

## Lecture 1

Lecturer: G. S. Paraoanu

*Department of Applied Physics, School of Science,  
Aalto University, P.O. Box 15100, FI-00076 AALTO, Finland*



- power density, i.e., how much heat they generate. Presently approaching  $6 \text{ W/mm}^2 = 600 \text{ W/cm}^2$ .

Compare with a light bulb  $\simeq 0.01 \text{ W/mm}^2 = 1 \text{ W/cm}^2$  and our Sun  $= 60 \text{ W/mm}^2$ .

### III. CLASSICAL WAVE PHYSICS

Recall plane waves have the form

$$\psi(x) = e^{ikx}, \quad (1)$$

where  $x$  denotes the position, and  $k$  the wavenumber. The wavelength  $\lambda$  relates to the wavenumber via  $\lambda = 2\pi/k$ . Furthermore, recognizing the dimensionless quantity  $\phi = kx$  as the phase, Eq. 1 is more compactly  $\psi(x) = e^{i\phi}$ .

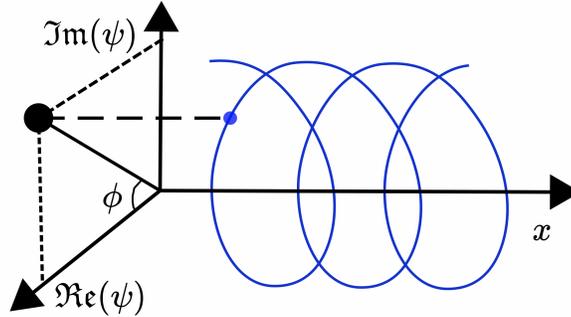


FIG. 2.

( $k, \omega$ )-space

-Defined by the respective Fourier transforms

$$\psi[k] = \int_{-\infty}^{\infty} dx e^{-ikx} \psi(x) \iff \psi(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} \psi[k] \quad (2)$$

$$\psi[k, \omega] = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt e^{-ikx + i\omega t} \psi(x, t) \iff \psi(x, t) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\omega e^{ikx - i\omega t} \psi[k, \omega]. \quad (3)$$

Some properties:

Real coordinates ( $x, t$ )	Fourier coordinates ( $k, \omega$ )
shifted by $x_0$	$x e^{-ikx_0}$
$x e^{ik_0x}$	shifted by $k_0$
shifted by $t_0$	$x e^{i\omega t_0}$
$x e^{-i\omega_0t}$	shifted by $\omega_0$

#### IV. QUANTUM MECHANICS

Recall, the time-dependent Schrödinger equation is

$$i\hbar \frac{d}{dt} \psi(x, t) = H \psi(x, t) , \quad (4)$$

where  $\psi(x, t)$  is the wavefunction. Also, the probability density is  $|\psi(x, t)|^2$  and the probability that a particle is between points a and b is

$$\int_a^b |\psi(x, t)|^2 dx . \quad (5)$$

- Typically  $H = \text{kinetic energy} + \text{potential energy}$ , i.e.,

$$H = \frac{p^2}{2m} + V , \quad (6)$$

where  $p$  is the momentum operator, which in the position representation reads

$$p = -i\hbar \frac{d}{dx} . \quad (7)$$

Importantly,  $p$  relates to the position operator  $x$  via the canonical commutation relation:

$$[x, p] = i\hbar \quad (8)$$

- Dirac notation, aka bra-ket notation.

1.  $\psi(x, t) = \langle x | \psi(t) \rangle$ .
2.  $\int_{-\infty}^{\infty} dx |\psi(x, t)|^2 = \int_{-\infty}^{\infty} dx \langle \psi(t) | x \rangle \langle x | \psi(t) \rangle = \langle \psi(t) | \psi(t) \rangle = 1$ , where we have used  $\int_{-\infty}^{\infty} |x\rangle \langle x| = \mathbb{I}$ .

3. Schrödinger equation:  $i\hbar \frac{d}{dt} = H|\psi(t)\rangle$

Note it is possible to have a time-dependent Hamiltonian  $H(t)$ . However, if  $H$  is time-independent, we can solve the Schrödinger equation by the method of separation of variables.

4. Time-evolution:  $|\psi(t)\rangle = e^{-i\frac{E}{\hbar}t}|\psi(0)\rangle$ .

5. Eigenvector-eigenvalue problem:  $H|\psi\rangle = E|\psi\rangle$ .

Example: Free-particle, i.e.,  $V(x) = 0$ .

The Schrödinger equation is  $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x)$ , where  $\psi(x) = \psi e^{\pm ikx}$ , with  $k = \sqrt{2mE/\hbar^2}$ . So overall,  $\psi(x, t) = \psi e^{\pm i(kx - \omega t)}$ , where  $\omega = E/\hbar$ .

### A. Infinite square well

Consider an infinite square well potential with the boundaries

$$V(x) = \begin{cases} 0, & x \in [-L/2, L/2] \\ \infty, & x \in (-\infty, -L/2) \cup (L/2, +\infty) . \end{cases} \quad (9)$$

We seek the eigenenergies and eigenstates.

**Solution:**

$$\psi(x) = A \sin(kx + kL/2).$$

The boundary conditions are

$$\begin{cases} x = -L/2 \rightarrow \psi(-L/2) = 0 \\ x = L/2 \rightarrow \psi(L/2) = A \sin(kL) = 0 , \end{cases} \quad (10)$$

where the second condition implies that  $k_n L = n\pi$ .

With normalization we have

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_{-L/2}^{L/2} dx A^2 \sin^2 \left( \frac{n\pi}{L} x + \frac{n\pi}{2} \right) = 1 , \quad (11)$$

which implies that  $A = \sqrt{2/L}$ . Moreover, the eigenstates are

$$\psi_n(x) = \sqrt{2/L} \sin \left( k_n x + \frac{k_n L}{2} \right) , \quad (12)$$

where  $n = 1, 2, 3 \dots$ .

The eigen-energies are recovered from the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) = E_n \psi_n(x), \quad (13)$$

where we find  $E_n = \hbar^2 k_n^2 / 2m$ .

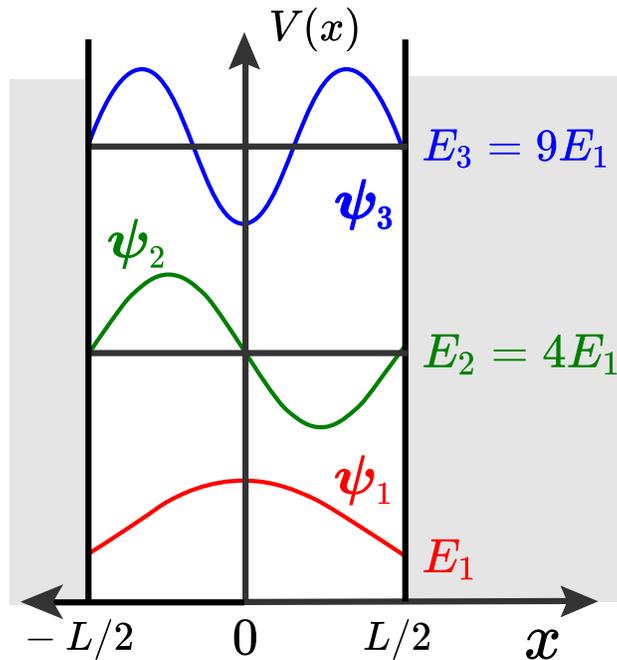


FIG. 3. 1-D infinite square well potential.

### Important observations:

- there exists a minimum non-zero energy  $E_1 = \hbar^2 \pi^2 / 2mL^2$ , corresponding to the ground state  $\psi_1$ . So a particle in a box always has some kinetic energy! This is very different from classical physics.
- energy levels are quantized – not every energy is allowed!– and form a discrete ladder.
- $E_n \propto 1/L^2$ . The larger the box, the smaller the gap between levels. Eventually, as  $L \rightarrow \infty$  we reach the continuum again.

## B. The quantum harmonic oscillator

The quantum harmonic oscillator has the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 . \quad (14)$$

We wish to find eigenenergies and eigenstates.

Solution:

$E_n = (n + 1/2)\hbar\omega$ , where  $n = 0, 1, 2, \dots$ .

$\psi_n(x) = N_n e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$ , where  $N_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$ , and  $H_n$  is a Hermite polynomial of degree  $n$ . Explicitly,  $H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} (e^{-z^2})$ , so

$$H_0(z) = 1$$

$$H_1(z) = 2z$$

$$H_2(z) = 4z^2 - 2$$

$$H_3(z) = 8z^3 - 12z$$

$$\bullet \quad a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{i}{m\omega} p\right) \quad x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$\bullet \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{i}{m\omega} p\right) \quad p = i\sqrt{\frac{\hbar m\omega}{2}} (a^\dagger - a)$$

- The number operator  $N = a^\dagger a$ ,  $N|n\rangle = n|n\rangle$ , where  $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$ . Note:  $a|0\rangle = 0$ . Therefore, in terms of the number operator, the Hamiltonian is  $H = \hbar\omega(N + 1/2)$ .

- Commutation relations:

$$[a, a^\dagger] = 1$$

$$[N, a^\dagger] = a^\dagger$$

$$[N, a] = -a$$

Important Observations:

- Energy levels are equally spaced by  $\hbar\omega$ .
- There exists a minimum energy of  $\hbar\omega/2$  which corresponds to the ground state, i.e., zero-point motion energy.

Example: Calculate the variance  $\langle(\Delta x)^2\rangle \equiv \langle x^2\rangle - \langle x\rangle^2$  for the vacuum state  $|0\rangle$ , where  $\Delta x$  denotes the standard deviation of  $x$ .

Solution:

With  $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ , we find  $\langle x\rangle = 0$ , and  $\langle x^2\rangle = \frac{\hbar}{2m\omega}$ . Therefore,  $\langle x^2\rangle = x_{zpf}^2$ , where  $x_{zpf} = \sqrt{\frac{\hbar}{2m\omega}}$  is the zero-point fluctuation.

### C. Spin-1/2 particles

- Comes from the Stern-Gerlach experiment where a beam of silver atoms running through a non-homogeneous magnetic field is split into two beams.
- Angular momentum

$$\mathbf{S} = \frac{\hbar}{2} \boldsymbol{\sigma} \qquad \boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$$

$s = 1/2$ :

$$|s, m\rangle = \begin{cases} |\frac{1}{2}, \frac{1}{2}\rangle & m = 1/2 \\ |\frac{1}{2}, -\frac{1}{2}\rangle & m = -1/2 \end{cases} \qquad (15)$$

$$S^2|\frac{1}{2}, \frac{1}{2}\rangle = \hbar^2 s(s+1)|\frac{1}{2}, \frac{1}{2}\rangle = \frac{3}{4}\hbar^2|\frac{1}{2}, \frac{1}{2}\rangle .$$

- In quantum information,

$$\left. \begin{array}{l} |\frac{1}{2}, \frac{1}{2}\rangle \equiv |0\rangle \\ |\frac{1}{2}, -\frac{1}{2}\rangle \equiv |1\rangle \end{array} \right\} \text{qubit states} \qquad (16)$$

General qubit state:  $|\psi\rangle = \cos \frac{\theta}{2}|0\rangle + e^{i\phi} \sin \frac{\theta}{2}|1\rangle .$

- Eigenvectors-eigenvalues:

Question: What is the analogue of zero-point fluctuations for spin-1/2?

$$\begin{array}{c}
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \left| \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \left| \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
\sigma_x |\chi_{\pm}^{(x)}\rangle = \pm |\chi_{\pm}^{(x)}\rangle \quad \sigma_y |\chi_{\pm}^{(y)}\rangle = \pm |\chi_{\pm}^{(y)}\rangle \quad \sigma_z |0\rangle = |0\rangle, \sigma_z |1\rangle = -|1\rangle \\
|\chi_{\pm}^{(x)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \quad |\chi_{\pm}^{(y)}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} \quad |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\end{array}$$

#### D. Many-particle quantum systems

In many-particle systems it is necessary to concatenate the Hilbert spaces of each particle.

$$\begin{array}{ll}
V, W \text{ Hilbert spaces} & |v\rangle \in V, |w\rangle \in W \\
V \otimes W = \text{tensor product} & |v\rangle \otimes |w\rangle \in V \otimes W
\end{array}$$

- But how do we write the wavefunctions?

Say we have two particles, is the wavefunction  $|v\rangle_1 |w\rangle_2$ ,  $|w\rangle_1 |v\rangle_2$  or  $\frac{1}{\sqrt{2}}(\alpha |v\rangle_1 |w\rangle_2 + \beta |w\rangle_1 |v\rangle_2)$ ?

- In nature there are only two types of particles:
  - bosons  $\rightarrow$  symmetric wavefunction
  - fermions  $\rightarrow$  anti-symmetric wavefunction

Good news, we do not necessarily need to work with cumbersome symmetrized or anti-symmetrized wavefunctions. Instead, a compact way of writing the wavefunction is provided by the Fock space:

$$|n_1, n_2, \dots\rangle$$

Bosons:

$$[a_i, a_j^\dagger] = \delta_{ij}$$

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0$$

$$N = \sum_i a_i^\dagger a_i$$

$$a_i^\dagger |\dots, n_i, \dots\rangle = \sqrt{n_i + 1} |\dots, n_i + 1, \dots\rangle$$

$$a_i |\dots, n_i, \dots\rangle = \sqrt{n_i} |\dots, n_i - 1, \dots\rangle$$

$$a_i |\dots, n_i = 0, \dots\rangle = 0$$

$$|n_1, n_2, \dots\rangle = \frac{1}{\sqrt{n_1! n_2! \dots}} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \dots |0, 0, \dots\rangle$$

Fermions:

$$c_i, c_j^\dagger = \delta_{ij}$$

$$c_i, c_j = c_i^\dagger, c_j^\dagger = 0$$

$$N = \sum_i c_i^\dagger c_i$$

$$c_i^\dagger |\dots, n_i, \dots\rangle = (1 - n_i) (-1)^{\sum_{j < i} n_j} |\dots, n_{i+1}, \dots\rangle$$

$$c_i |\dots, n_i, \dots\rangle = n_i (-1)^{\sum_{j < i} n_j} |\dots, n_{i-1}, \dots\rangle$$

$$c_i |\dots, n_i = 0, \dots\rangle = 0$$

$$c_i^\dagger |\dots, n_i = 1, \dots\rangle = 0 \longrightarrow \text{Pauli exclusion principle.}$$

$$|n_1, n_2, \dots\rangle = (c_1^\dagger)^{n_1} (c_2^\dagger)^{n_2} \dots |0, 0, \dots\rangle$$

## V. ELEMENTS OF SOLID STATE PHYSICS

Electrons – they are fermions; i.e., Pauli exclusion principle applies.

– at  $T = 0$ , we fill all the states until we use all of the electrons.

For example, take a wire (just because we have a single  $k$ -vector  $\dots$ ).

At  $T \neq 0$  the distribution of electrons is described by the Fermi-Dirac distribution:

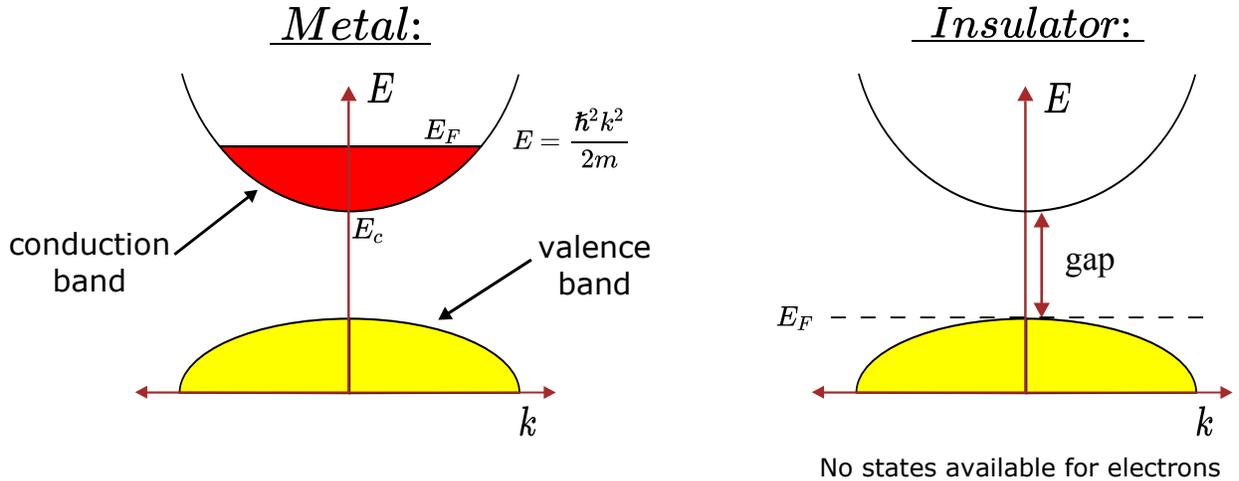


FIG. 4. Energy bands of a metal and insulator.

$$f_{FD}(E) = \frac{1}{\exp[(E - E_F)/k_B T] + 1} \quad (17)$$

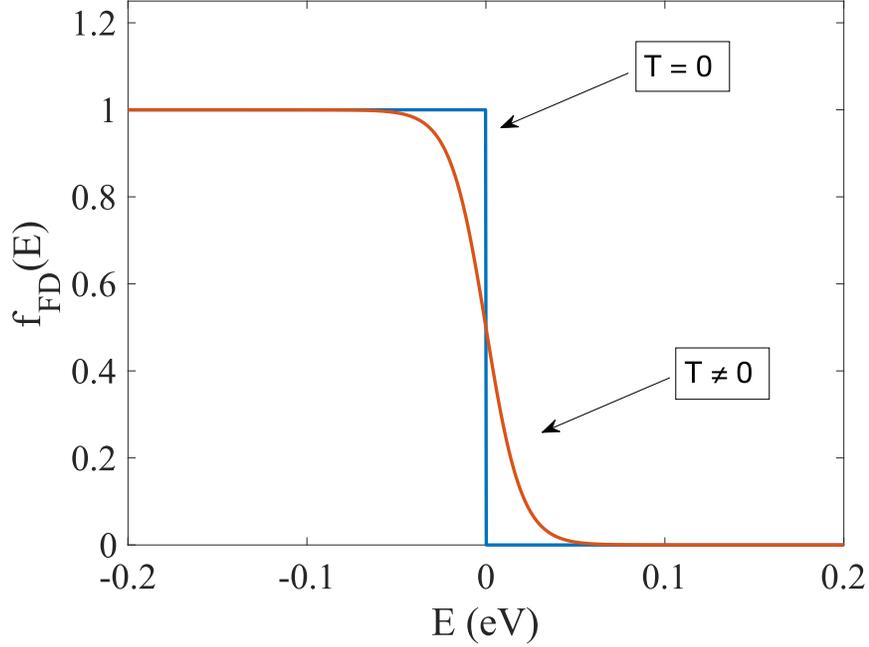


FIG. 5.

Two limits:

- degenerate limit:  $f_{FD}(E) \approx \Theta(E_F - E)$ .
- non-degenerate limit:  $f_{FD} = \exp[-(E - E_F)/k_B T]$   
when  $E - E_F \gg k_B T$ .

Density of states:

Free electron wavefunction:  $\psi(\vec{r}) = \frac{e^{ik_x \cdot x}}{\sqrt{L}} \cdot \frac{e^{ik_y \cdot y}}{\sqrt{L}} \cdot \frac{e^{ik_z \cdot z}}{\sqrt{L}} = \frac{1}{\sqrt{V}} e^{ik \cdot r}$ . Here,  $V$  is the volume in  $k$ -space and  $E = \hbar^2 k^2 / 2m$  is the dispersion relation, where  $k_x = 2\pi n_x / L$ ,  $k_y = 2\pi n_y / L$ , and  $k_z = 2\pi n_z / L$ .

We want to calculate the number of states per volume within an energy interval  $dE$ . This is known as the density of states.

The volume element in k-space is  $V_{3D} = \left(\frac{2\pi}{L}\right)^3$  and the volume of shell between  $k$  and  $k + dk$  is  $V_{dk} = 4\pi k^2 dk$ .

The number of states in this shell is  $2 \cdot \frac{V_{dk}}{V_{3D}} = \frac{k^2 dk}{\pi^2} \cdot L^3$ , where the factor of 2 comes from

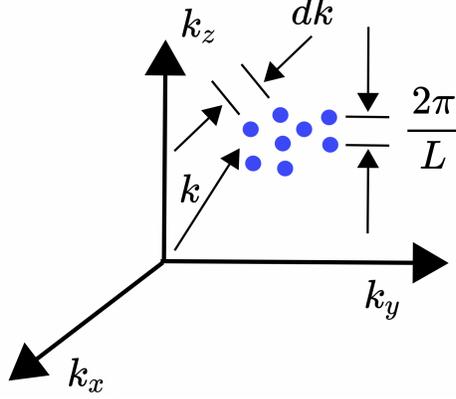


FIG. 6.

the electron spin.

$$E = \hbar^2 k^2 / 2m \implies dk = \frac{1}{\sqrt{2mE/\hbar^2}} \frac{m}{\hbar^2} dE$$

Therefore, the number of states in the interval  $dE$  per unit volume is

$$\mathcal{N}_{3D}(E)dE = \frac{k^2 dk}{\pi^2} = \frac{1}{2\hbar^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} dE . \quad (18)$$

## VI. ELECTROMAGNETISM

Maxwell's equations (in SI units):

$$\begin{aligned} \nabla \times \vec{\mathcal{H}} &= \vec{\mathcal{J}} + \frac{\partial \vec{\mathcal{D}}}{\partial t} && \text{Faraday's Law} \\ \nabla \times \vec{E} &= -\frac{\partial \vec{\mathcal{B}}}{\partial t} && \text{Ampère's Law} \\ \vec{\nabla} \cdot \vec{\mathcal{D}} &= \rho && \text{Coulomb's Law} \\ \vec{\nabla} \cdot \vec{\mathcal{B}} &= 0 && \text{Gauss' Law ,} \end{aligned} \quad (19)$$

where  $\vec{\mathcal{J}}$  is the current density and  $\rho$  is the charge density.

Constitutive relations:

$$\vec{D} = \epsilon \vec{E}$$

$$\begin{aligned} \epsilon &= \epsilon_0 \epsilon_r = \text{electrical permittivity,} \\ \epsilon_0 &= 8.854 \times 10^{-12} \text{ F/m} = \text{vacuum permittivity} \\ \epsilon_r &= \text{relative permittivity} \end{aligned}$$

$$c = \frac{1}{\sqrt{\epsilon_0 \mu_0}} = \text{speed of light in vacuum.}$$

$$\vec{B} = \mu \vec{H}$$

$$\begin{aligned} \mu &= \mu_0 \mu_r = \text{magnetic permeability} \\ \mu_0 &= 4\pi \times 10^{-7} \text{ H/m} = \text{vacuum permeability.} \\ \mu_r &= \text{relative permeability.} \end{aligned}$$

In AC fields:  $\epsilon \rightarrow \epsilon = \epsilon' - i\epsilon''$  &  $\tan \delta \equiv \frac{\epsilon''}{\epsilon'}$  = loss tangent.

Other fundamental relations:

- Ohm's law  $\vec{J} = \vec{\sigma} \cdot \vec{E}$
- Continuity equation:  $-\frac{\partial \rho}{\partial t} = \vec{\nabla} \cdot \vec{J}$

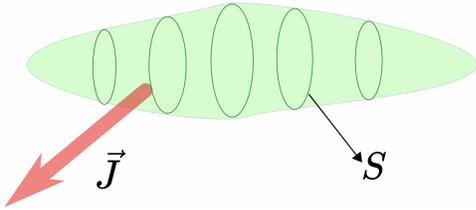


FIG. 7.

- Gauss-Ostrogradsky theorem:  $-\frac{\partial}{\partial t} \iiint_V dV \cdot \vec{\rho} = \oiint_S d\vec{s} \cdot \vec{J}$ , i.e, the rate of decrease of positive charge = total current flux flowing out of the closed surface.

## VII. THERMODYNAMICS

- First law of thermodynamics:  $\Delta U = Q - W$

This is conservation of energy, where  $\Delta U$  denotes the change in internal energy,  $Q$  is the heat supplied to the system, and  $W$  is the work done by the system onto the environment.

- Second law of thermodynamics:  $\delta Q = TdS$  (for reversible processes)

This says that the total entropy of an isolated system can never decrease.  $\delta Q$  denotes the amount of heat transferred and  $dS$  is the change in entropy produced by the transferred heat.

Corollary: It is impossible to construct a cyclic engine that produces work from the energy extracted from a single reservoir (Planck).

- Third law of thermodynamics.

The entropy approaches a constant value when  $T \rightarrow 0$

$$\lim_{T \rightarrow 0} S = \text{const} .$$

### A. Equipartition Theorem

- In thermal equilibrium, energy is shared equally between the degrees of freedom ( $\frac{1}{2}k_B T$  per degree of freedom).

#### Example:

**Ideal gas:**  $E = \frac{1}{2}mv_x^2 + \frac{1}{2}mv_y^2 + \frac{1}{2}mv_z^2 =$  average energy  $= \frac{1}{2}k_B T + \frac{1}{2}k_B T + \frac{1}{2}k_B T = \frac{3}{2}k_B T \implies v_{rms} = \sqrt{\langle v^2 \rangle} = \sqrt{\frac{3k_B T}{m}}$ .

**Harmonic oscillator:**  $E = \frac{p^2}{2m} + \frac{1}{2}kx^2 =$  average energy  $\frac{1}{2}k_B T + \frac{1}{2}k_B T = k_B T$

where  $k_B = 1.38 \times 10^{-23} \frac{\text{m}^2 \text{kg}}{\text{s}^2 \text{K}}$  – Boltzmann's constant.

## VIII. FURTHER READING

Any introductory textbook on quantum mechanics, solid state physics, and electromagnetism should suffice. For example, *cf.*

- The Open University: SM358 The Quantum World  
Science Level 3 Books 1-3
- David J. Griffiths – Introduction to Quantum Mechanics
- Charles Kittel – Introduction to Solid State Physics

- Martin Sibley – Introduction to Electromagnetism

There is a plethora of information, lecture notes, and video lectures on the internet!

---