \frac{2 \mu_t + \mu_l}{3}. \quad (16.58)$$

In (16.58), τ_{pn} is the momentum-relaxation time of the electrons, m_t the transverse mass, and m_l the longitudinal mass;²⁶ it follows

²⁶ In the parabolic-band approximation, the energy-momentum relation of the electrons near each minimum of the conduction band is a quadratic form generated by a 3×3 diagonal matrix; in the

$$a_n = 3 \frac{m_l(m_l + 2m_t)}{(m_t + 2m_l)^2}, \quad (16.59)$$

namely, a_n of (16.56) is a known parameter. A similar derivation, albeit more involved due to the presence of two maxima of the valence band, applies to a_p of (16.57). The total current density $\mathbf{J} = \mathbf{J}_n + \mathbf{J}_p$ then reads

$$\mathbf{J} = \sigma \mathbf{E} + r \sigma^2 \mathbf{E} \wedge \mathbf{B}, \quad (16.60)$$

where $\sigma = q \mu_p p + q \mu_n n$ is the electric conductivity and

$$r = \frac{q}{\sigma^2} (a_p \mu_p^2 p - a_n \mu_n^2 n) = \frac{a_p \mu_p^2 p - a_n \mu_n^2 n}{q (\mu_p p + \mu_n n)^2} \quad (16.61)$$

is the *Hall coefficient*. The two quantities σ and r can be measured independently as shown below; while σ is positive definite, r has a sign. In particular, the following limiting cases hold: for the *p*-type dopant it is $p \gg n$, whence $\sigma \simeq q \mu_p p$ and $r \simeq a_p/(q p) > 0$; thus,

$$p = \frac{a_p}{q r}, \quad \mu_p = \frac{r}{a_p} \sigma \quad (p \gg n). \quad (16.62)$$

Similarly, for the *n*-type dopant it is $n \gg p$, whence $\sigma \simeq q \mu_n n$ and $r \simeq -a_n/(q n) < 0$; thus,

$$n = -\frac{a_n}{q r}, \quad \mu_n = -\frac{r}{a_n} \sigma \quad (n \gg p). \quad (16.63)$$

From (16.62) and (16.63) it follows that the concentration and mobility of the majority carriers can be determined independently, provided σ and r are known. In turn, the measurement of σ and r is easily carried out by applying (16.60) to the prismatic sample of Fig. 16.19. Let \mathbf{i}_L be the unit vector of the longitudinal direction, and \mathbf{i}_W the unit vector parallel to \mathbf{B} , so that $\mathbf{B} = B \mathbf{i}_W$. Observing that $E_W = 0$, $J_W = 0$, and $\mathbf{E} \wedge \mathbf{B} = E_L B \mathbf{i}_H - E_H B \mathbf{i}_L$, it follows

$$J_L = \sigma E_L - r \sigma^2 E_H B, \quad J_H = \sigma E_H + r \sigma^2 E_L B, \quad (16.64)$$

with $J_H = 0$. In turn, B is small enough to make the following approximations possible:

$$J = J_L \simeq \sigma E_L, \quad E_H = -r \sigma E_L B \simeq -r J B. \quad (16.65)$$

On the other hand it is $E_L \simeq V_L/L$, $E_H \simeq V_H/H$, and $J = I/(WH)$, where the block's length L , height H , and width W are indicated in Fig. 16.19; thus, $V_H = -r BI/W$ and $I/(WH) = \sigma V_L/L$. In conclusion,

$$\sigma = \frac{LI}{WHV_L}, \quad r = -\frac{WV_H}{BI}, \quad (16.66)$$

latter, two diagonal entries are equal to m_t and one diagonal entry is equal to m_l [61, Sect. 17.6.2]. See also note 24.

namely, the two parameters are obtained by combining the Hall voltage with other known physical and geometrical parameters. Typical applications of the measurement scheme shown in this section are the measurements of concentrations and mobilities as functions of temperature and dopant concentration.

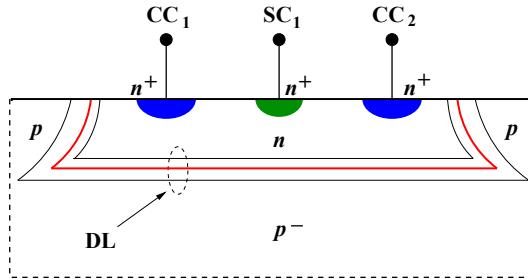


Fig. 16.20 Integrated Hall plate realized with the bipolar process (lateral view). The drawing is an elaboration on Fig. 4 of [4]

Figure 16.20 shows the lateral view of an integrated Hall plate realized with the bipolar process [4]; Fig. 16.21 shows the top view of the same device. The region of the plate is of the n type, and is epitaxially grown on a lightly-doped, p -type substrate; the position of the p - n junction is marked with the red line in the figure. The lateral isolation of the plate is obtained by diffusing p regions like those visible on the sides. The contacts between which current I flows (marked with CC_1 and CC_2 in the figure) and the side contacts between which the Hall voltage is measured (marked with n^+ diffusions) are obtained with n^+ diffusions. The voltages at CC_1 and CC_2 are such that the p - n junction is reversely biased; since the depleted layer DL extends mainly in the substrate, the geometry of the device is not influenced significantly by the functioning regime.

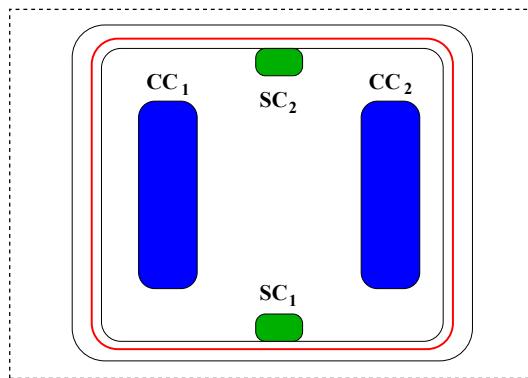


Fig. 16.21 Top view of the integrated Hall plate of Fig. 16.20. The drawing is an elaboration on Fig. 4 of [4]

Figure 16.22 shows the lateral view of an integrated Hall plate realized with an MOS transistor [4];²⁷ Fig. 16.23 shows the top view of the same device. In this device the Hall plate is provided by the inversion layer of the channel; with respect to the standard structure of the MOS transistor, here the two side contacts SC_1 and SC_2 are added.

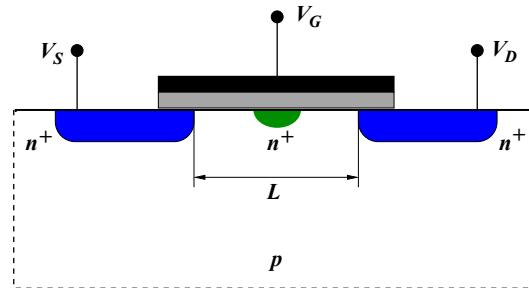


Fig. 16.22 Integrated Hall plate realized with the MOS process (lateral view). The drawing is an elaboration on Fig. 9 of [4]

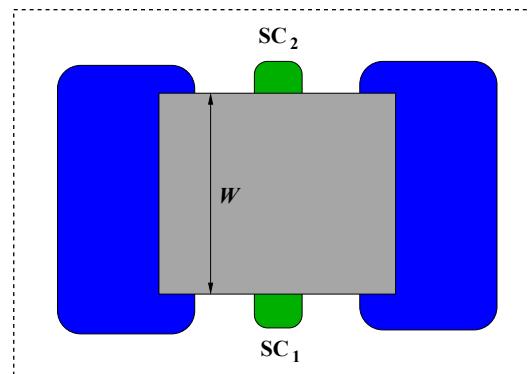


Fig. 16.23 Top view of the integrated Hall plate of Fig. 16.22. The drawing is an elaboration on Fig. 9 of [4]

16.9 Hall Effect — Samples with Arbitrary Aspect Ratio

The measurement technique based on the Hall effect, outlined above, is based on the hypothesis that the sample under investigation is slender, so that the flow lines of the current density are aligned with the longitudinal direction, whose unit vector is \mathbf{i}_L , and the contacts where the Hall voltage is measured are far away from the contacts onto which the external perturbation is applied. The typical arrangement is

²⁷ The magnetic sensors based on the architecture of the MOS transistor are sometimes indicated as MAGFETs.

that shown in Fig. 16.19, where the contacts used for measuring the Hall voltage are in the mid section of the sample, and the condition $L \gg H, W$ is fulfilled.

In more realistic situations the device of interest exhibits geometrical features that do not allow for the approximations indicated above. As a typical example, consider the device shown in Fig. 16.24, which is used for measuring the conductivity and the Hall voltage. The former quantity is measured by the four-contact, van der Pauw method [61, Sect. 25.7]: for this, the contacts labeled c_1, c_2, c_3, c_4 , also termed *Hall probes*, are used, while the two lateral contacts k_1, k_2 are left open. In turn, the Hall voltage V_H is measured at a pair of Hall probes, e.g., c_1 and c_3 , after applying the external perturbation to the lateral contacts and a magnetic induction \mathbf{B} normal to the x, y plane. Here it is assumed for simplicity that the external perturbation is a constant current I forced into the device. The portions of the boundary corresponding to the lateral contacts k_1, k_2 are equipotential; therefore, they influence the value of the Hall voltage measured at a pair of Hall probes.²⁸

If the sample under investigation, like that of Fig. 16.24, is not slender, the influence of the lateral contacts can not be neglected even if the pair of Hall probes is placed at the midpoint $L/2$ of the longitudinal extension of the sample; the current field is in fact two-dimensional, and is expressible (see, e.g., [61, Sect. 25.5] and references therein) as $\mathbf{J} = \text{rot}(\psi \mathbf{k})$, where \mathbf{k} is the unit vector of the z axis. Here, ψ is a function of x, y only, which is sometimes called *stream function*, and fulfills the Laplace equation $\nabla^2 \psi = 0$; the solution of the latter eventually leads to the expression of the Hall voltage at any position along the longitudinal direction of the sample:

$$V_H(y) = V_{H0} \left[1 - \frac{8}{\pi^2} S(y) \right], \quad (16.67)$$

where

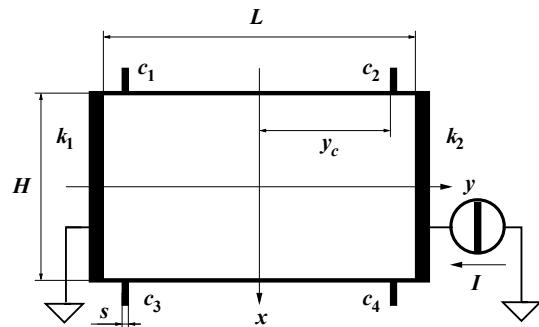


Fig. 16.24 Scheme for the combined conductivity and Hall-voltage measurements

²⁸ Specifically, placing a pair of Hall probes at a shorter and shorter distance from a lateral contact makes the Hall voltage smaller and smaller, regardless of the values of other parameters involved (compare with the comments to (16.67) below).

$$V_{H0} = -r \frac{BI}{W}, \quad S(y) = \sum_{n=0}^{\infty} \frac{\cosh(k_n y)}{(2n+1)^2 \cosh(k_n L/2)}. \quad (16.68)$$

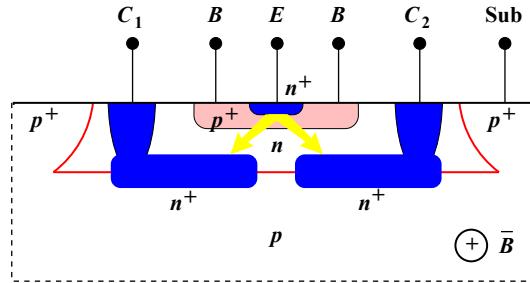
In (16.68), r is the Hall coefficient (16.61), W is the thickness of the device in the z direction, and $k_n = (2n+1)\pi/H$. For $y = 0$ the series in (16.68) attains the minimum, $S(0) = \sum_{n=0}^{\infty} [(2n+1)^2 \cosh(k_n L/2)]^{-1}$, whose leading term is $1/\cosh[\pi L/(2H)]$; this shows that the contribution of the series at $y = 0$ is small when $H \ll L$. In this limiting case the result of the standard theory is recovered, $V_H(0) \simeq V_{H0}$; in the other cases, instead, the measured Hall voltage differs significantly from V_{H0} [62]. Also, observing that $\sum_{n=0}^{\infty} (2n+1)^{-2} = \pi^2/8$, it also follows $V_H(\pm L/2) = 0$, which is consistent with the condition imposed by the lateral contacts.

20.4 Detecting the Magnetoresistive Effect

Figure 20.9 shows the lateral view of a magnetotransistor of the vertical type, realized with a bipolar process carried out over a p -type substrate [33]. The transistor is of the $n-p-n$ type, whose collector region is epitaxially grown on the substrate; the position of the $p-n$ junction between substrate and collector is marked with the red line in the figure. The lateral isolation of the device is obtained by diffusing p^+ regions like those visible on the sides. The device has two collectors, symmetrically placed with respect to the emitter and base regions as shown in the figure; the n^+ , blue regions connected to the collectors are the buried layers. When no magnetic induction is present, the current injected by the emitter (sketched by the yellow arrows) equally distributes between the two collectors.

The circuit representing the magnetotransistor is shown in Fig. 20.10, where the two load resistors R are equal to each other. When a magnetic induction is applied, normal to the device section (as exemplified by symbol \mathbf{B} in Fig. 20.9), the flow lines of the current density are modified due to the magnetoresistive effect, as illustrated in Sect. 16.7; this, in turn, unbalances the distribution of the emitter current between the two collectors and, consequently, unbalances the voltage drop over the load resistors. This produces a voltage ΔV between the two collectors, which constitutes the output signal of the sensor.

Fig. 20.9 Lateral view of an integrated magnetotransistor of the vertical type, realized with the bipolar process. The drawing is an elaboration on Fig. 17 of [33]



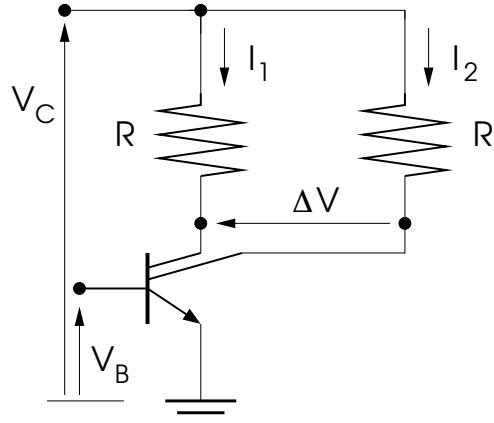


Fig. 20.10 Detection scheme of the magnetotransistor signal. The unbalance of the I_1 and I_2 currents produces a voltage drop $\Delta V \neq 0$ between the two collectors

$$\rightarrow F = m_n a, \quad \frac{du}{dt} = -\frac{q}{m_n} (E + u \wedge B)$$

we know for an e^- in a crystal the inertia is not given by the Mass of the free particle but it's given by the Effective Mass.

- There are two types of Effective Mass
 - (i) Average made out of components of Mass Tensor that is used in the definition of Density of States in Energy -

we use
in this
calculation

- (ii) Effective Mass for the Transport

m_n

→ If an external force acts on the e^- then the acceleration and force are related by

$$F = m_n a$$

effective Mass incorporates all the other forces that are due to the lattice

Now we proceed with analysis with simultaneous presence of Electric & Magnetic field

$$F = m_n a = m_n \frac{du}{dt} = -q(E + u \Lambda B)$$

$$\Rightarrow \frac{du}{dt} = -\frac{q}{m_n} (E + u \Lambda B) \quad \text{Torsion Force}$$

'u': velocity of individual e^-

$$\Rightarrow u(t) - u(t-\tau) = \left[-\frac{q}{m_n} (E + u(t) \Lambda B) \right] dt$$

$$\approx -\frac{q}{m_n} (E + u(t) \Lambda B) \tau$$

$\tau \Rightarrow$ Time that elapses b/w instant of last collision suffered by the e^- and the present one

* Some quantitative considerations

- The typical time b/w collisions is some fraction of ps (picoseconds)
i.e. τ' is very very short time
 \therefore Even ^{factor} change in E & M will not be have any effect in between the collision time which is why we consider E, B as constants in the Integral

$$u(t) - u(t-\tau) = -\frac{q}{m_n} \int_{t-\tau}^t (E + u(t') \Lambda B) dt'$$

↓

$$\approx -\frac{q}{m_n} (E + u(t) \Lambda B) \tau$$

and also u varies little during the collision time because e^-s are subjected to

external force and these external forces are not very intense; also 'i' change a little

→ At this point we will take average over all the e^i 's (it is a statistical average)
it is like taking a picture of all e^i 's at the instant of time and then we average all the terms that appear in the formula:

$$\langle u(t) \rangle - \underline{\langle u(t-\tau) \rangle} \approx -\frac{q}{m_n} (E\langle v \rangle + \langle u(t)\tau \rangle AB)$$

average at
instant
 $t-\tau$

* E & B are same for all e^i 's, but τ is different for all the e^i 's

→ We remember from previous lesson

$$\langle u(t-\tau) \rangle = 0 \quad \text{why?}$$

Any Because when e^i 's suffer collisions, the collisions are randomized that means that

the e^- may have any velocity oriented any direction. This interaction cancels all the possible memories w.r.t previous motion \Rightarrow
 e^-s we can dispose of $\langle u(t-\tau) \rangle$

Definition:

$\langle u(t) \rangle = \underset{\substack{\text{statistical} \\ |}}{\text{Average of } e^-s \text{ at time instant } t} = v_n$

$\langle \tau \rangle = \boxed{z_{pn}}$ \Rightarrow Momentum relaxation time
 for e^-s

$\langle u(t) \tau \rangle = v_n z_{pn}$ product of two approximations



original eqⁿ transforms into

$$v_n = -\frac{q}{m_n} z_{pn} (E + v_n \wedge B)$$

$$v_n \Rightarrow -m_n (E + v_n \wedge B)$$

• We know

$$J_n = -q_n v_n = -q_n (-\mu_n (\vec{E} + v_n \wedge \vec{B}))$$

(current density)

$$\Rightarrow q \mu_n \wedge \vec{E} + (q n v \wedge \mu_n \vec{B})$$

conductivity

$$J_n \Rightarrow \sigma_n \vec{E} - (J_n \wedge \mu_n \vec{B})$$

Here $\mu_n \wedge \vec{B}$

have inverse units
 \therefore Their product is
 just a Number

$$J_n \Rightarrow \sigma_n \vec{E} + (\mu_n \vec{B} \wedge J_n)$$

$$\mu_n \vec{B} \wedge J_n = \mu_n \vec{B} \wedge (\sigma_n \vec{E} + \mu_n \vec{B} \wedge J_n)$$

We know, $a \wedge (b \wedge c) = (a \cdot c)b - (a \cdot b)c$

$$\vec{B} \wedge (\vec{B} \wedge J) = (\vec{B} \cdot J)\vec{B} - (\vec{B} \cdot \vec{B})J$$

T

$\therefore \downarrow$ B & J are \perp law
 $B \cdot J = 0$

$$\Rightarrow B \wedge (B \wedge J) = -B^2 J$$

$$\rightarrow \therefore \mu_n B \wedge J_n = \mu_n B \wedge \sigma_n E - \mu_n^2 B^2 J_n$$

$$\therefore J_n = \sigma_n E + \mu_n B \wedge J_n$$

$$\Rightarrow \sigma_n E + \mu_n B \wedge \sigma_n E - \mu_n^2 B^2 J_n$$

$$J_n + \mu_n^2 B_n^2 J_n = \sigma_n (E + \mu_n B \wedge E)$$

$$\Rightarrow J_n (1 + \mu_n^2 B_n^2) = \sigma_n (E + \mu_n B \wedge E)$$

$$\Rightarrow J_n = \frac{\sigma_n (E + \mu_n B \wedge E)}{1 + \mu_n^2 B_n^2}$$

This ratio is less than 1 merely decreasing the conductance

define $J_{n_0} = \sigma_n E$ current in the absence of MF, B .

This is called Magneto Resistance.

$$\Rightarrow J_n = \frac{1}{1 + \mu_n^2 B_n^2} \left(\sigma_n E + \mu_n B_n \sigma_n E \right)$$

$$J_h \Rightarrow \frac{1}{1 + \mu_n^2 B_n^2} \left(J_{n0} + \mu_n B_n \Delta J_{n0} \right)$$

This term signifies

the change in current density
because the current density lines
get deflected in the presence of MF.
(B)



Explanation of the Hall effect - III

$$J_n = \sigma_n B (E + \mu_n^* B \times E)$$

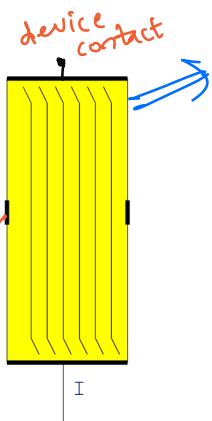
$$J_{ny} = 0$$

$$E_y + \mu_n^* B_z E_x = 0$$

$$E_y = -\mu_n^* B_z E_x = -\mu_n^* B_z J_{nx} / \sigma_n$$

$$R_H = -\mu_n^* / \sigma_n = -r_n / qn$$

measure must
to Hall voltage



for measuring Device properties using Hall effect the Device must be elongated

MAGNETORESISTANCE EFFECT

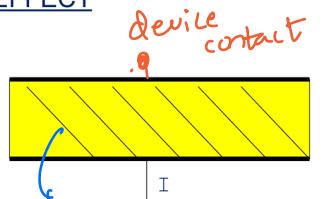
$$J_n = \sigma_n B (E + \mu_n^* B \times E)$$

$$E_y = 0$$

$$J_{nx} = \sigma_n B E_x$$

$$\sigma_n B = \frac{\sigma_n}{1 + \mu_n^{*2} B_z^2}$$

$$\frac{\rho_n B}{\rho_n} = 1 + \mu_n^{*2} B_z^2$$



The flowline of current density are clearly bent.

Instead if we want to exploit the Device as a Sensor the Geometry must be opposite (i.e. The device is very short)

∴ Qualitatively the current lines are bent it is forced to take a longer path from one contact to other in presence of Magnetic Field.
This effect is called MagnetoResistance

Magnetic Field Sensors (MFSs)

1. Measured quantities (H and B)

Measurement Units for the magnetic field (H) and induction (B)

$$\nabla \times \mathbf{H} = \epsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} + \mathbf{J}_I$$

H – magnetic field: A/m

$$\mathbf{B} = \mu_r \mu_0 \mathbf{H}$$

B – magnetic induction: Tesla

μ_r is the relative permeability of the specific medium;

$\mu_0 = 4\pi 10^{-7}$ H/m is the vacuum permeability

T = 1 Weber/m² = 10⁴ Gauss

Magnetic Field Sensors (MFSs)

2. Applications:

- Earth magnetic field measurements
- Reading of magnetic tapes and disks
- Recognition of magnetic ink patterns in banknotes
- Reading of credit cards

Indirect applications:

- Contactless switching
- Detection of a current through H
- Linear and angular displacement detection through the mechanical displacement of a magnet

Range of interesting values for the magnetic induction field B

geomagnetic field	30-60 μT
data storage (hard-disk, floppy-disk, videotapes)	$\approx 10\mu\text{T}-10\text{mT}$
reading of magnetic patterns (credit cards)	$\approx 10\mu\text{T}-10\text{mT}$
reading of magnetic ink of banknotes	$\approx 10\mu\text{T}-10\text{mT}$
permanent magnets used in switches and sensors	5 \div 100 mT
permanent magnets used in measuring instrumentations	4 \div 5 T

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→ System of Interacting Particles

- We begin another topic which is related to the Elastic property of the Materials in view of the Analysis of the Mechanical SENSORS
- We shall see how Elastic properties are related to the Microscopic properties i.e interaction of individual atoms
- For the moment we consider a system of particles not necessarily a crystal.
we assume the S/S is made of no. of particles that may be different from each other.

Total no. of particles = N

- Although the description of Atoms can be carried out using QM this kind of analysis can be done using CM
- Classically we can define each particle in S/S w.r.t its Position Vector.
Ex: R_1, R_2, \dots, R_N

System of Interacting Particles — I

Consider a conservative system made of N interacting (not necessarily identical) particles. The coordinates associated to them are $\mathbf{R} \equiv (\mathbf{R}_1, \dots, \mathbf{R}_N)$, the scalar components for each particle are $(X_{j1}, X_{j2}, X_{j3}) \equiv \mathbf{R}_j$. The Hamiltonian function of the system reads

$$T_a + V_a = \sum_{j=1}^N \frac{P_j^2}{2m_j} + V_a = \frac{1}{2} \sum_{j=1}^N m_j (\dot{X}_{j1}^2 + \dot{X}_{j2}^2 + \dot{X}_{j3}^2) + V_a,$$

with $V_a = V_a(\mathbf{R}) = V_a(X_{11}, X_{12}, \dots)$. Let $V_{a0} = V_a(\mathbf{R}_0)$, where \mathbf{R}_0 corresponds to an equilibrium position of the particles. As a consequence, V_{a0} is a minimum: $V_{a0} < V_a(\mathbf{R})$ for all \mathbf{R} in the vicinity of \mathbf{R}_0 . In particular, if the displacement $\mathbf{R} - \mathbf{R}_0$ of the particles with respect to the equilibrium position is small, V_a can be expanded to second order around \mathbf{R}_0 : let $s_1 \doteq X_{11}, s_2 \doteq X_{12}, \dots, s_{3j+k-3} \doteq X_{jk}, \dots, s_{3N} \doteq X_{N3}$ and $\xi_n \doteq s_n - s_{n0}$, $n = 1, 2, \dots, 3N$, where s_{n0} corresponds to the equilibrium position. As $(\partial V_a / \partial \xi_k)_0 = 0$, it is

$$V_a \simeq V_{a0} + \frac{1}{2} \sum_{k,n=1}^{3N} c_{kn} \xi_k \xi_n, \quad c_{kn} = \left(\frac{\partial^2 V_a}{\partial \xi_k \partial \xi_n} \right)_0.$$

→ At some point we will put all these vectors together in an enormous vector with many components.

Assumption: We assume the forces acting on the S/S are conservative which means

that they can be derived from a
Potential Energy.

- We may argue that the Atoms interact with each other through the EM force & Magnetic part is not really conservative
- However the velocities of particles inside a solid piece of Matter are small that means Magnetic part of the Force is Negligible because Qualitatively the

Magnetic part of the Force on particle due

$$\text{to EMF} = \frac{V}{C} \text{ Electric}$$

In the solid $\nabla \ll C \therefore$ the
Magnetic part is Neglected

→ In conclusion as the Forces are conservative we can say Total Energy = constant

$$T.E = T_a + V_a \quad P.E \text{ of atom}$$

K.E of atom

$T_a = \text{Sum of K.E's of individual particles}$

$$T_a + V_a = \sum_{j=1}^N \frac{P_j^2}{2m_j} + V_a = \frac{1}{2} \sum_{j=1}^N m_j (\dot{X}_{j1}^2 + \dot{X}_{j2}^2 + \dot{X}_{j3}^2) + V_a,$$

* The Potential Energy ' V_a ' instead depends on co-ordinates of each particle. consider a Columbic type of interaction b/w particles each particle is subjected to interaction by all remaining particles so the P.E. enbds co-ordinates of all particles \therefore in general is not separable (i.e V_a cannot be written in pieces, where each piece contains only one (or maybe components))

→ \therefore The above description is impossible to solve, unless an enormous set of eqⁿ. are processed.

• However, there is a way out, this way out is very elegant In a piece of solid matter

The Atoms are Tightly Bound to each other

i.e in Solids the Atoms vibrate at frequency of vibrations are strong.

But the amplitude of vibration is Not very High

This phenomenon is Helpfull in the Analysis of the S/S. In mechanics we define Equilibrium position of the particle as the

position in which P.E = minimum value

$$T_a + V_a = \sum_{j=1}^N \frac{P_j^2}{2m_j} + V_a = \frac{1}{2} \sum_{j=1}^N m_j (\dot{X}_{j1}^2 + \dot{X}_{j2}^2 + \dot{X}_{j3}^2) + V_a,$$

with $V_a = V_a(\mathbf{R}) = V_a(X_{11}, X_{12}, \dots)$. Let $V_{a0} = V_a(\mathbf{R}_0)$, where \mathbf{R}_0 corresponds to an equilibrium position of the particles. As a consequence, V_{a0} is a minimum: $V_{a0} < V_a(\mathbf{R})$ for all \mathbf{R} in the vicinity of \mathbf{R}_0 . In particular, if the displacement $\mathbf{R} - \mathbf{R}_0$ of the particles with respect to the equilibrium position is small, V_a can be expanded to second order around \mathbf{R}_0 : let $s_1 \doteq X_{11}, s_2 \doteq X_{12}, \dots, s_{3j+k-3} \doteq X_{jk}, \dots, s_{3N} \doteq X_{N3}$ and $\xi_n \doteq s_n - s_{n0}, n = 1, 2, \dots, 3N$, where s_{n0} corresponds to the equilibrium position. As $(\partial V_a / \partial \xi_k)_0 = 0$, it is

$$V_a \simeq V_{a0} + \frac{1}{2} \sum_{k,n=1}^{3N} c_{kn} \xi_k \xi_n,$$

$$c_{kn} = \left(\frac{\partial^2 V_a}{\partial \xi_k \partial \xi_n} \right)_0.$$

This matrix is Symmetric & PD
positive definite



$$V_a \approx V_{a0} + \frac{1}{2} \sum_{k,n=1}^{3N} c_{kn} \xi_k \xi_n$$

- since V_{a0} is the minimum value of PE at equilibrium then ' V_a ' at a different position

from a_0 is larger by construction.

- That means that the double sum is strictly positive for any choice of the displacement. This is due to the property of the Matrix C_{kn}

This Matrix
 $n, k = 0 \text{ to } 3N$
 is not only Symmetric but also Positive Definite

- By the way C_{kn} is called Elastic Matrix.

* One Dimensional Counter part of Elastic Matrix is we have only one Atom and this atom can move along only one axis.

Then $C_{kn} = C$ (because of only One Dimension & one Atom)

$$\therefore V_a \approx V_{a0} + \frac{1}{2} C_n \xi_n^2$$

$$\therefore V_a = V_{a0} + \frac{1}{2} C \xi_n^2$$

$\xi = n = 1$

→ Now Force = Derivative of P.E
(conservative system)

$$F = - \frac{d}{dx} (V_a) = - \frac{d}{dx} \left(V_{a_0} + \frac{1}{2} C \xi_n^2 \right) \quad \xi_n \propto x$$

$$\Rightarrow - \frac{1}{2} C (2 \xi_n)$$

$$F \Rightarrow -C \xi_n$$

so the Force is of the Elastic type proportional to the Elongation wrt to the origin.

* This formula generalizes to many Dimensions like the Man connected to origin with Spring or Pendulum.

Q) What happens when we want to calculate in the General situation i.e $\eta, F = (0, 3N)$?

Ans Due to definition of P.E if we take the derivative of P.E

$$F_{j,k} = - \frac{\partial V_a}{\partial x_{j,k}} \quad \begin{array}{l} j \Rightarrow \text{atom} \\ k \Rightarrow \text{axis} \end{array}$$

System of Interacting Particles — II

The $3N \times 3N$ matrix \mathbf{C} of entries c_{kn} is by definition symmetrical, and is positive definite as it equals $V_a - V_{a0} > 0$. The force acting on the j th particle along the k th axis is $F_{jk} = -\partial V_a / \partial X_{jk}$ or, using $r = 3j + k - 3$,

$$F_r = -\frac{\partial V_a}{\partial s_r} = -\frac{\partial V_a}{\partial \xi_r} = -\sum_{n=1}^{3N} c_{rn} \xi_n, \quad \text{Force} \rightarrow F \propto -\xi_n$$

namely, it is a linear function of the displacements. Indicating with ξ the column vector of elements ξ_1, ξ_2, \dots , it follows

$$V_a = V_{a0} + \frac{1}{2} \xi^T \mathbf{C} \xi, \quad \text{Quadratic form}$$

where ξ^T is the row vector transpose of ξ . Define

$$\mathbf{M} \doteq \begin{bmatrix} m_1 & & & & & \\ & m_1 & & & & \\ & & m_1 & & & \\ & & & \ddots & & \\ & & & & m_N & \\ & & & & & m_N \\ & & & & & & m_N \end{bmatrix}.$$

FORCE & STIFFNESS MATRIX NO. OF PARTICLES
COMPONENTS 1, 2, 3

Here
 $F \propto -\xi_n$
 displacement

∴ The Mass oscillates
 that is called
 the Linear
 Harmonic
 oscillator

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→ Q) What is the next issue?

Any We remember that we started with general form of the T.E., we understood the kinetic part which is sum of individual pieces but P.E. was not separable

Total Energy $\Rightarrow T_a + V_a = \sum_{j=1}^N \frac{P_j^2}{2m_j} + V_a = \frac{1}{2} \sum_{j=1}^N m_j (\dot{X}_{j1}^2 + \dot{X}_{j2}^2 + \dot{X}_{j3}^2) + V_a,$

Now we have derived a simpler expression for P.E is a mixture of all co-ordinates :.
 it is Non separable and we will do something to make it separable.

* * Rest of analysis for today will be devoted to how to separate the P.E. so that after separation we can analyze the motion of each individual degree of freedom separately from the rest of the system.

→ To do so, it's better to introduce a Matrix and vector Notation

i.e $\mathbf{C}_{2N \times 3N}$ with entries being C_{kn}
 $k, n = (0, 2N)$

- We also introduce a column vector whose elements are the Displacements & so, if we want to express the P.E after the expansion to the second order in vector form, we may write the Quadratic form

$$V_a = V_{ao} + \frac{1}{2} \boldsymbol{\xi}^T C \boldsymbol{\xi}$$

→ Now, we define a Mass Matrix

$$\mathbf{M} \doteq \begin{bmatrix} m_1 & & & & \\ & m_1 & & & \\ & & m_1 & & \\ & & & \ddots & \\ & & & & m_N \\ & & & & & m_N \\ & & & & & & m_N \end{bmatrix}.$$

Dashed red arrows
Components 1, 2, 3 above

System of Interacting Particles — III

\mathbf{M} turns out to be a $3N \times 3N$ diagonal matrix. Letting

$$\mu_{3j-2} = \mu_{3j-1} = \mu_{3j} \doteq m_j, \quad j = 1, \dots, N,$$

the entries of \mathbf{M} and \mathbf{M}^{-1} read

$$[\mathbf{M}]_{kn} = \mu_n \delta_{kn}, \quad [\mathbf{M}^{-1}]_{kn} = \frac{\delta_{kn}}{\mu_n}.$$

The Hamiltonian function takes the form

$$\text{Total Energy} = T_a + V_a = \frac{1}{2} \boldsymbol{\xi}^T \mathbf{M} \boldsymbol{\xi} + \frac{1}{2} \boldsymbol{\xi}^T \mathbf{C} \boldsymbol{\xi} + V_{ao},$$

which can be diagonalized by means of the eigenvalue equation

$$\mathbf{C} \boldsymbol{\eta}_\sigma = \lambda_\sigma \mathbf{M} \boldsymbol{\eta}_\sigma, \quad \sigma = 1, \dots, 3N.$$

The eigenvalues λ_σ are real because \mathbf{C} and \mathbf{M} are real and symmetrical, hence the eigenvectors $\boldsymbol{\eta}_\sigma$ are real as well. In addition, as \mathbf{C} and \mathbf{M} are positive definite, the eigenvalues are positive and the eigenvectors are linearly independent. They can also be taken orthonormal with respect to \mathbf{M} :

$$\boldsymbol{\eta}_\sigma^T \mathbf{M} \boldsymbol{\eta}_\tau = \delta_{\sigma\tau}.$$

- Here Total Energy is the sum of two Quadratic forms and $K.E = T_a$ is Diagonal because Matrix \mathbf{M}' is Diagonal.

→ on The other Hand for $P \cdot E = \frac{1}{2} \xi^T C \xi$
'C' is not Diagonal . At this point we can
recall on How to Diagonalise the Matrix !

• When we have a Symmetric Matrix The Eigen
values of the Matrix are Real

which implies Eigen vectors can also be taken
as Real.

• Besides being Symmetric C is also
Positive Definite i.e The Eigen values
besides being Real are also positive.

→ ∵ C is Symmetric & Positive Definite
if you rotate a Matrix or the P.E is
what you do is introduce a change in the
vector size (ξ) This may diagonalize the
P.E but destroy KE which is already diagonal

* ∵ The issue is to find transformation that
makes 'C' diagonal & transforms 'M'

into something that is still diagonal.

This is accomplished by a Eigenvalue λ_σ

$$C\eta_\sigma = \lambda_\sigma M\eta_\sigma \quad \sigma = 1, \dots, 3N$$



$$C\eta_\sigma = \lambda_\sigma M\eta_\sigma, \quad \sigma = 1, \dots, 3N.$$

The eigenvalues λ_σ are real because C and M are real and symmetrical, hence the eigenvectors η_σ are real as well. In addition, as C and M are positive definite, the eigenvalues are positive and the eigenvectors are linearly independent. They can also be taken orthonormal with respect to M :

$$\eta_\sigma^T M \eta_\tau = \delta_{\sigma\tau}.$$

- * Here possible Eigenvalues λ_σ are $3N$.
They will be positive but may not be different from each other. To each Eigenvalue we associate an Eigenvector.

- We can always select the EV's so that they are mutually orthogonal. and EV's would be linearly independent and finally considering that the EV η_σ is homogeneous. The EV's

are defined apart from a Multiplicative Constant.

Due to special form of EV eqn i.e

$$C\eta_\sigma = \lambda_\sigma M \eta_\sigma$$

- The orthogonality condition we impose on EV's will also be special it has the form that is on the last line.

$$\eta_\sigma^T M \eta_T = \delta_{\sigma T}$$

$$\text{for } \sigma = T \quad \delta_{\sigma T} = 1$$

$$\sigma \neq T \quad \delta_{\sigma T} = 0$$

i.e The EV's are mutually orthogonal w.r.t Matrix 'M'

→ The difficult part of above analysis is

to solve the eigen value eqⁿ

$$C\eta_\sigma = J_\sigma M \eta_\sigma$$

$$\sigma = 1, \dots, 2N$$

because it is a system of order $2N$ which is enormous.

- We shall see in a crystal this eqⁿ simplifies very much. This is thanks to periodicity of the crystal

→ Assume for now, we have a solⁿ i.e

all values of J_σ & η_σ

for $\sigma = 1, \dots, N$

and we also know that the EV's are mutually independent.

Total Energy

Diagonalization of the Hamiltonian Function — I

Let \mathbf{G} be the $3N \times 3N$ matrix whose columns are made of the eigenvectors:

$$\mathbf{G} = \begin{bmatrix} \eta_{11} & \eta_{21} & \cdots & \eta_{3N,1} \\ \eta_{12} & \eta_{22} & & \eta_{3N,2} \\ \vdots & & \ddots & \vdots \\ \eta_{1,3N} & \eta_{2,3N} & \cdots & \eta_{3N,3N} \end{bmatrix}.$$

all columns of
 ' \mathbf{G} ' are linearly independent \Rightarrow ' \mathbf{G} ' is Non Singular Matrix
 $\therefore \mathbf{G}^{-1}$ exists

- As the eigenvectors are orthonormal with respect to \mathbf{M} , the following hold:

$$\mathbf{G}^T \mathbf{M} \mathbf{G} = \mathbf{I}$$

$$\Rightarrow \begin{cases} \mathbf{G}^T \mathbf{M} = \mathbf{G}^{-1}, & \mathbf{M} \mathbf{G} = (\mathbf{G}^T)^{-1} \\ \mathbf{G} \mathbf{G}^T \mathbf{M} = \mathbf{I}, & \mathbf{M} \mathbf{G} \mathbf{G}^T = \mathbf{I} \end{cases}$$

→ To conclude this part we will use the above equations into the original expression for Total Energy

The Hamiltonian function takes the form

$$\text{Total Energy} = T_a + V_a = \frac{1}{2} \dot{\boldsymbol{\xi}}^T \mathbf{M} \dot{\boldsymbol{\xi}} + \frac{1}{2} \boldsymbol{\xi}^T \mathbf{C} \boldsymbol{\xi} + V_{a0},$$

which can be diagonalized by means of the eigenvalue equation

We will use for the Identity Matrix 'I' one of the expressions we derived from $G^T M G = I$



Diagonalization of the Hamiltonian Function — II

Let L be the $3N \times 3N$ diagonal matrix made of the eigenvalues:

$$L \doteq \begin{bmatrix} \lambda_1 & & & & & \\ & \lambda_2 & & & & \\ & & \lambda_3 & & & \\ & & & \ddots & & \\ & & & & \lambda_{3N-2} & \\ & & & & & \lambda_{3N-1} \\ & & & & & & \lambda_{3N} \end{bmatrix}.$$

The set of $3N$ eigenvalue equations can then be given the compact form

$$CG = MGL \Rightarrow G^T C G = \underbrace{G^T M G}_I L = L.$$

As a consequence,

- $\xi^T C \xi = \xi^T (\underbrace{MGG^T}_I) C (\underbrace{GG^T M}_I) \xi =$
 $= (\xi^T MG)(G^T CG)(G^T M \xi) = (\xi^T MG)L(G^T M \xi).$
- Let $b \doteq G^{-1}\xi = G^T M \xi$, whence $\xi = Gb$, $\xi^T = b^T G^T$, and
 $\xi^T MG = b^T G^T MG = b^T \Rightarrow \xi^T C \xi = b^T L b.$

Similarly,

$$\xi^T M \xi = b^T G^T MG b = b^T b.$$

Non Diagonal Quadratic form for the P.E

we have transformed it to a Diagonal form

$i.e \quad \xi^T C \xi = b^T L b$

Here the QF for the E still stays Diagonal

$$\dot{\xi}^T M \dot{\xi} = \dot{b}^T \dot{b}$$

Conclusion: We have successfully made Total Energy Diagonal.

\dot{b} = derivative of ' b '

Diagonalization of the Hamiltonian Function — III

- The eigenvalues λ_σ are positive and are the inverse of a time squared. In conclusion, letting $\omega_\sigma^2 = \lambda_\sigma$,

$$T_a + V_a = \frac{1}{2} \dot{b}^T \dot{b} + \frac{1}{2} b^T L b + V_{a0},$$

$$T_a + V_a = \sum_{\sigma=1}^{3N} H_\sigma + V_{a0}, \quad H_\sigma \doteq \frac{1}{2} \dot{b}_\sigma^2 + \frac{1}{2} \omega_\sigma^2 b_\sigma^2.$$

- From the expression of H_σ it follows

$$\frac{\partial H_\sigma}{\partial \dot{b}_\sigma} = \dot{b}_\sigma, \quad \frac{\partial H_\sigma}{\partial b_\sigma} = \omega_\sigma^2 b_\sigma.$$

- The above show that H_σ can be identified with the Hamiltonian function of a linear harmonic oscillator of unit mass and canonical coordinates $q_\sigma = b_\sigma$, $p_\sigma = \dot{b}_\sigma$, whence

$$\dot{p}_\sigma = \ddot{b}_\sigma, \quad \dot{p}_\sigma = -\frac{\partial H_\sigma}{\partial b_\sigma} = -\omega_\sigma^2 b_\sigma \Rightarrow \ddot{b}_\sigma = -\omega_\sigma^2 b_\sigma.$$

Q) What are the units of L ?

Ans $\because 'L'$ is a Diagonal matrix made of the eigen values (λ_σ)

$$T_a + V_a = \frac{1}{2} \dot{b}^T \dot{b} + \frac{1}{2} b^T L b + V_{a0}$$

both quantities should have same unit

$\therefore 'L'$ must have the units of Inverse of

Time Square

$$\therefore \omega^2 = \dot{\vartheta}_\sigma$$

ω = Angular frequency

we can write

$$\dot{b}_\sigma^T \dot{b}_\sigma = \dot{b}_\sigma^2 \quad \& \quad b_\sigma^T b_\sigma = b_\sigma^2$$

$$T_a + V_a = \sum_{\sigma=1}^{3N} H_\sigma + V_{a0}$$

$$H_\sigma = \frac{1}{2} \dot{b}_\sigma^2 + \frac{1}{2} \omega_\sigma^2 b_\sigma^2$$

$$T_a + V_a = \sum_{\sigma=1}^{3N} H_\sigma + V_{a0}, \quad H_\sigma = \frac{1}{2} \dot{b}_\sigma^2 + \frac{1}{2} \omega_\sigma^2 b_\sigma^2.$$

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The sum of

$$\frac{1}{2} \dot{b}_\sigma^2 + \frac{1}{2} \omega_\sigma^2 b_\sigma^2 = H_\sigma$$

In conclusion: we have separated the Total system's sum of individual degree of freedom

It is total energy associated to single degree of freedom of the system & the total energy apart from from the constant V_{a0} can be written as

$$T_a + V_a = \sum_{\sigma=1}^{3N} H_\sigma + V_{ao}$$

∴ Since the individual degrees of freedom are separate. They do not exchange energy from each other.

~~That means that the Total energy of the S/S is conserved also the Individual degrees of Freedom are also conserved.~~

→ H_σ is the Hamiltonian function of individual degree of freedom

• we remember that the derivative of Hamiltonian w.r.t the co-ordinate is (- derivative of momentum)
i.e (- Force)

• and derivative of Hamiltonian w.r.t Momentum
= velocity of the degrees of freedom

- The above show that H_σ can be identified with the Hamiltonian function of a linear harmonic oscillator of unit mass and canonical coordinates $q_\sigma = b_\sigma$, $p_\sigma = \dot{b}_\sigma$, whence

$$\dot{p}_\sigma = \ddot{b}_\sigma, \quad \dot{p}_\sigma = -\frac{\partial H_\sigma}{\partial b_\sigma} = -\omega_\sigma^2 b_\sigma \Rightarrow \ddot{b}_\sigma = -\omega_\sigma^2 b_\sigma.$$

This does not mean atoms behave like linear harmonic oscillators.

because $\xi = G b$

Diagonalization of the Hamiltonian Function — IV

Finally,

$$b_\sigma(t) = b_{\sigma 0} \cos(\omega_\sigma t + \varphi_\sigma) = \\ = \frac{1}{2} \{ \tilde{b}_{\sigma 0} \exp(-j\omega_\sigma t) + \tilde{b}_{\sigma 0}^* \exp(j\omega_\sigma t) \},$$

where $b_{\sigma 0}$, φ_σ are two constants depending on the initial conditions $b_\sigma(0)$, $\dot{b}_\sigma(0)$, while $\omega_\sigma \doteq \sqrt{\omega_\sigma^2}$ and $\tilde{b}_{\sigma 0} \doteq b_{\sigma 0} \exp(-j\varphi_\sigma)$.

The $3N$ quantities b_σ are called *normal coordinates* or *principal coordinates*. The oscillation of the normal coordinate of index σ is also called a *mode* of the vibrating system. Once the normal coordinates have been determined, the displacements are calculated from

$$\xi = G b, \quad \xi_r = s_r - s_{r0} = \sum_{\sigma=1}^{3N} \eta_{\sigma r} b_\sigma,$$

- hence they are superpositions of oscillatory functions. The initial conditions $b_\sigma(0)$, $\dot{b}_\sigma(0)$ are derived from those on ξ_r by means of

$$b(0) = G^{-1} \xi(0), \quad \dot{b}(0) = G^{-1} \dot{\xi}(0).$$

* All the calculations have been performed fully in the

Classical Mechanics environment. But when we have reached this point it's relatively easy to Quantize the system because the Quantization of LHO is a very well known problem of QM

Diagonalization of the Hamiltonian Function — V

From

$$T_a + V_a - V_{a0} = \sum_{\sigma=1}^{3N} H_{\sigma},$$

where each H_{σ} corresponds to one degree of freedom, it follows that the system is completely separable in the normal coordinates, and that each normal coordinate evolves as a linear harmonic oscillator. The total energy can be expressed in terms of the initial conditions as

$$T_a + V_a = V_{a0} + \sum_{\sigma=1}^{3N} E_{\sigma}, \quad E_{\sigma} \doteq \frac{1}{2} \dot{b}_{\sigma}^2(0) + \frac{1}{2} \omega_{\sigma}^2 b_{\sigma}^2(0).$$

One also sees that to calculate the displacements it is necessary to preliminarily determine the eigenvalues ω_{σ}^2 and the eigenvectors η_{σ} . For this, one must solve the eigenvalue equation

$$\mathbf{C}\boldsymbol{\eta}_{\sigma} = \omega_{\sigma}^2 \mathbf{M}\boldsymbol{\eta}_{\sigma}, \quad [\mathbf{C}]_{kn} = \left(\frac{\partial^2 V_a}{\partial \xi_k \partial \xi_n} \right)_0, \quad [\mathbf{M}]_{kn} = \mu_n \delta_{kn}.$$

The real difficulty is to solve this Eigenvalue eqⁿ we didn't solve it.

The solution is easy if the structure is periodic



Calculation of the Normal Coordinates — I

To calculate the normal coordinates that describe the dynamics of the nuclei in a crystal, it is necessary solve the eigenvalue equation

$$\mathbf{C}\boldsymbol{\eta}_\sigma = \omega_\sigma^2 \mathbf{M}\boldsymbol{\eta}_\sigma, \quad [\mathbf{C}]_{kn} = \left(\frac{\partial^2 V_a}{\partial \xi_k \partial \xi_n} \right)_0, \quad [\mathbf{M}]_{kn} = \mu_n \delta_{kn},$$

where V_a is the potential energy, ξ_k the displacement of the k th degree of freedom with respect to the equilibrium position, and μ_k the mass associated to the k th degree of freedom.

The calculation of the normal coordinates is in principle the same for any system of particles. However, if the system has special properties, they reflect into the form of the normal coordinates. A particularly important case is that of a periodical structure, such as a crystal.

Let the crystal be made of N_c elementary cells, with a basis made of N_b nuclei. It follows that the total number of nuclei is $N = N_b N_c$, and the total number of degrees of freedom is $3N$.

→ we an Eigen value to solve, the Matrix ' C ' is the Elastic Matrix so it made of the 2nd derivative of Potential Energy w.r.t co-ordinates calculated at the Equilibrium. and Matrix ' M ' is the matrix of the masses it is a Diagonal Matrix The masses are indicated as $\mu_n \delta_{kn}$

- we assume that the δ_{kn} that we are

Considering is a crystal i.e. a Periodic structure we remember that we introduced a concept of Elementary cell & There are the elementary cells of a Direct lattice.

- The cells are equal to each other, they cover completely the crystal and assume that the no. of cells is some N_c

Basis: Group of atoms that replicate itself periodically, basis is made of N_b nuclei

∴ Total no. of Nuclei is

$$N = N_b N_c$$



Calculation of the Normal Coordinates — II

- With respect to a given origin, the m th cell is identified by the corresponding translational vector of the direct lattice, \mathbf{l}_m . Such a vector determines the local origin within the m th cell. In turn, the equilibrium position of the α th nucleus of the m th cell with respect to the local origin is identified by a vector ρ_α of the direct lattice.
- It is convenient to number the degrees of freedom in such a way as to distinguish the indices of the cells from those of the basis and of the coordinate axes. To this purpose, one observes that the component along the u th coordinate axis of the equilibrium position of the j th nucleus is

$$X_{ju0} = s_{q0}, \quad q = u + 3(j-1), \quad j = \alpha + N_b(m-1),$$

with coordinate axis

$$u = 1, 2, 3,$$

$$\rho_\alpha$$

$$\alpha = 1, \dots, N_b,$$

$$\ln$$

$$m = 1, \dots, N_c.$$

- The same applies to the displacements, which are more conveniently expressed in terms of three indices:

$$\xi_q \leftarrow \xi_{max}, \quad \xi_r \leftarrow \xi_{n\beta w}.$$

To proceed further we must be able to identify each individual cell of the crystal.

and must also identify the atoms that form the Basis.

For each atom of the Basis we must be able to identify the equilibrium position and the displacement.

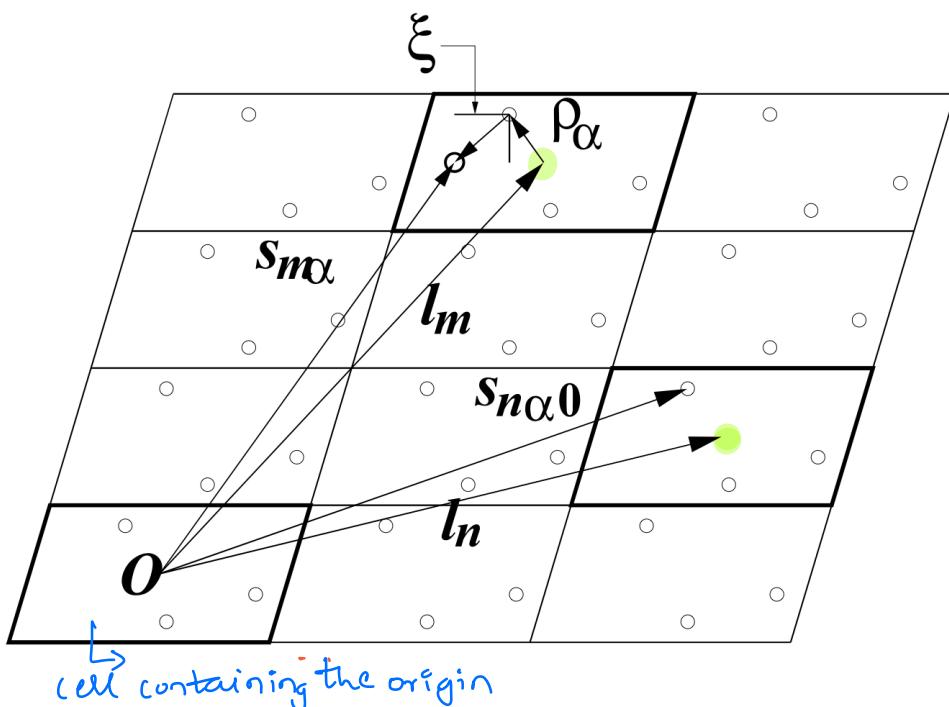
→ Technical difficulty is that now we have to quit the very convenient method of one index (i.e. we numbered all the degrees of freedom with one index) which we can do it anymore

we must distinguish indices for the cells,

- indices for the Equilibrium position of atom inside the cell.

- also the indices for the Displacements

The notion will become very difficult but eventually because of the periodicity we will be able to arrive at a simpler solution.



→ Q) How does notation change because of many indices?

Calculation of the Normal Coordinates — III

- The entries of \mathbf{C} are identified in the same manner:

$$c_{qr} = \left(\frac{\partial^2 V_a}{\partial \xi_q \partial \xi_r} \right)_0 \quad \leftarrow \quad c_{m\alpha u}^{n\beta w} = \left(\frac{\partial^2 V_a}{\partial \xi_{m\alpha u} \partial \xi_{n\beta w}} \right)_0,$$

with elastic matrix with '2' indices elastic matrix with '4' indices

$m, n = 1, \dots, N_c, \quad \alpha, \beta = 1, \dots, N_b, \quad u, w = 1, 2, 3.$

- As the order of derivation is irrelevant, it is $c_{m\alpha u}^{n\beta w} = c_{n\beta w}^{m\alpha u}$. It should also be noted that, as the number of nuclei is finite, the crystal is not actually periodical. Periodicity can formally be recovered by imposing periodical boundary conditions to the quantities of interest.
- With this provision, the entries of \mathbf{C} become invariant with respect to the lattice translations. The latter are related only to the cell indices m, n and are obtained by the replacements

$$\mathbf{l}_m \leftarrow \mathbf{l}_m + \mathbf{l}_\nu, \quad \mathbf{l}_n \leftarrow \mathbf{l}_n + \mathbf{l}_\nu, \quad \text{translation}$$

with ν any integer. In particular, taking $\mathbf{l}_\nu = -\mathbf{l}_n$ yields

$$c_{m\alpha u}^{n\beta w} = c_{\alpha u}^{\beta w}(\mathbf{l}_m, \mathbf{l}_n) = c_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n, 0) = c_{\alpha u}^{\beta w}(\mathbf{l}_m - \mathbf{l}_n).$$

↓
force applied on an atom placed in
cell no 'm' due to the action of another atom
that belongs to the cell no 'n'

Now this action must depend on the relative position of the two cells not on the absolute position because the force b/w two atoms cannot depend on the origin of reference.



Calculation of the Normal Coordinates — IV

- The above shows that the entries of \mathbf{C} depend only on the relative positions of the cells. The periodic boundary conditions are actually an approximation; however, the interatomic interactions typically give rise to short-range forces, hence the above reasoning holds for all the cells that are not too close to the boundaries.
- Due to the invariance of \mathbf{C} with respect to the lattice translations one sees that, given α, u and β, w , there are only N_c distinct entries of \mathbf{C} out of N_c^2 , namely, those such that

$$m - n = 0, \quad m - n = 1, \quad \dots, \quad m - n = N_c - 1.$$

- In fact, all the remaining $N_c^2 - N_c$ entries are derived from the first N_c ones by suitable translations of the indices.
- In turn, using the new indices the entries of \mathbf{M} read

$$\mu_r \delta_{qr} \leftarrow \mu_{n\beta w} \delta_{m\alpha u}^{n\beta w} = \mu_\beta \delta_{m\alpha u}^{n\beta w},$$

- where the last equality is due to the fact that the mass of a given nucleus of the cell does not depend on the cell position within the crystal nor on the coordinate axis.

∴ we also need to simplify Mass Matrix.

