

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

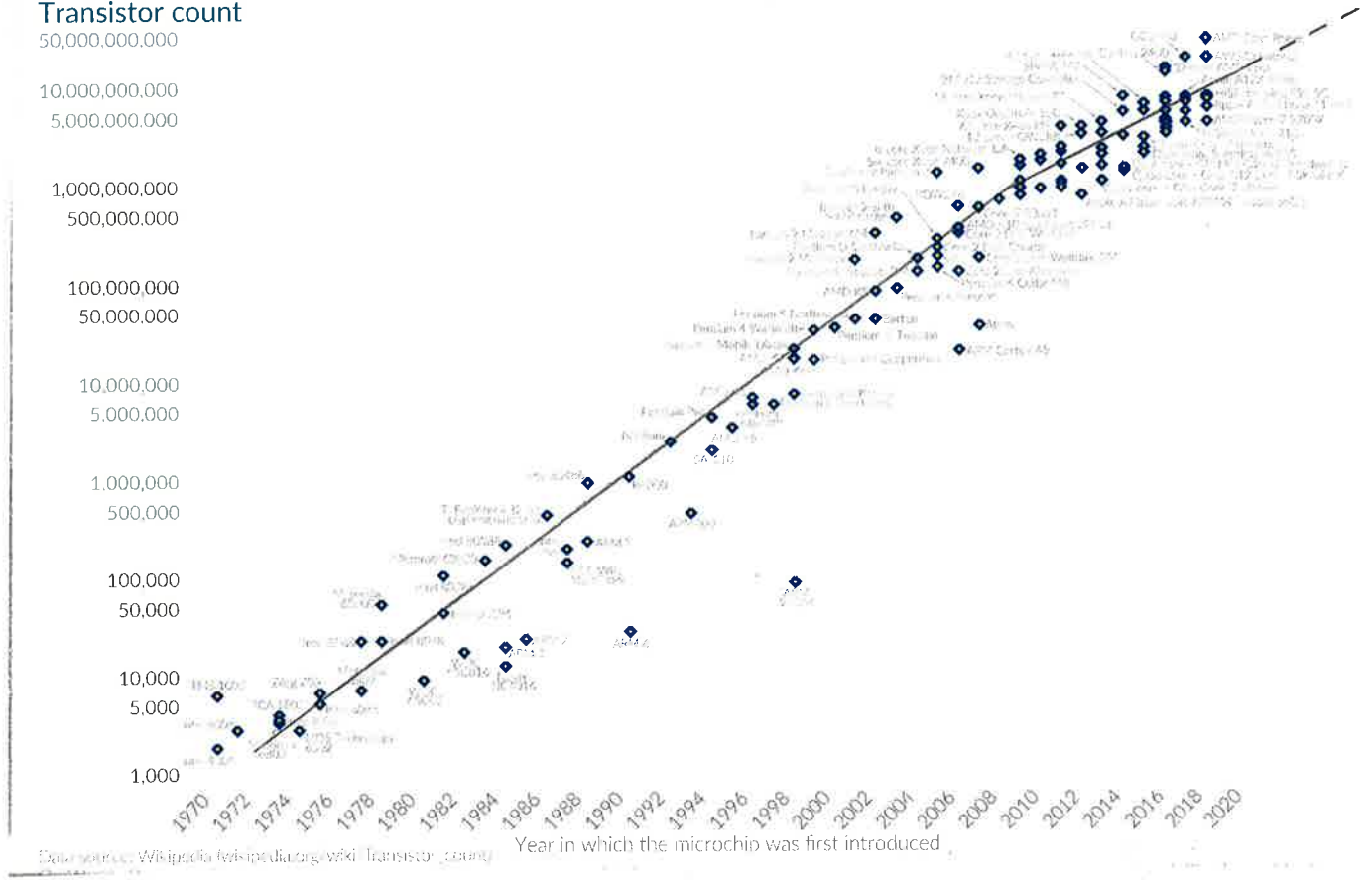
Motivation: Moore's law  $\rightarrow$  doubling of the no. of transistors/chip every 18-24 months.

Moore's Law: The number of transistors on microchips doubles every two years



Moore's law describes the empirical regularity that the number of transistors on integrated circuits doubles approximately every two years. This advancement is important for other aspects of technological progress in computing – such as processing speed or the price of computers.

Transistor count  
50,000,000,000



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

# Classical wave physics

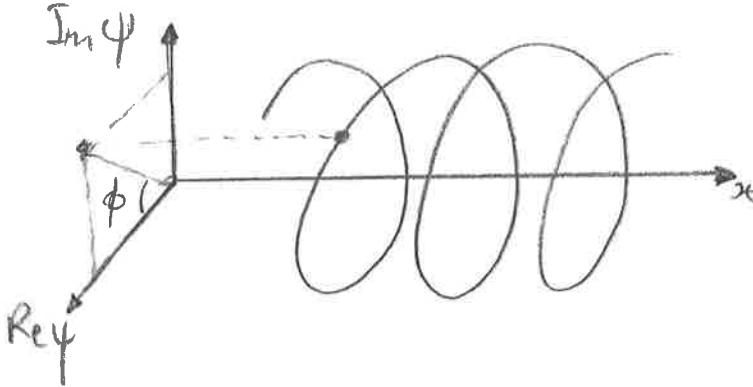
Plane waves:

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

$k = \text{wavenumber}$   
 $x = \text{position}$

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

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



Time-dependence:

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

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

$T = \text{period}$

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

(k, ω) - space

- Defined by the respective Fourier transforms

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

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

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

Some properties:

Real coordinates (x, t)	Fourier coordinates (k, ω)
shift by $x_0$	$x e^{-ikx_0}$
$x e^{ik_0 x}$	shift by $k_0$
shift by $t_0$	$x e^{i\omega t_0}$
$x e^{-i\omega t}$	shift by $\omega_0$

# Quantum physics

- $i\hbar \frac{d}{dt} \psi(x,t) = H \psi(x,t)$        $\psi(x,t)$  = 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  
 $H = \frac{p^2}{2m} + V$        $p$  = momentum operator  
 $p = -i\hbar \frac{d}{dx}$        $[x, p] = i\hbar$

- Dirac notations "bra" - "ket"

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

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

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

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.

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

eigenvector-eigenvalue problem

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

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

$$\downarrow$$

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

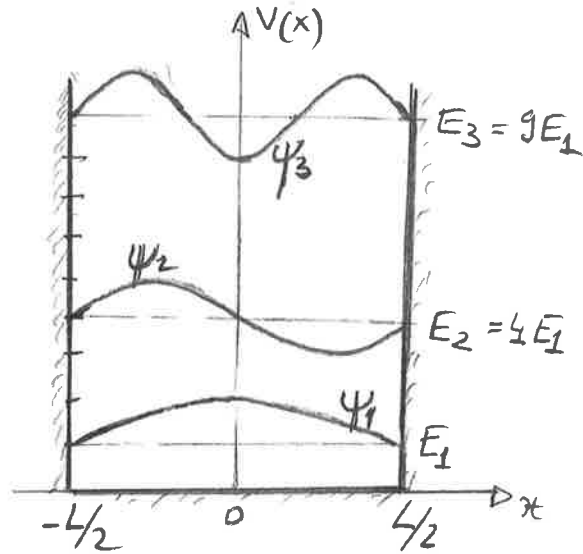
So overall,

$$\psi(x,t) = \psi e^{\pm i(kx - \omega t)} \quad \text{where} \quad \omega = \frac{E}{\hbar}$$

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



• Boundary conditions:

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

$$x = L/2 \rightarrow \psi(L/2) = A \sin kL = 0 \Rightarrow \underline{k_n L = n\pi}$$

• 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  $\underline{\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(k_n x + \frac{k_n L}{2}\right)}$   $n = 1, 2, 3, \dots$

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

Important observations:

- there exists a minimum non-zero energy  $E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$ , corresponding to the ground state  $\psi_1$ .

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

-  $E_n \sim 1/L^2$ . The larger the box, the lower the gap between levels. Eventually, as  $L \rightarrow \infty$  we reach again the continuum.

# The quantum harmonic oscillator

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

$$H\psi = E\psi$$

Solution:

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

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

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

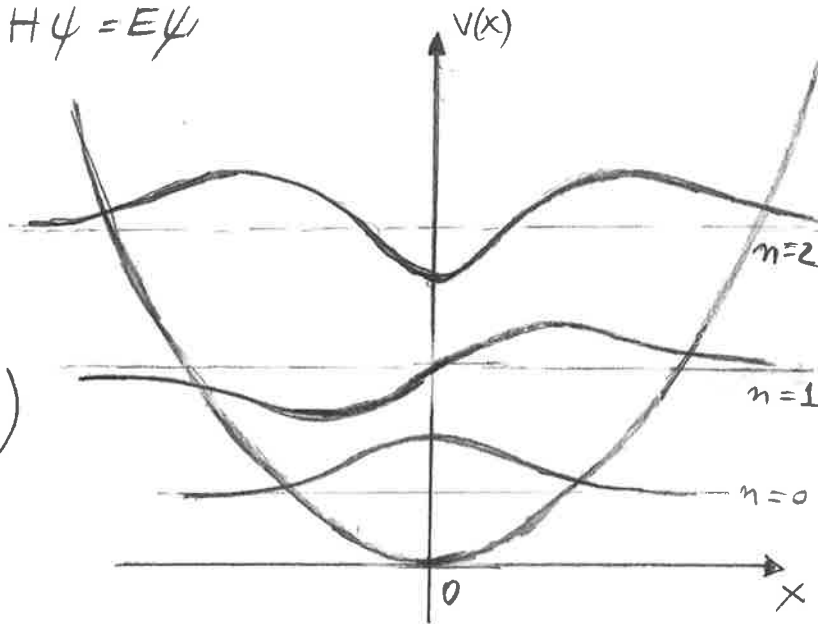
$H_n(z)$  = Hermite polynomial of degree  $n$

$$H_0(z) = 1$$

$$H_1(z) = 2z$$

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

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



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

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

o Ladder operators:

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

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

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

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

$$N = a^\dagger a = \text{number operator}$$

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

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

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

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

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

$$a|0\rangle = 0$$

Important observations:

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

o energy levels are equally spaced by  $\hbar\omega$

o there exists a minimum energy of  $\hbar\omega/2$  which corresponds to the ground state ( $\equiv$  zero-point motion energy).

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

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

$\Delta x \equiv x - \langle x \rangle$   
(standard deviation)

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

$$\langle x \rangle = 0$$

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

zero-point fluctuation  
 $x_{ZPF} \equiv \sqrt{\frac{\hbar}{2m\omega}}$   $\langle x^2 \rangle = x_{ZPF}^2$

# 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  $\vec{S} = \frac{\hbar}{2} \vec{v}$       $\vec{v} = (v_x, v_y, v_z)$

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

$s = \frac{1}{2}$

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

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

general state

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

Eigenvectors - eigenvalues:

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

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

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

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

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

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

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

$$\downarrow$$
$$v_z |0\rangle = |0\rangle$$

$$v_z |1\rangle = -|1\rangle$$

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

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

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.

$$V, W = \text{Hilbert space} \quad |v\rangle \in V, |w\rangle \in W$$

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

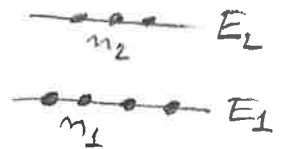
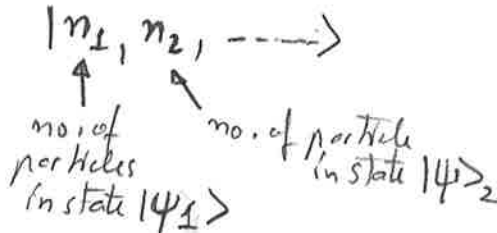
- But how do we write the wavefunctions? Is it  $|v\rangle_1 |w\rangle_2, |w\rangle_1 |v\rangle_2$  or  $\frac{1}{\sqrt{2}} (\alpha |v\rangle_1 |w\rangle_2 + \beta |w\rangle_1 |v\rangle_2)$  (say we have 2 particles)

In nature there are

- only 2 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:



## BOSONS:

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

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

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

$$[a_i, a_j] = [a_i^+, a_j^+] = 0$$

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

$$N = \sum_i a_i^+ a_i$$

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

## FERMIONS:

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

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

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

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

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

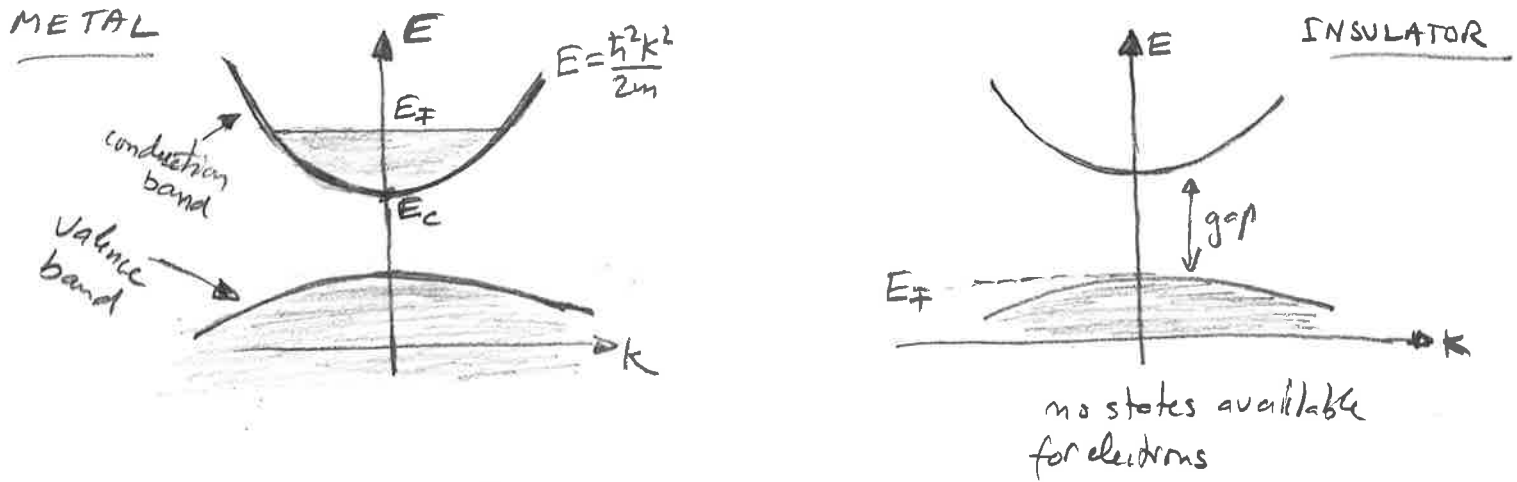
$$c_i^+ | \dots, n_i = 1, \dots \rangle = 0$$

$\rightarrow$  Pauli exclusion principle

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

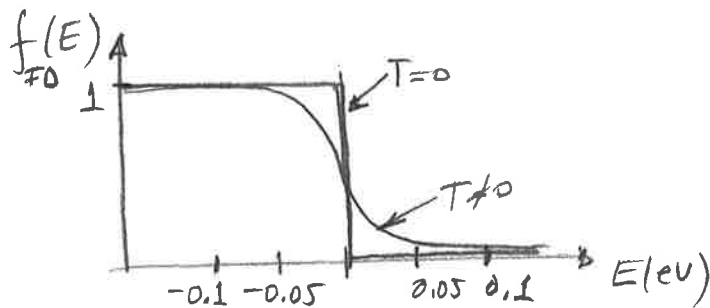
Elements of solid-state physics: Fermi energy, density of states, etc

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 ...)



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

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



Two limits:

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

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

• non-degenerate limit:

$$f_{FD} \approx \exp\left[-\frac{(E - E_F)}{k_B T}\right]$$

when  $E - E_F \gg k_B T$



# Density of states

Free electron wavefunction:  $\psi(\vec{r}) = \frac{e^{ik_x x}}{\sqrt{L}} \cdot \frac{e^{ik_y y}}{\sqrt{L}} \cdot \frac{e^{ik_z z}}{\sqrt{L}}$   
 $= \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}}$

$V = \text{volume}$

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

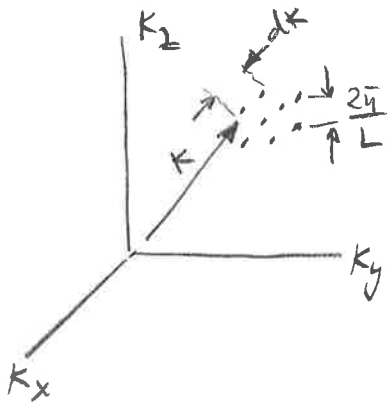
$k_x = \frac{2\pi n_x}{L}$

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

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

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 =  $2 \cdot \frac{V_{dk}}{V_{3D}} = \frac{k^2 dk}{\pi^2} \cdot L^3$   
 ↑  
 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

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

# 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

$\rho$  = charge density

• Constitutive relations:  $\vec{D} = \epsilon \vec{E}$

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

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

Potentials:

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$\vec{A}$  = magnetic vector potential

$V$  = electric potential

$$\vec{E} = -\vec{\nabla} V - \frac{\partial \vec{A}}{\partial t}$$

$\epsilon = \epsilon_0 \epsilon_r$  = electrical permittivity

$$\epsilon_0 = 8.854 \times 10^{-12} \text{ F/m}$$

= vacuum permittivity

$\epsilon_r$  = relative permittivity

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

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

= vacuum permeability

$\mu_r$  = relative permeability

• Other fundamental relationships:

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

- Continuity equation

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

$$-\frac{\partial}{\partial t} \iiint_V \rho \, dV = \iint_S \vec{J} \cdot \vec{S} \, dS$$



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

by Gauss-Ostrogradsky Theorem

# In ac fields:

$$\epsilon \rightarrow \epsilon = \epsilon' - j\epsilon''$$

$$\tan \delta \equiv \frac{\epsilon''}{\epsilon'} = \text{loss tangent}$$

# Thermodynamics

• first law of thermodynamics:

# conservation of energy

$$\Delta U = Q - W$$

$\Delta U$ : change in internal energy  
 $Q$ : heat supplied to the system  
 $W$ : work done by the system on the environment

• second law of thermodynamics:

# total entropy of an isolated system can never decrease

$$\int \frac{dQ}{T} = dS \quad (\text{for reversible processes})$$

$\int \frac{dQ}{T}$ : amount of heat transferred  
 $dS$ : 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  $T \rightarrow 0$   
 $\lim_{T \rightarrow 0} S = \text{const.}$

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

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

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

harmonic oscillator

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

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

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

- Boltzmann constant

## Further reading

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

For example:

- 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 Sibly - Introduction to Electromagnetism
- Plenty of information, lecture notes, video lectures available on the internet.