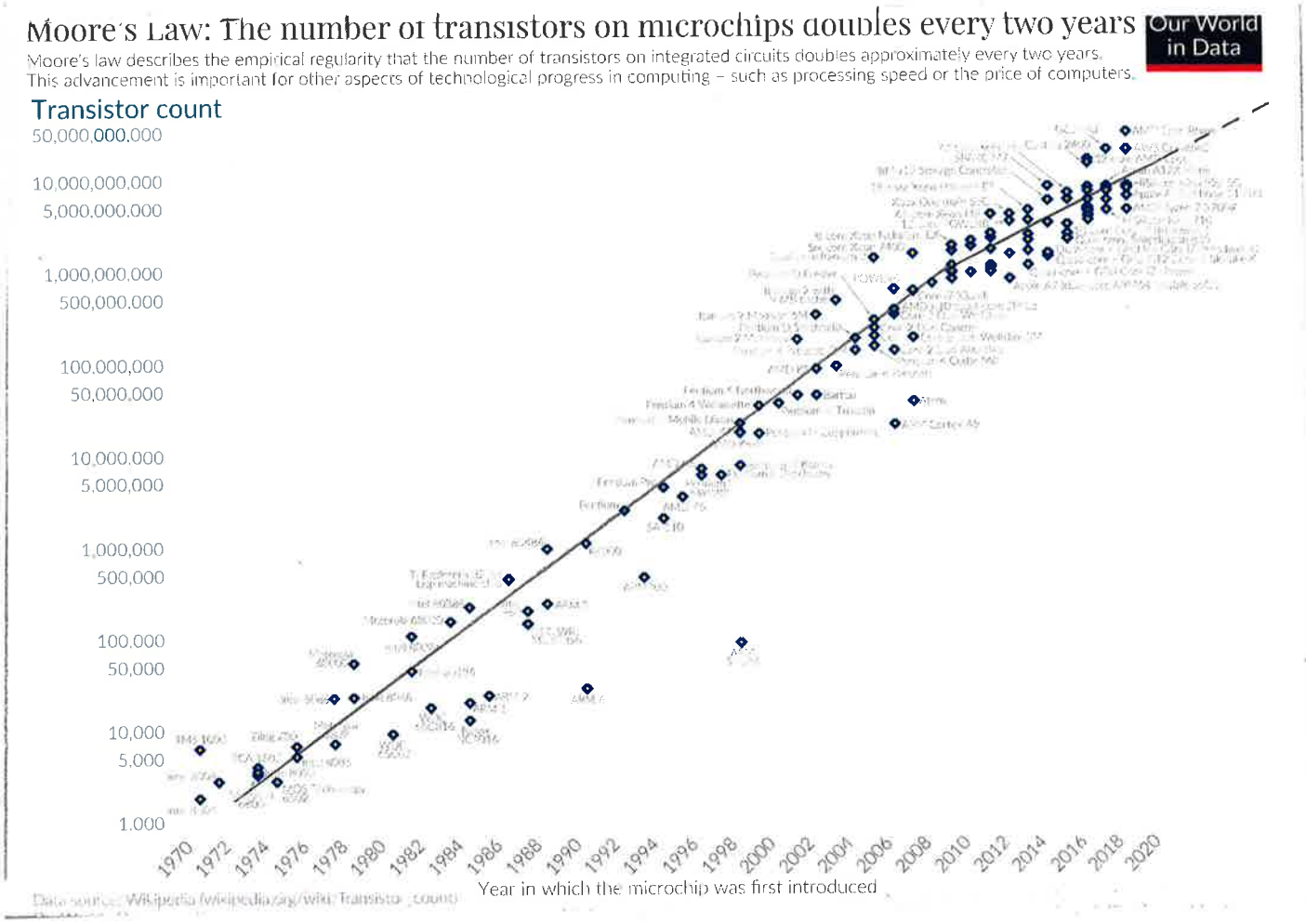
Key concepts from quantum mechanics, electromagnetism, and solid-state physics

- **Motivation:** Moore's law → doubling of the no. of transistors/chip every 18-24 months.



- dimension of gate = 7 nm presently! Already near the molecular scale and approaching atomic scale.
  - quantum effects (tunneling) will become important
- density: with 7nm technology, it approaches $\simeq 10^8$ transistors/mm^2
- power density → how much heat they generate
  presently approaching $\simeq 6\ W/mm^2 = 600\ W/cm^2$
  Comparison: a light bulb $\simeq 0.01\ W/mm^2 = 1\ W/cm^2$ our Sun $= 60\ W/mm^2$

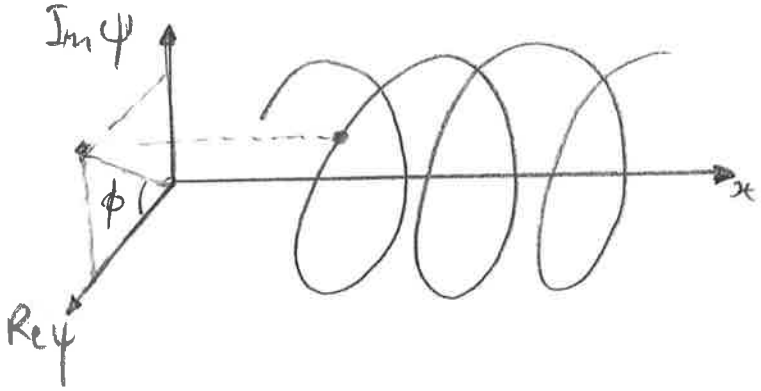
Classical wave physics

Plane waves:

$$\psi(x) = e^{ikx}$$ k = wavenumber, x = position

$$\lambda = \frac{2\pi}{k} = \text{wavelength}$$

$$\phi = kx = \text{phase}$$



Time-dependence:

$$\psi(x,t) = e^{i(kx-\omega t)}$$

$$\omega = \frac{2\pi}{T} = \text{angular frequency}$$

T = period

$\nu = \frac{1}{T}$ = frequency

(k,ω)-space

- Defined by the respective Fourier transforms

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

$$\psi[k,\omega] = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt\, e^{-ikx+i\omega t}\psi(x,t)$$

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

Some properties:

Real coordinates (x,t)	Fourier coordinates (k,ω)
shift by x_0	$\times e^{-ikx_0}$
$\times e^{ik_0x}$	shift by k_0
shift by t_0	$\times e^{i\omega t_0}$
$\times e^{-i\omega_0 t}$	shift by ω_0

Quantum physics

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

  $|\psi(x,t)|^2$ = probability density ; $\int_a^b |\psi(x,t)|^2 dx$ = probability that a particle is located between a and b

  H = Hamiltonian

- Typically H = kinetic energy + potential energy

  $H = \frac{p^2}{2m} + V$ $\quad\quad$ p = momentum operator

  $p = -i\hbar \frac{d}{dx}$ $\quad\quad$ $[x,p] = i\hbar$

- Dirac notations "bra" – "ket"

$$\psi(x,t) = \langle x|\psi(t)\rangle$$

$$\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 = \int_{-\infty}^{\infty} dx\, \langle\psi(t)|x\rangle\langle x|\psi(t)\rangle = \langle\psi(t)|\psi(t)\rangle = 1$$

$$\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = \mathbb{I}$$

Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

↓ in general it is possible to have a time-dependent Hamiltonian $H(t)$.

But, if H is time-independent, we can solve the Schrödinger eq. by the method of separation of variables.

$|\psi(t)\rangle = e^{-i\frac{E}{\hbar}t}|\psi\rangle$ and $H|\psi\rangle = E|\psi\rangle$.

eigenvector – eigenvalue problem

~ Example: free particle $V(x) = 0$

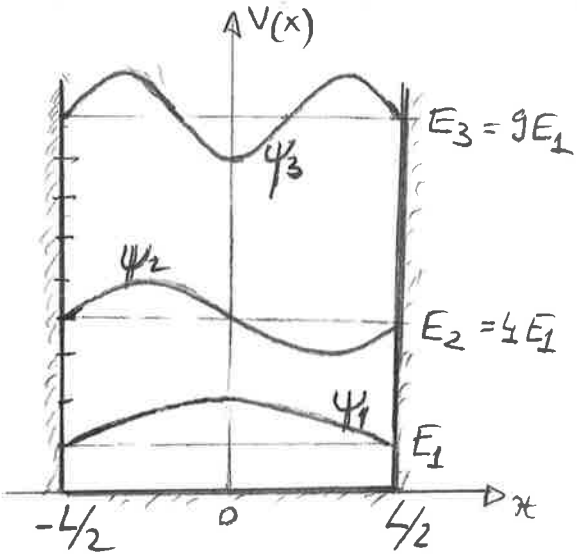
$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

$$\psi(x) = \psi e^{\pm ikx} \quad \text{with } k = \sqrt{\frac{2mE}{\hbar^2}}$$

So overall, $\psi(x,t) = \psi e^{\pm i(kx-\omega t)}$ where $\omega = E/\hbar$

The infinite square well

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



Solution: $\psi(x) = A \sin\left(Kx + K\frac{L}{2}\right)$

- Boundary conditions:

$x = -L/2 \rightarrow \psi(-\frac{L}{2}) = 0$

$x = L/2 \rightarrow \psi(\frac{L}{2}) = A \sin KL = 0 \Rightarrow K_n L = n\pi$

- Normalization:

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

So $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(K_n x + \frac{K_n L}{2}\right)$ $\quad n = 1, 2, 3 \ldots$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n \psi_n(x) \Rightarrow E_n = \frac{\hbar^2 K_n^2}{2m}.$$

Important observations:

- there exists a minimum non-zero energy $E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$, corresponding to the ground state ψ_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
- $E_n \sim 1/L^2$. The larger the box, the lower the gap between levels.
  Eventually, as $L \to \infty$ we reach again the continuum.

The quantum harmonic oscillator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \qquad H\psi = E\psi$$

Solution:

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$n = 0, 1, 2, \dots$

$$\psi_n(x) = N_n e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

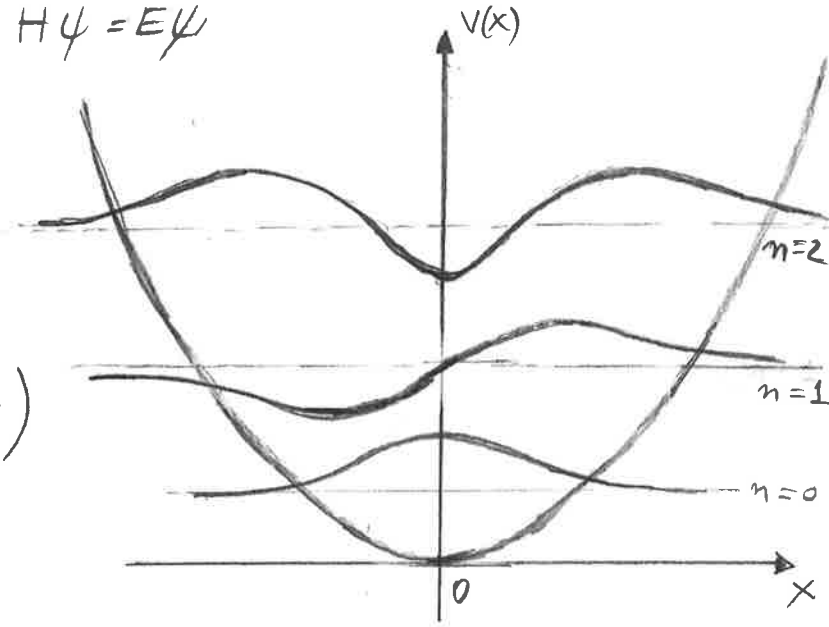
$H_n(z)$ = Hermite polynomial of degree n

$H_0(z) = 1$

$H_1(z) = 2z$

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

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



$$N_n = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}\left(e^{-z^2}\right)$$

- Ladder operators:

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

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

$N = a^\dagger a$ = number operator

$$[a, a^\dagger] = 1 \qquad [N, a^\dagger] = a^\dagger \qquad [N, a] = -a$$

$$N|n\rangle = n|n\rangle$$

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

$$a|0\rangle = 0$$

$$H = \hbar\omega\left(N + \frac{1}{2}\right)$$

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 (≡ zero-point motion energy).

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

Calculate the variance $\langle(\Delta x)^2\rangle \equiv \langle x^2\rangle - \langle x\rangle$ for the vacuum state $|0\rangle$

Δx = standard deviation

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

$$\langle x\rangle = 0$$

$$\langle x^2\rangle = \langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}$$

zero-point fluctuation

$$x_{ZPF} \equiv \sqrt{\frac{\hbar}{2m\omega}} \qquad \langle x^2\rangle = x_{ZPF}^2$$

Spin -1/2 particles

- Comes from the Stern-Gerlach experiment

  A beam of Ag atoms running through a non-homogeneous magnetic field is split into 2 beams.

Angular momentum $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ $\qquad \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$

$$|s, m\rangle = \begin{cases} |\tfrac{1}{2}, \tfrac{1}{2}\rangle & m = 1/2 \\ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle & m = -1/2 \end{cases} \qquad s = 1/2$$

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

- In quantum information, $|\tfrac{1}{2}, \tfrac{1}{2}\rangle \equiv |0\rangle$, $|\tfrac{1}{2}, -\tfrac{1}{2}\rangle \equiv |1\rangle$ — qubit states

general state

$$|\psi\rangle = \cos\tfrac{\theta}{2}|0\rangle + e^{i\varphi}\sin\tfrac{\theta}{2}|1\rangle$$

Eigenvectors - eigenvalues:

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\sigma_x |\chi_\pm^{(x)}\rangle = \pm |\chi_\pm^{(x)}\rangle$

$|\chi_\pm^{(x)}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \pm 1 \end{bmatrix}$

$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$\sigma_y |\chi_\pm^{(y)}\rangle = \pm |\chi_\pm^{(y)}\rangle$

$|\chi_\pm^{(y)}\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \pm i \end{bmatrix}$

$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\sigma_z |0\rangle = |0\rangle$

$\sigma_z |1\rangle = -|1\rangle$

$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Question: what is the analog of zero-point fluctuations for spin-1/2?

Many-particle quantum systems

How to "concatenate" the Hilbert spaces of each particle.

V, W = Hilbert space $\quad |v\rangle \in V, \; |w\rangle \in W$

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

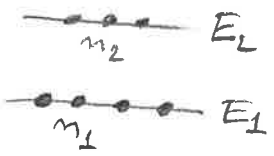
- But how do we write the wavefunctions? Is it $|v\rangle_1 |w\rangle_2$, $|w\rangle_1 |v\rangle_2$ or $\frac{1}{\sqrt{2}}\left(\alpha |v\rangle_1 |w\rangle_2 + \beta |w\rangle_1 |v\rangle_2\right)$ (say we have 2 particles)

In nature there are only 2 types of particles: bosons → symmetric wavefunction
fermions → 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:

$|n_1, n_2, \dots\rangle$

n_1: no. of particles in state $|\psi_1\rangle$; n_2: no. of particles in state $|\psi\rangle_2$



BOSONS:

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

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

$N = \sum_i a_i^\dagger a_i$

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

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

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

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

FERMIONS:

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

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

$N = \sum_i c_i^\dagger c_i$

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

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

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

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

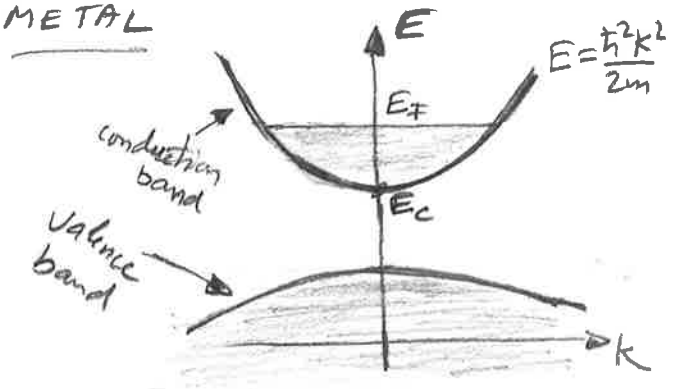
$$|n_1, n_2, \dots\rangle = \left(c_1^\dagger\right)^{n_1} \left(c_2^\dagger\right)^{n_2} \dots |0, 0, \dots\rangle$$

Elements of solid-state physics : Fermi energy, density of states, etc

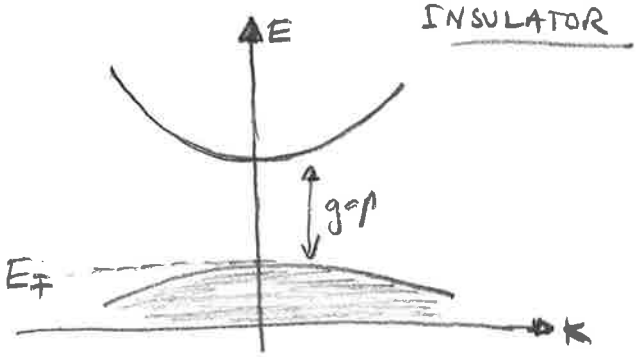
Electrons — they are fermions ; i.e. Pauli exclusion principle applies.
— at $T=0$, we fill all the states until we use all the electrons.

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

METAL



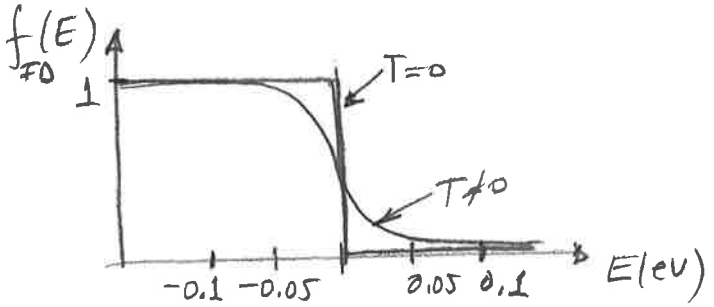
INSULATOR



no states available for electrons

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

$$f_{FD}(E) = \frac{1}{\exp\left[(E-E_F)/k_BT\right]+1}$$



Two limits:

- degenerate limit: $f_{FD}(E) \approx \Theta(E_F - E)$

  ↑ step function

  For example, this can happen at $T \simeq 0$ or if the Fermi level is such that $E_F - E_c \gg kT$ so that the thermal blurring can be neglected

- non-degenerate limit:

$$f_{FD} \approx \exp\left[-(E-E_F)/k_BT\right]$$

when $E - E_F \gg k_BT$

Density of states

Free electron wavefunction : $\psi(\vec{r}) = \frac{e^{ik_x \cdot x}}{\sqrt{L}} \cdot \frac{e^{ik_y \cdot y}}{\sqrt{L}} \cdot \frac{e^{ik_z \cdot z}}{\sqrt{L}}$

$$= \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

V = volume

$$E = \frac{\hbar^2 k^2}{2m} = \text{dispersion relation}$$

$$k_x = \frac{2\pi n_x}{L}$$

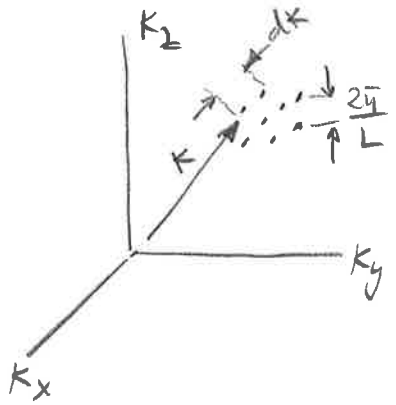
$$k_y = \frac{2\pi n_y}{L}$$

$$k_z = \frac{2\pi n_z}{L}$$

We want to calculate the no. of states / volume within an energy interval dE.

= density of states.

3D case:



Volume element in k-space

$$V_{3D} = \left(\frac{2\pi}{L}\right)^3$$

Volume of shell between k and $k+dk$

$$V_{dk} = 4\pi k^2 dk$$

no. of states in this shell $= 2 \cdot \frac{V_{dk}}{V_{3D}} = \frac{k^2 dk}{\pi^2} \cdot L^3$

(2 ↑ electron spin)

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\Rightarrow dk = \frac{1}{\sqrt{\frac{2mE}{\hbar^2}}} \frac{m}{\hbar^2} dE$$

$\Rightarrow$ no. of states in the interval dE per unit volume

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

Electromagnetism

Maxwell's equations (SI units)

$$\vec{\nabla} \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{D} = \rho$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$\vec{J}$ = current density

ρ = charge density

- Constitutive relations: $\vec{D} = \varepsilon \vec{E}$

$\varepsilon = \varepsilon_0 \varepsilon_r$ = electrical permittivity

$\varepsilon_0 = 8{,}854 \times 10^{-12}$ F/m = vacuum permittivity

ε_r = relative permittivity

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$$ = speed of light in vacuum

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

$\mu = \mu_0 \mu_r$ = magnetic permeability

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

μ_r = relative permeability

- Other fundamental relationships:

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

  # In ac fields: $\varepsilon \to \varepsilon = \varepsilon' - i\varepsilon''$

  $\tan\delta \equiv \varepsilon''/\varepsilon'$ = loss tangent

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

$$-\frac{\partial}{\partial t} \iiint dV \, \rho = \oiint_S d\vec{S} \cdot \vec{J}$$

by Gauss-Ostrogradsky theorem

↓ rate of decrease of positive charge = total current flux flowing out of the closed surface

Thermodynamics

- first law of thermodynamics: $\Delta U = Q - W$
  - ΔU: change in internal energy
  - Q: heat supplied to the system
  - W: work done by the system onto the environment
  - # conservation of energy
- second law of thermodynamics: $\delta q = T\,dS$ (for reversible processes)
  - δq: amount of heat transferred
  - dS: change in entropy produced by the transferred heat
  - # total entropy of an isolated system can never decrease

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 $T \to 0$

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

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 (translational): $E = \frac{1}{2} m v_x^2 + \frac{1}{2} m v_y^2 + \frac{1}{2} m v_z^2$

$\Rightarrow$ average energy $= \frac{1}{2} k_B T + \frac{1}{2} k_B T + \frac{1}{2} k_B T = \frac{3}{2} k_B T$

$\Rightarrow v_{RMS} = \sqrt{\langle v^2 \rangle} = \sqrt{\frac{3 k_B T}{m}}$

harmonic oscillator $E = \frac{p^2}{2m} + \frac{1}{2} k x^2$

average energy $= \frac{1}{2} k_B T + \frac{1}{2} k_B T = k_B T$

$k_B = 1.38 \times 10^{-23} \frac{m^2 kg}{s^2 K^{-1}}$ - Boltzmann constant

Further reading

- Any textbook on quantum mechanics, solid-state physics, and electromagnetism would do it.

For example:

- The Open University S M358 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

- Plenty of information, lecture notes, video lectures available on the Internet.