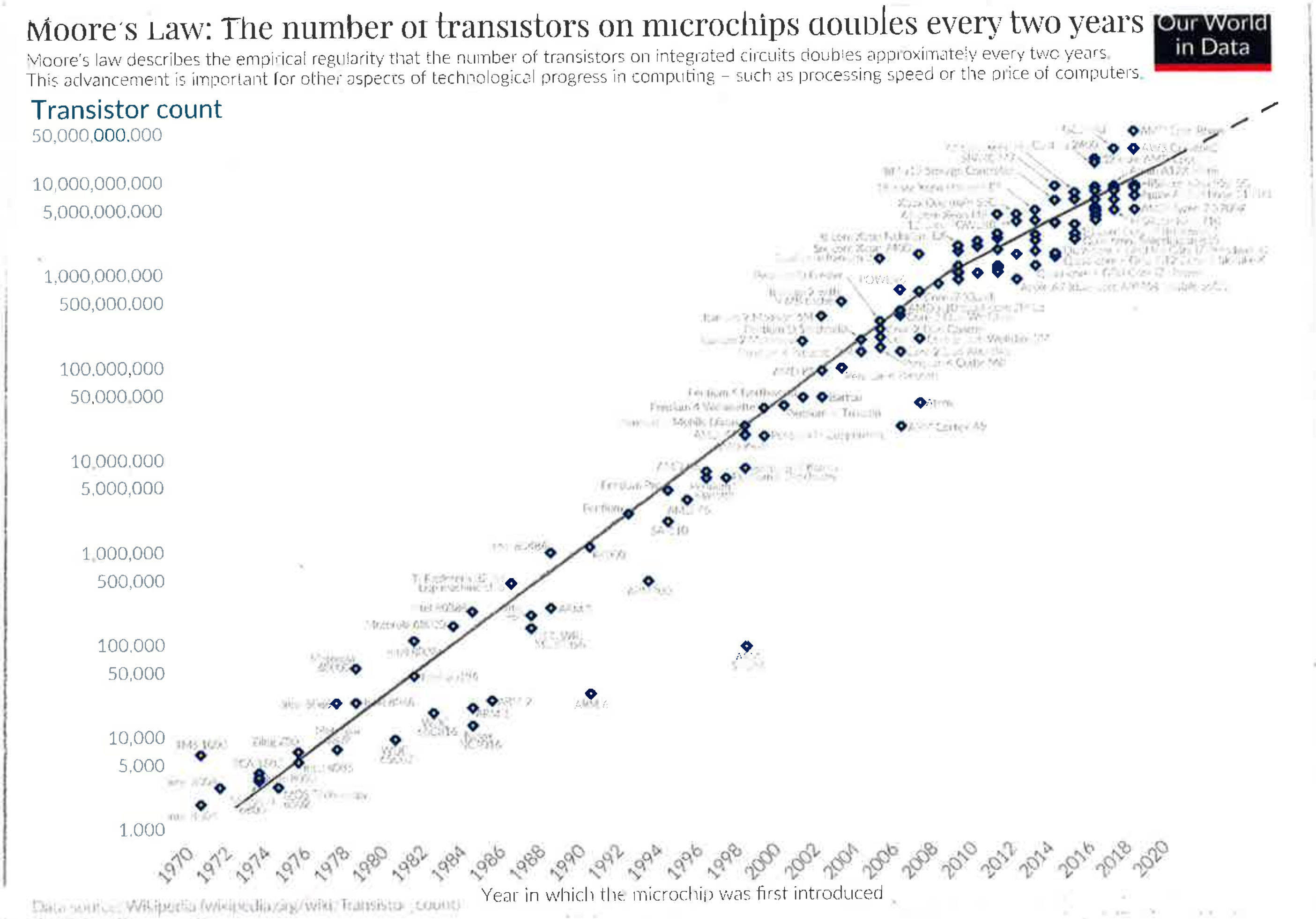
Key concepts from quantum mechanics, electromagnetism, and solid-state physics

- **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 7 nm technology, it approaches $\simeq 10^8$ transistors$/\mathrm{mm}^2$
- power density → how much heat they generate
  presently approaching $\simeq 6\,\mathrm{W}/\mathrm{mm}^2 = 600\,\mathrm{W}/\mathrm{cm}^2$

Comparison: a light bulb $\simeq 0.01\,\mathrm{W}/\mathrm{mm}^2 = 1\,\mathrm{W}/\mathrm{cm}^2$ our Sun $= 60\,\mathrm{W}/\mathrm{mm}^2$

Classical wave physics

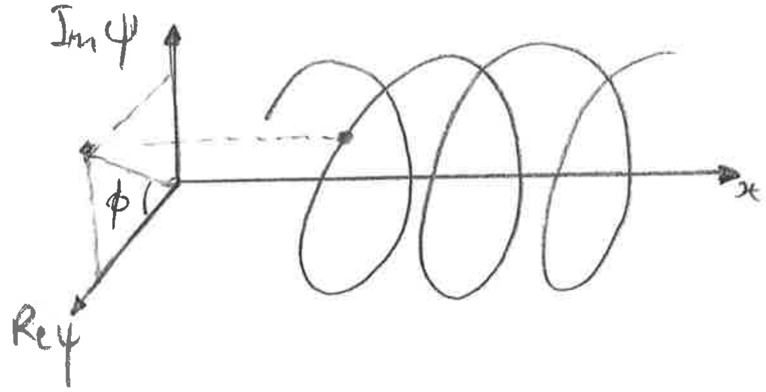
Plane waves:

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

k = wavenumber
x = position

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

$\phi = kx$ = phase



Time-dependence:

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

$\omega = \frac{2\pi}{T}$ = angular frequency
T = period
$\nu = \frac{1}{T}$ = frequency

(k,ω)-space

- Defined by the respective Fourier transforms

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

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

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

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

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

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

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

- 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.

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

eigenvector – eigenvalue problem

~ **Example:** free particle

$$V(x) = 0$$

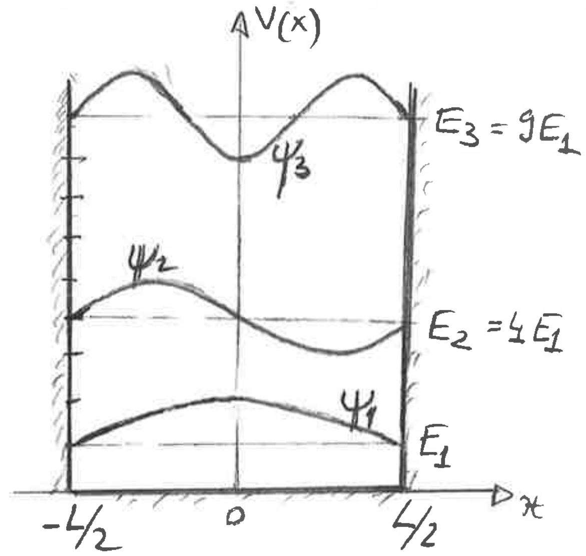
$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

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

So overall,

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

The infinite square well



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

Solution: $\psi(x) = A \sin\left(kx + k L/2\right)$

- Boundary conditions:

$$x = -L/2 \rightarrow \psi\left(-\tfrac{L}{2}\right) = 0$$

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

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

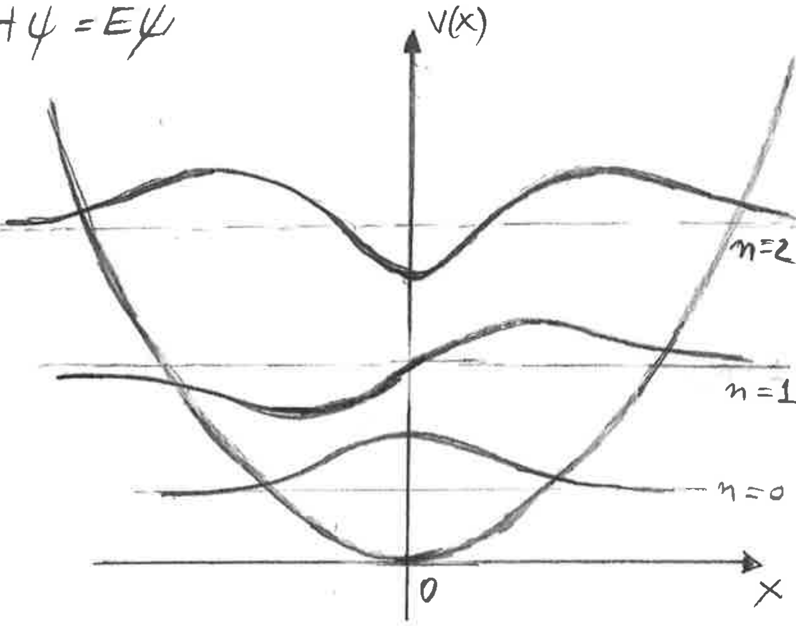
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n \psi_n(x) \Rightarrow \underline{E_n = \frac{\hbar^2 k_n^2}{2m}}.$$

Important observations:

- there exists a minimum non-zero energy $E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$, corresponding to the ground state ψ_1.
  So a particle in a box <u>always</u> 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

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



Solution:

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

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

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

$H_n(z)$ = 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:

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

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

$N = a^+a$ = number operator

$[a, a^+] = 1 \qquad [N, a^+] = a^+ \qquad N|n\rangle = n|n\rangle$

$[N, a] = -a$

$$H = \hbar\omega\left(N + \frac{1}{2}\right) \qquad |n\rangle = \frac{(a^+)^n}{\sqrt{n!}}|0\rangle$$

$a|0\rangle = 0$

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).

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

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

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

$\langle x\rangle = 0$

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

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

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

$s = 1/2$

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

- In quantum information,

$$\left.\begin{aligned} |\tfrac{1}{2}, \tfrac{1}{2}\rangle &\equiv |0\rangle \\ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle &\equiv |1\rangle \end{aligned}\right] \text{qubit states}$$

general state

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

Eigenvectors - eigenvalues:

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

$\downarrow$

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

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

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

$\downarrow$

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

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

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

$\downarrow$

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

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

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

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

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 $\qquad |v\rangle \in V \; , \; |w\rangle \in W$

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

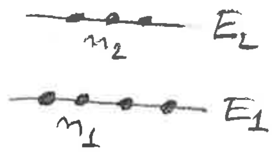
- But how do we write the wavefunctions? Is it $|v\rangle_1 |w\rangle_2$, $|w\rangle_1 |v\rangle_2$ or $\frac{1}{\sqrt{2}}\left(\alpha |v\rangle_1 |w\rangle_2 + \beta |w\rangle_1 |v\rangle_2\right)$ (say we have 2 particles)

In nature there are only 2 types of particles: bosons $\longrightarrow$ symmetric wavefunction
fermions $\longrightarrow$ 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:

$$|n_1, n_2, \cdots\rangle$$

no. of particles in state $|\psi_1\rangle$ $\qquad$ no. of particle in state $|\psi\rangle_2$



BOSONS:

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

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

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

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

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

$N = \sum_i a_i^+ a_i$

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

FERMIONS:

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

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

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

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

$N = \sum_i c_i^+ c_i$

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

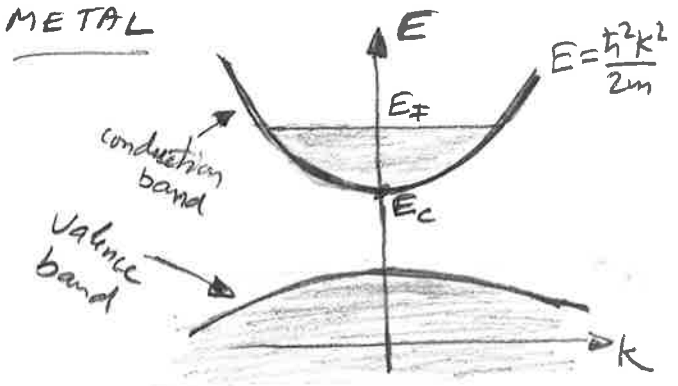
$$c_i^+ |\cdots, n_i = 1, \cdots\rangle = 0 \longrightarrow \text{Pauli exclusion principle}$$

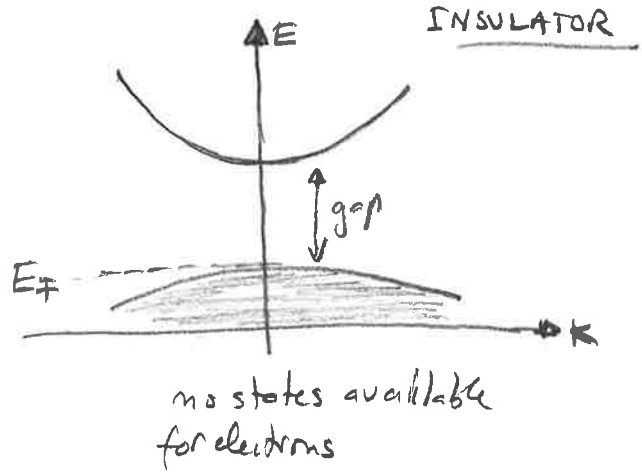
$$|n_1, n_2, \cdots\rangle = (c_1^+)^{n_1} (c_2^+)^{n_2} \cdots |0, 0, \cdots\rangle$$

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.

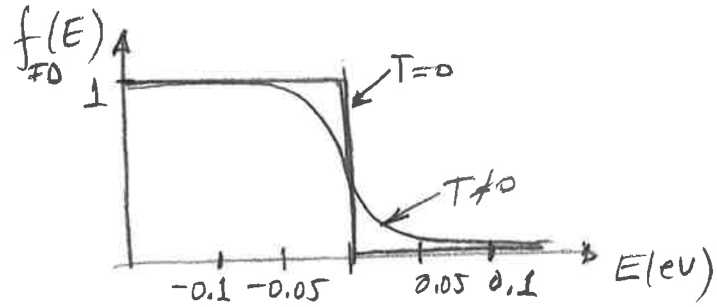
For example take a wire (just because we have a single K-vector ...)





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

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



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:

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

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

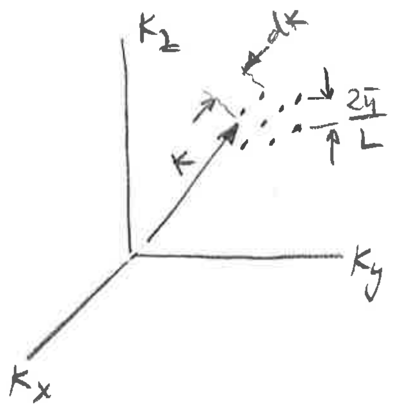
$$E = \frac{\hbar^2 k^2}{2m} = \text{dispersion relation}$$

$$k_x = \frac{2\pi n_x}{L} \qquad k_y = \frac{2\pi n_y}{L} \qquad k_z = \frac{2\pi n_z}{L}$$

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 $k+dk$

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

$$\text{no. of states in this shell} = \underset{\substack{\uparrow \\ \text{electron spin}}}{2} \cdot \frac{V_{dk}}{V_{3D}} = \frac{k^2 dk}{\pi^2} \cdot L^3$$

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

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

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

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

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: $\vec{D} = \varepsilon \vec{E}$

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

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

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

ε_r = relative permittivity

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

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

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

μ_r = relative permeability

- Other fundamental relationships:
  - Ohm's law $\vec{J} = \sigma \vec{E}$
  - 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

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 Sibley – Introduction to Electromagnetism

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