# Lecture 1

Lecturer: G. S. Paraoanu

*Department of Applied Physics, School of Science,*

*Aalto University, P.O. Box 15100, FI-00076 AALTO, Finland*

## I. INTRODUCTION

In this lecture we will review key concepts from quantum mechanics, electromagnetism, and solid-state physics which will be essential for this course.

## II. MOTIVATION

Moore's Law – Doubling of the number of transistors per chip every 18-24 months.

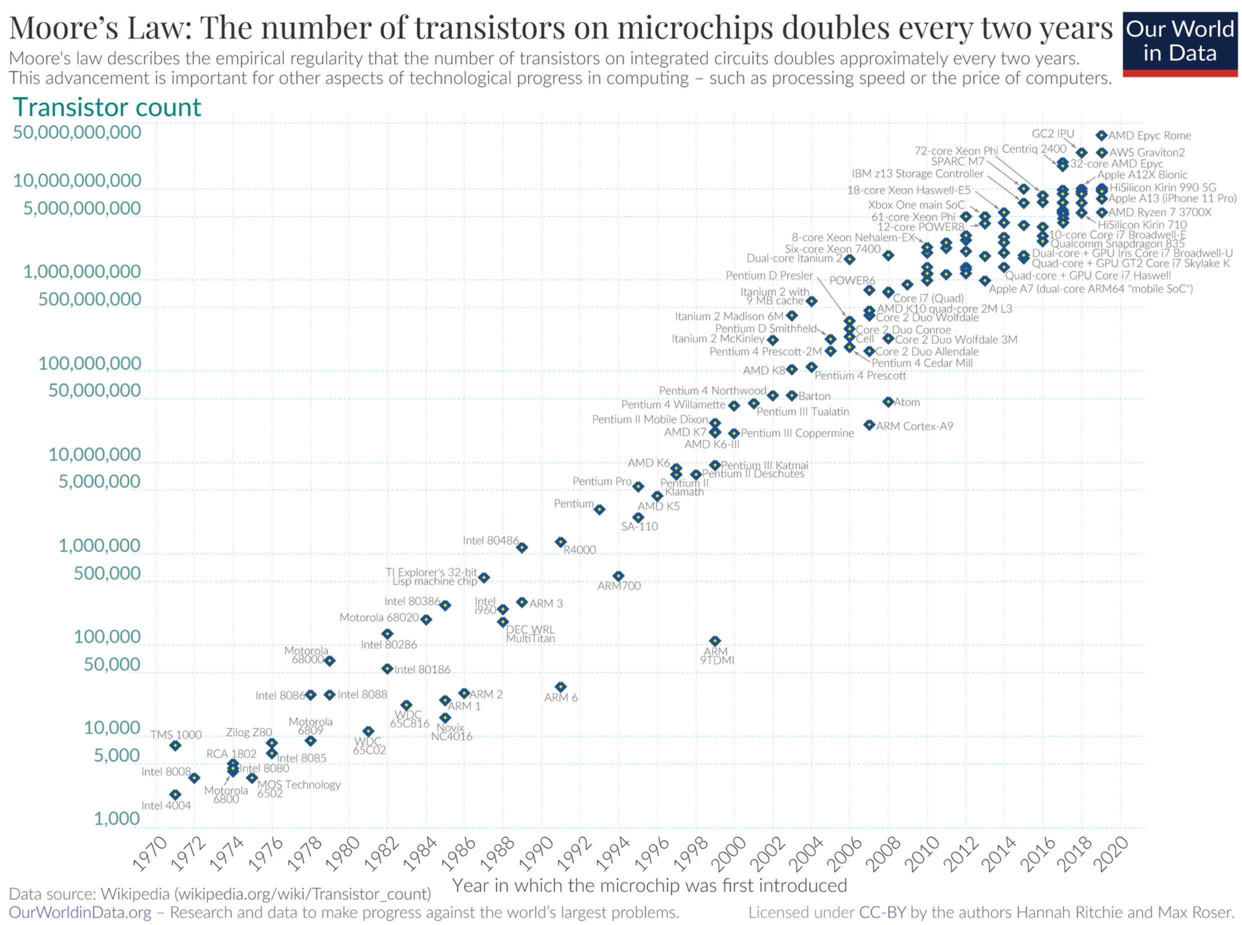


FIG. 1. Moore's Law

– dimension of gate = 5 nm presently! Very near the molecular scale and approaching atomic scale, where quantum effects (tunneling) will become important.

– density: with 5 nm technology has $\simeq 10^8/mm^2$.

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

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

## III. CLASSICAL WAVE PHYSICS

Recall plane waves have the form

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

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 $\psi(x) = e^{i\phi}$.

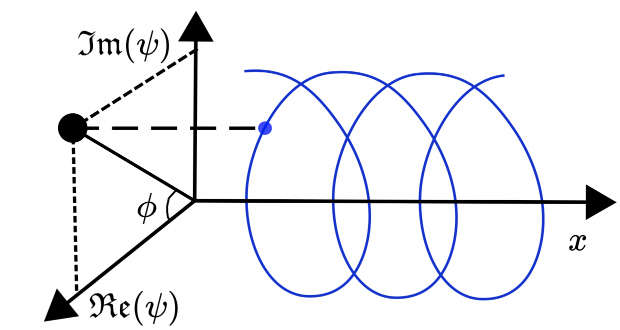


FIG. 2.

(k,$\omega$)-space

-Defined by the respective Fourier transforms

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

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

Some properties:

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

## IV. QUANTUM MECHANICS

Recall, the time-dependent Schrödinger equation is

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

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

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

- Typically $H$ = kinetic energy + potential energy, i.e.,

$$H = \frac{p^2}{2m} + V \ , \tag{6}$$

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

$$p = -i\hbar\frac{d}{dx} \ . \tag{7}$$

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

$$[x,p] = i\hbar \tag{8}$$

- 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 that 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: $H|\psi\rangle = E|\psi\rangle$.

### A. Free particle

For a free particle by definition $V(x) = 0$.

**Solution:**

The time-dependent Schrödinger equation is $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$, and can be solved by $\psi(x) = \psi e^{\pm ikx}$, with $k = \sqrt{2mE/\hbar^2}$.

Then, using the method above, we can write the solution of the time-dependent Schr$\acute{}$odinger equation $i\hbar\frac{d}{dt} = H|\psi(t)\rangle$ as $\psi(x,t) = \psi e^{\pm i(kx-\omega t)}$, where $\omega = E/\hbar$.

### B. Infinite square well

Consider an infinite square well potential with the boundaries

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

We seek the eigenenergies and eigenstates.

**Solution:**

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

The boundary conditions are

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

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

With normalization we have

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

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

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

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

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

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

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

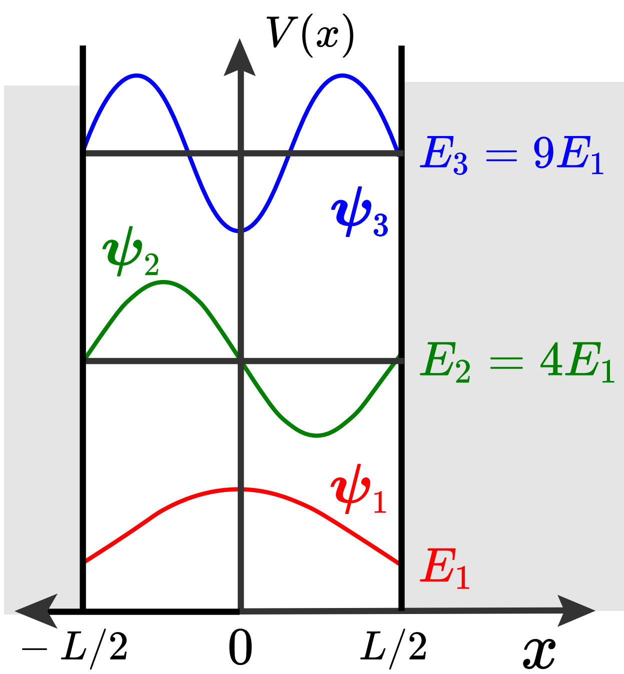


FIG. 3. 1-D infinite square well potential.

**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 $L \to \infty$ we reach the continuum again.

### C. The quantum harmonic oscillator

The quantum harmonic oscillator has the Hamiltonian

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

We wish to find eigenenergies and eigenstates.

<u>**Solution:**</u>

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

$\psi_n(x) = N_n e^{-\frac{-m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$, 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, $H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}\left(e^{-z^2}\right)$, so

$H_0(z) = 1$

$H_1(z) = 2z$

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

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

Introduce the ladder operators $a$ (lowering) and $a^\dagger$ (raising)

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

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

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

  $[N, a] = -a$

<u>Important Observations:</u>

- 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 $\langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$ for the vacuum state $|0\rangle$, where $\Delta x \equiv x- < x >$.

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.

### D. 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

  $\mathbf{S} = \frac{\hbar}{2}\,\sigma \qquad\qquad \sigma = (\sigma_\mathbf{x}, \sigma_\mathbf{y}, \sigma_\mathbf{z})$

  $s = 1/2$:

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

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

- In quantum information,

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

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

- Eigenvectors-eigenvalues:

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

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

### E. Many-particle quantum systems

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

$V$, $W$ Hilbert spaces $\qquad |v\rangle \in V$, $|w\rangle \in W$

$V \otimes W =$ tensor product $\qquad |v\rangle \otimes |w\rangle \in V \otimes W$

- 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 $\frac{1}{\sqrt{2}}\big(\alpha|v\rangle_1|w\rangle_2 + \beta|w\rangle_1|v\rangle_2\big)$?

- 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:

$|n_1, n_2, \cdots\rangle$

Bosons:

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

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

$N = \sum_i a_i^\dagger a_i$

$a_i^\dagger|\cdots, n_i, \cdots\rangle = \sqrt{n_i + 1}|\cdots, n_{i+1}, \cdots\rangle$

$a_i|\cdots, n_i, \cdots\rangle = \sqrt{n_i}|\cdots, n_{i-1}, \cdots\rangle$

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

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

Fermions:

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

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

$N = \sum_i c_i^\dagger c_i$

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

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

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

$c_i^\dagger|\cdots, n_i = 1, \cdots\rangle = 0 \longrightarrow$ Pauli exclusion principle.

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

## 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 $\cdots$).

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

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

Two limits:

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

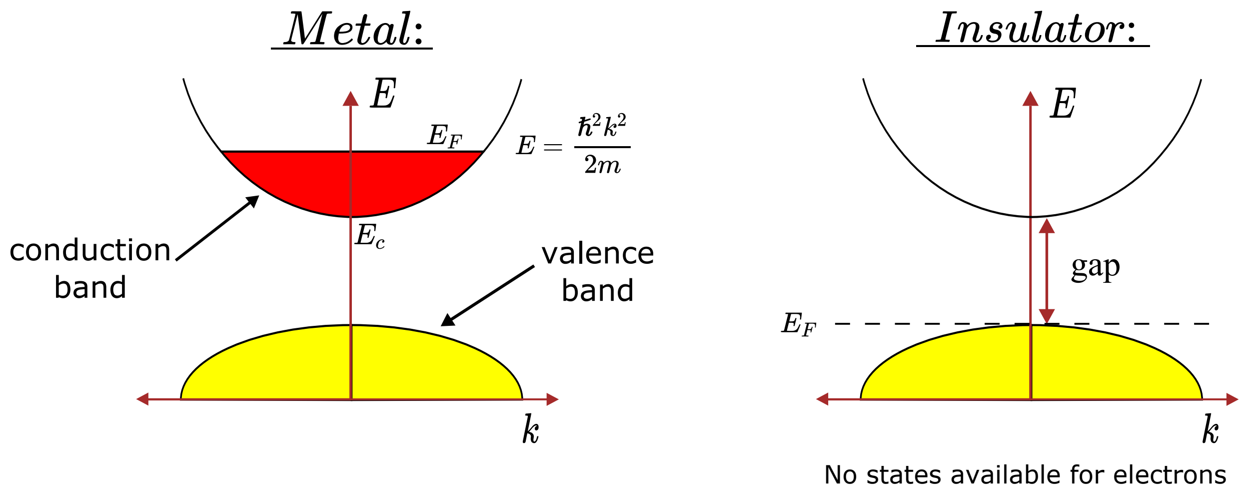


FIG. 4. Energy bands of a metal and insulator.

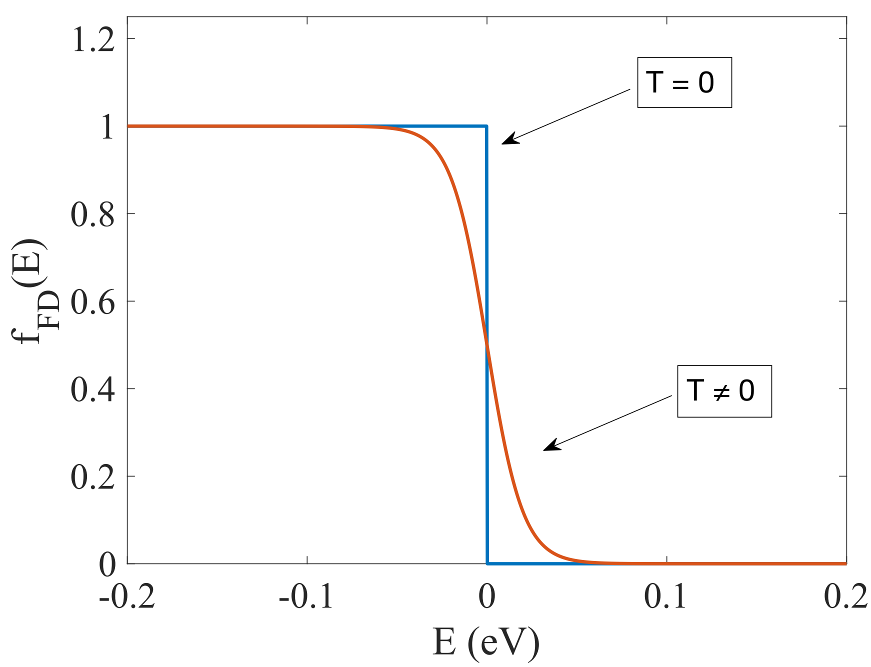


FIG. 5.

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

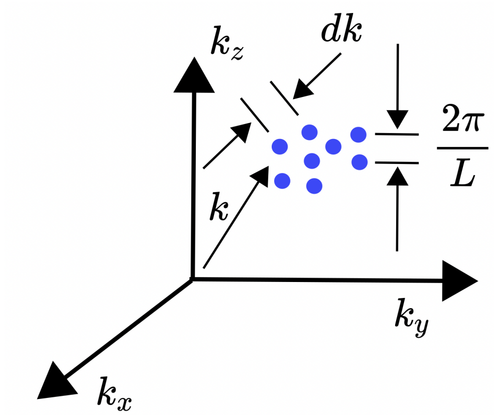


FIG. 6.

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

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

## VI. ELECTROMAGNETISM

Maxwell's equations (in SI units):

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

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

Electromagnetic potentials:

* magnetic vector potential $\vec{\mathcal{A}}$ defined as $\vec{B} = \vec{\nabla} \times \vec{A}$.

* electric potential V.

Electric field in terms of potentials: $\vec{E} = -\vec{\nabla} V - \frac{\partial}{\partial} \vec{A}$.

Constitutive relations:

| | |
|---|---|
| $\vec{D} = \varepsilon \vec{E}$ | $\varepsilon = \varepsilon_0 \varepsilon_r$ = electrical permittivity,<br>$\varepsilon_0 = 8.854 \times 10^{-12}\ F/m$ = vacuum permittivity<br>$\varepsilon_r$ = relative permittivity |
| $c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$ = speed of light in vacuum.<br>$\vec{B} = \mu \vec{H}$ | $\mu = \mu_0 \mu_r$ = magnetic permeability<br>$\mu_0 = 4\pi \times 10^{-7}\ H/m$ = vacuum permeability.<br>$\mu_r$ = relative permeability. |

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

Other fundamental relations:

- Ohm's law $\vec{\mathcal{J}} = \vec{\sigma} \cdot \vec{E}$

- Continuity equation: $-\frac{\partial \rho}{\partial t} = \vec{\nabla} \cdot \vec{\mathcal{J}}$

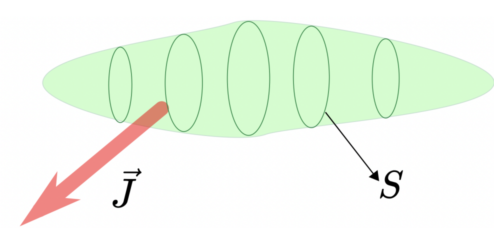


FIG. 7.

- Gauss-Ostrogradsky theorem: $-\frac{\partial}{\partial t} \iiint_V dV \cdot \vec{\rho} = \oiint_S d\vec{s} \cdot \vec{\mathcal{J}}$, 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 $T \to 0$

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

### A. Equipartition Theorem

– In thermal equilibrium, energy is shared equally between the degrees of freedom ($\frac{1}{2}k_BT$ 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 $= \frac{1}{2}k_BT + \frac{1}{2}k_BT + \frac{1}{2}k_BT = \frac{3}{2}k_BT \implies v_{rms} = \sqrt{\langle v^2\rangle} = \sqrt{\frac{3k_BT}{m}}$.

**Harmonic oscillator:** $E = \frac{p^2}{2m} + \frac{1}{2}kx^2 =$ average energy $\frac{1}{2}k_BT + \frac{1}{2}k_BT = k_BT$
where $k_B = 1.38 \times 10^{-23}\frac{m^2kg}{s^2K}$ – 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!