

FYS3410 - Vår 2018 (Kondenserte fasers fysikk)

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**Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17, 18, 20)**

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2019 FYS3400 Lecture Plan (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17-20)

Module I – Periodity and Disorder (Chapters 1-3, 19, 20)

	calender week
Ti 15/1 09-10 Introduction. Crystal bonding. Periodicity and lattices. Lattice planes and Miller indices. Reciprocal space.	3
To 17/1 10-12 Bragg diffraction and Laue condition	
Ti 22/1 09-10 Ewald construction, interpretation of a diffraction experiment, Bragg planes and Brillouin zones	4
To 24/1 10-12 Surfaces and interfaces. Disorder. Defects crystals. Equilibrium concentration of vacancies	
Ti 29/1 09-10 Diffusion phenomena in solids	5
To 31/1 10-12 Mechanical properties of solids. Summary of Module I	

Module II – Phonons (Chapters 4, 5, and 18 pp.557-561)

Ti 05/2 09-10 Vibrations in monoatomic and diatomic chains of atoms; examples of dispersion relations in 3D	6
To 07/2 10-12 Periodic boundary conditions (Born – von Karman); phonons and its density of states (DOS)	
Ti 12/2 09-10 Effect of temperature - Planck distribution;	7
To 14/2 10-12 Lattice heat capacity: Dulong-Petit, Einstein, and Debye models	
Ti 19/2 09-10 Comparison of different lattice heat capacity models	8
To 21/2 10-12 Thermal conductivity and thermal expansion	
Ti 26/2 09-10 Summary of Module II	9

Module III – Electrons (Chapters 6, 7, 11 - pp 315-317, 18 - pp.528-530, 19, and Appendix D)

To 28/2 10-12 Free electron gas (FEG) versus free electron Fermi gas (FEFG)	
Ti 05/3 09-10 DOS of FEFG in 3D; Effect of temperature – Fermi-Dirac distribution	10
To 07/3 10-12 Heat capacity of FEFG in 3D	
Ti 12/3 09-10 Transport properties of electrons electrons – examples for thermal, electric and magnetic fields	11
To 14/3 10-12 DOS of FEFG in 2D - quantum wells, DOS in 1D – quantum wires, and in 0D – quantum dots	
Ti 19/3 09-10 Origin of the band gap;	12
To 21/3 10-12 Nearly free electron model; Kronig-Penney model;	
	undervisningsfri uke 13
Ti 02/4 09-10 Effective mass method	14
To 04/4 10-12 cancelled	
Ti 09/4 09-10 Electronic/thermal phenomena in disordered systems (Joakim Bergli)	15
To 11/4 10-12 Electronic/thermal phenomena in disordered systems (Joakim Bergli)	

Easter 16
17

Module IV – Advanced Theory and Examples (Chapters 8, 9 pp 223-231, and 17, 19)

To 25/4 10-12 Effective mass method for calculating localized energy levels for defects in crystals	
Ti 30/4 09-10 canceled	18
To 02/5 10-12 Intrinsic and extrinsic electrons and holes in semiconductors	
Ti 07/5 09-10 Carrier statistics in semiconductors	19
To 09/5 10-12 p-n junctions	
Ti 14/5 09-10 Advanced theory of disordered systems (Marcel Moura and Gaute Linga)	20
To 16/5 10-12 Interesting properties of disordered systems (Marcel Moura and Gaute Linga)	
Ti 21/5 09-10 Summary of Module IV	21

Summary and repetition

To 23/5 10-12 Repetition - course in a nutshell

FYS3400 in a nutshell

- **Condensed Matter Physics à la FYS3400;**
- **Waves periodic lattices and defects;**
- **Phonons;**
- **Electrons;**
- **Advanced properties.**

Condensed Matter Physics

Condensed Matter Physics



Solid State Physics of Crystals

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in **Periodic Lattices**

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in **Periodic Lattices**



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in **Periodic Lattices**



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion

Electron waves in lattices

Free electrons

Electron DOS

Fermi-Dirac distribution



Electronic properties:

Electron concentration and transport,
contribution to the heat capacity

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion

Electron waves in lattices

Free electrons

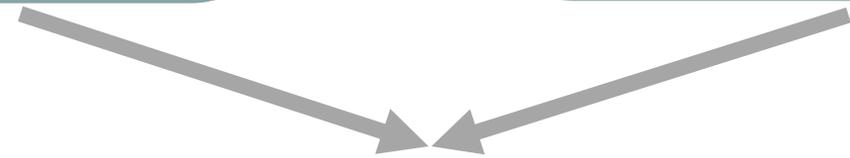
Electron DOS

Fermi-Dirac distribution



Electronic properties:

Electron concentration and transport,
contribution to the heat capacity



Advanced theory and novel materials properties

Condensed Matter Physics

Solid State Physics of Crystals

Disordered systems

Properties of Waves in Periodic Lattices

Elastic waves in lattices
Vibrations
Phonon DOS
Planck distribution

Disordered systems

Thermal properties:
heat capacity and conductance,
thermal expansion

Electron waves in lattices
Free electrons
Electron DOS
Fermi-Dirac distribution

Disordered system

Electronic properties:
Electron concentration and transport,
contribution to the heat capacity

Advanced theory and novel materials properties

Disordered systems

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in **Periodic Lattices**

Properties of Waves in Periodic Lattices

Questions: (i) why in periodic lattices?

(ii) why waves?

Answers: (i) because organizing atoms in periodic structures minimizes the energy – in other words – periodicity is a common feature of the matter;

(ii) waves are used as probes to study crystals, but most importantly waves are inside the crystals in form of vibrations (phonons) and electrons.

Even though the waves having different nature, the principles of the wave interaction with a periodic lattice are common, e.g. in terms of the Bragg's diffraction law.

Typically, the waves are characterized with the wave vectors $k = 2\pi/\lambda$; notably k is given in units of the reciprocal length; How to plot/align “ k ” at the lattice points, than? Use the reciprocal space to visualize the wave-lattice interactions !!

The "physics" part can be reduced to Waves in Periodic Lattices

Two questions: (i) why in periodic lattices?
(ii) why waves?

Secondly, let's discuss (ii); check the following question/inputs for the discussion:

Why do we talk about waves at all, are there waves inside the crystals?

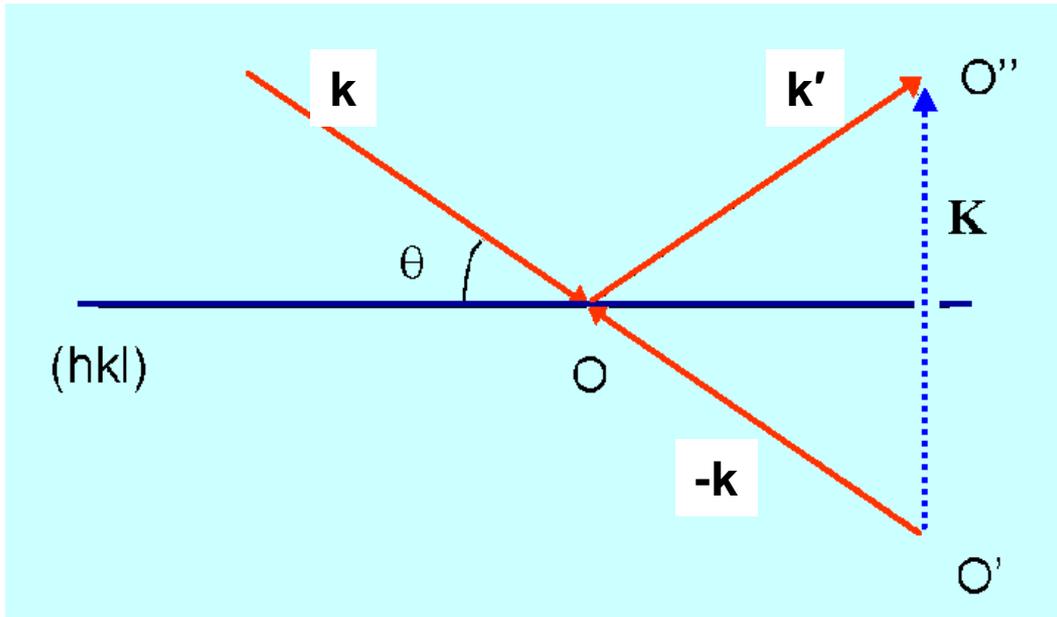
Or possibly, we are after waves exposed on crystals to be used as probes to collect the information?

Anyhow, even waves having different nature, its interaction principles with a periodic lattice are common, e.g. in terms of the Bragg's diffraction law;

Typically, waves are characterized with wave vectors $k = 2\pi/\lambda$; notably k is given in units of the reciprocal length; How to plot k at lattice points, than?

Use the reciprocal space to visualize the wave-lattice interactions !!

Laue condition



$$|\mathbf{K}| = 2|k| \sin \theta_{hkl} = \frac{2 \sin \theta_{hkl}}{\lambda}$$

$\vec{\mathbf{K}}$ is perpendicular to the (hkl) plane, so can be defined as:

$$\vec{\mathbf{K}} = \left[\frac{2 \sin \theta_{hkl}}{\lambda} \right] \hat{\mathbf{n}}$$

\mathbf{G} is also perpendicular to (hkl) so $\hat{\mathbf{n}} = \frac{\mathbf{G}_{hkl}}{|\mathbf{G}_{hkl}|}$

$$\Rightarrow \mathbf{K} = \frac{2}{\lambda |\mathbf{G}_{hkl}|} \sin \theta_{hkl} \mathbf{G}_{hkl}$$

and $|\mathbf{G}_{hkl}| = \frac{1}{d_{hkl}}$ from previous

$$\Rightarrow \mathbf{K} = \frac{2d_{hkl} \sin \theta_{hkl}}{\lambda} \mathbf{G}_{hkl}$$

But Bragg: $2d \sin \theta = \lambda$

$$\mathbf{K} = \mathbf{G}_{hkl}$$

the Laue condition

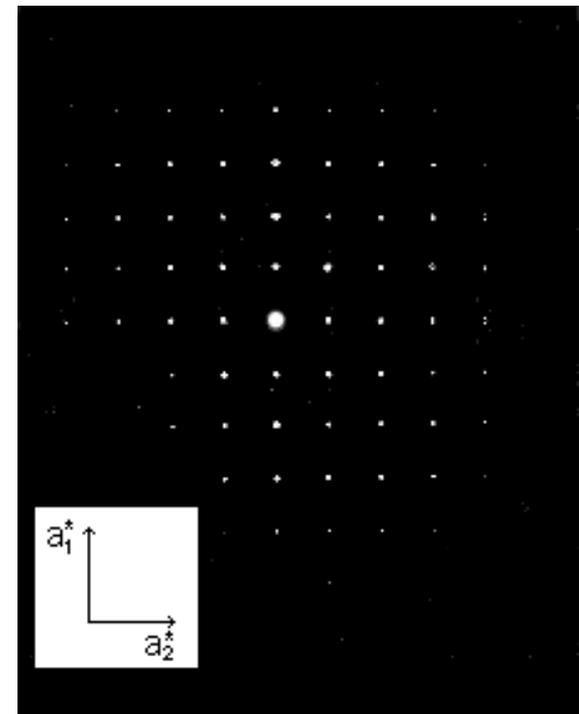
Reciprocal lattice

The reciprocal lattice is composed of all points lying at positions \vec{G}_{hkl} from the origin, so that there is one point in the reciprocal lattice for each set of planes (hkl) in the real-space lattice.

This seems like an unnecessary abstraction. Is there a benefit for defining such a reciprocal lattice?

YES, the reciprocal lattice simplifies the interpretation of x-ray diffraction from crystals because:

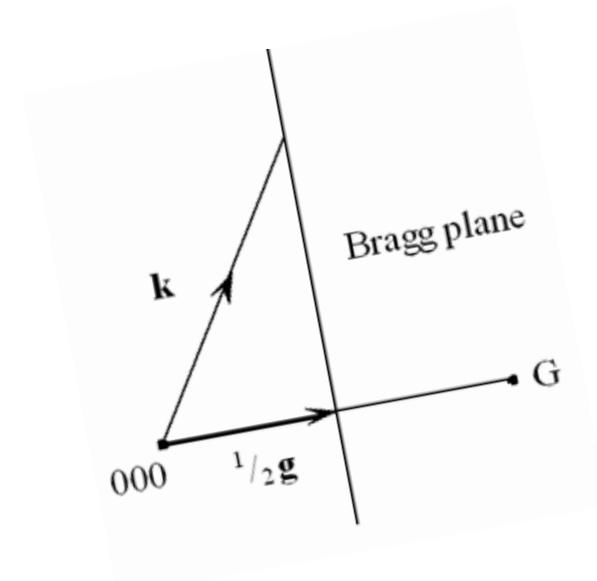
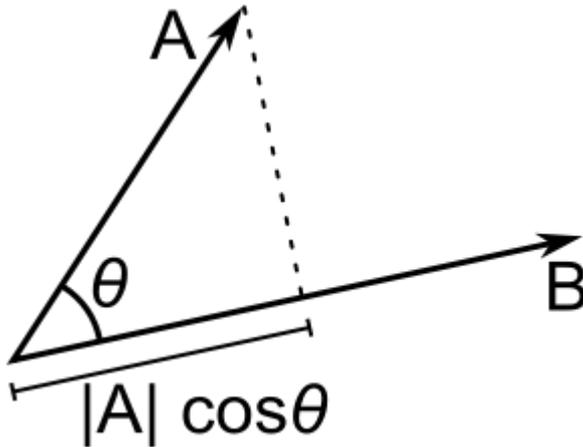
- Diffraction pattern is not a direct representation of the crystal lattice
 - Diffraction pattern is a representation of the *reciprocal lattice*



Bragg planes and Brillouin zone construction

$\mathbf{k} \cdot (\frac{1}{2}\mathbf{g}) = (\frac{1}{2}\mathbf{g}) \cdot (\frac{1}{2}\mathbf{g})$ When this holds – diffraction occurs – that's the law

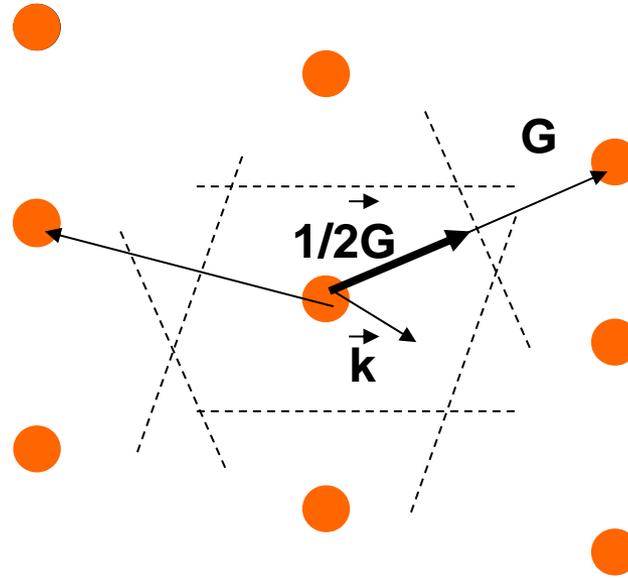
Let's considering when this "dot" products will do coincide?
What the dot product by the way?



Fundamental conclusion is:

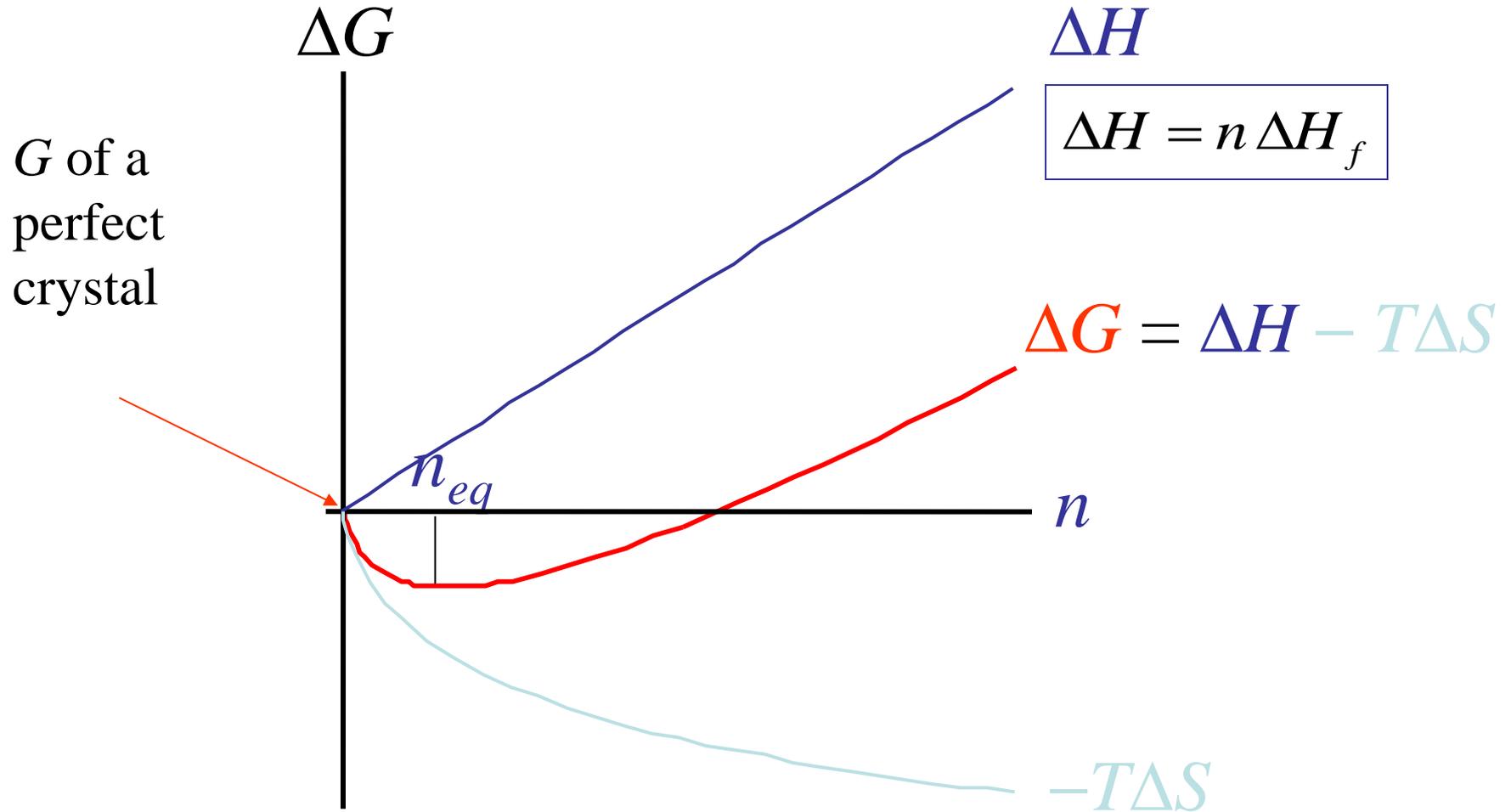
A wave with a wave vector $< k$ has no chance to get diffracted

Bragg planes and Brillouin zone construction



- Brillouin Zone formed by perpendicular bisectors of G vectors
- Consequence: No diffraction for any k inside the first Brillouin Zone

Equilibrium concentration of vacancies – temperature dependence



Equilibrium concentration of vacancies – temperature dependence

$$\left. \frac{\partial \Delta G}{\partial n} \right|_{n=n_{eq}} = 0$$

$$\frac{n_{eq}}{N} = \exp\left(-\frac{\Delta H_f}{kT}\right)$$

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

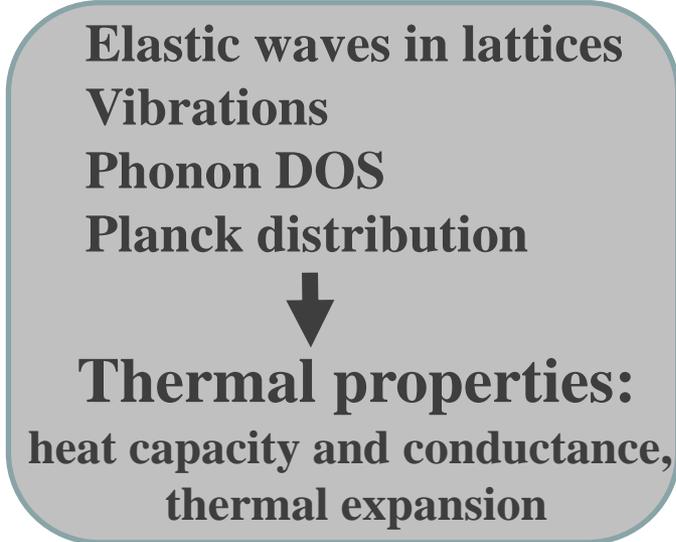
Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion



Temperature dependence of experimentally measured heat capacity

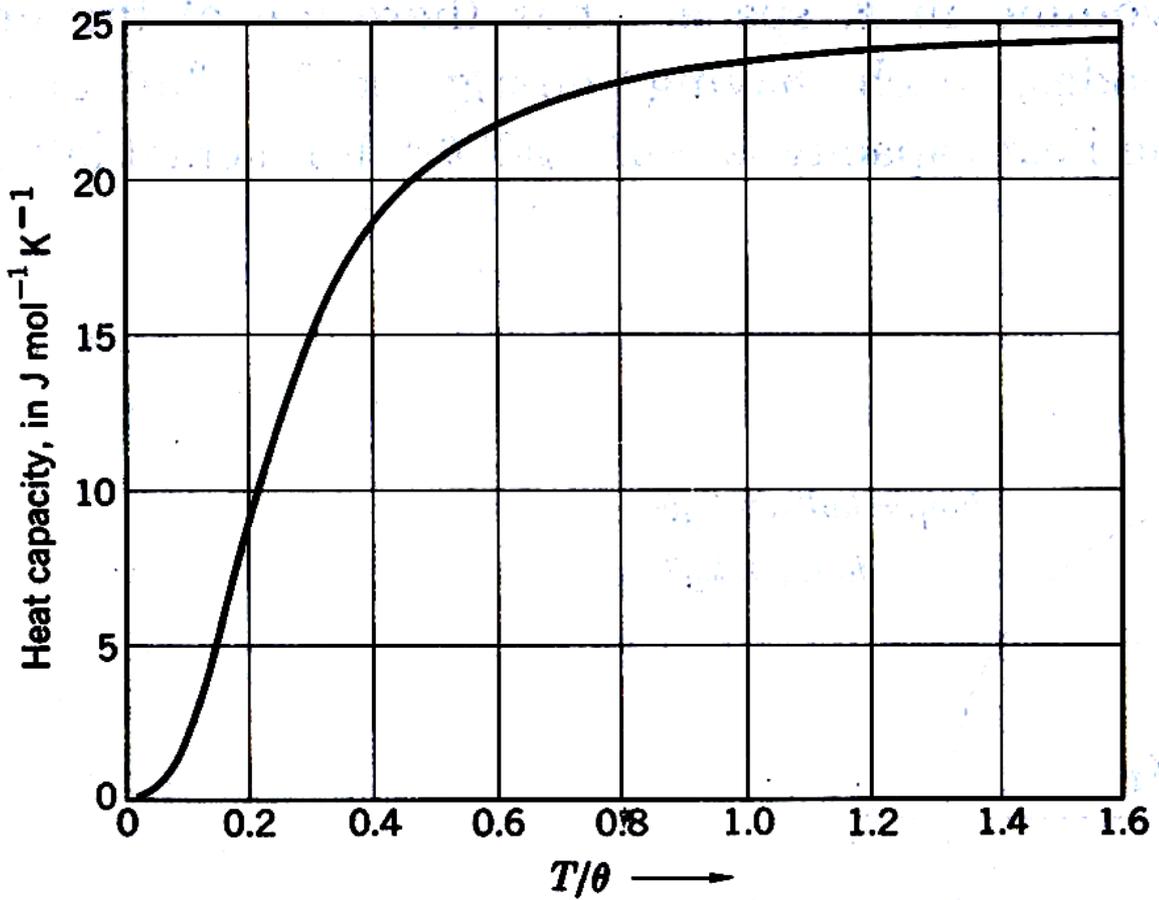
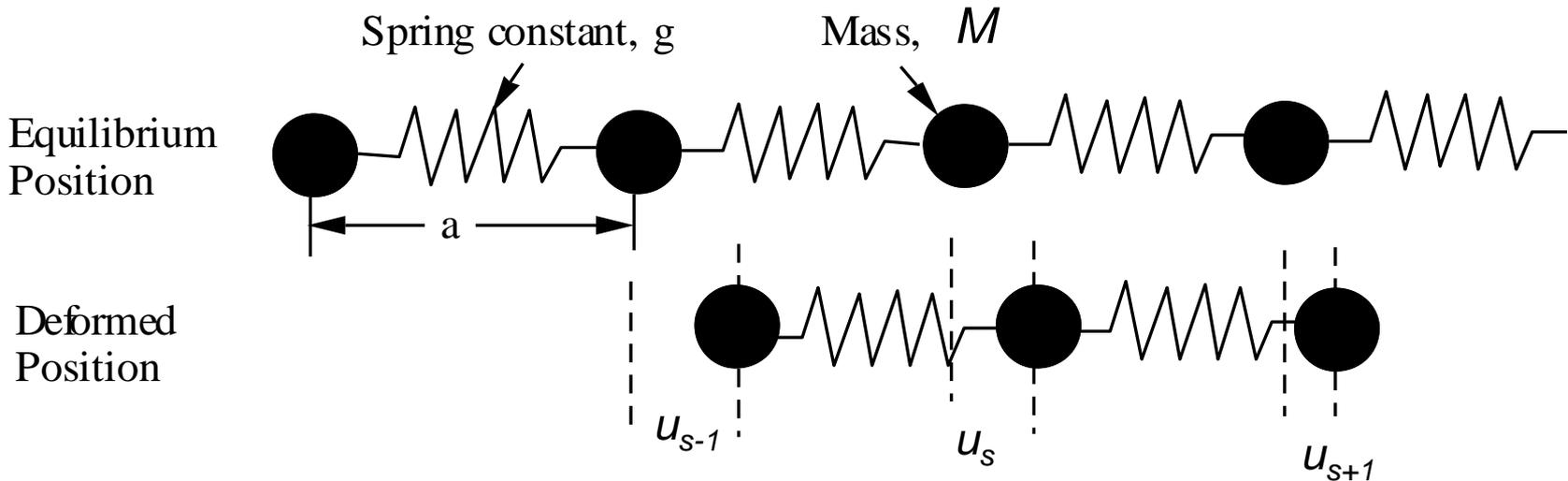
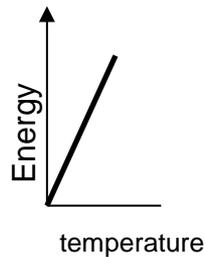


Figure 9a. Heat capacity C_V of a solid, according to the Debye approximation. The vertical scale is in $\text{J mol}^{-1} \text{K}^{-1}$. The horizontal scale is the temperature normalized to the Debye temperature θ . The region of the T^3 law is below 0.1θ . The asymptotic value at high values of T/θ is $24.943 \text{ J mol}^{-1} \text{ deg}^{-1}$.

Vibrations of crystals with monatomic basis



u_s : displacement of the s^{th} atom from its equilibrium position

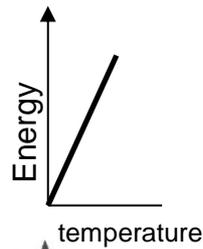


Classical oscillators

Any energy state is accessible for any oscillator in form of $k_B T$, i.e. no distribution function is applied and the total energy is

$$\bar{E} = N\bar{E}_1 = 3Nk_B T$$

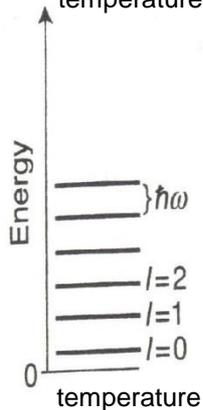
Classical versus quantum oscillators



Classical oscillators

Any energy state is accessible for any oscillator in form of $k_B T$, i.e. no distribution function is applied and the total energy is

$$\bar{E} = N\bar{E}_1 = 3Nk_B T$$



Quantum oscillators

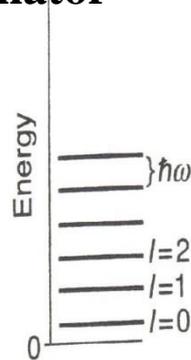
Not all energies are accessible, but only those in quants of $\hbar\omega$, and Planck distribution is employed to calculate the occupancy at temperature T , so that

$$E = 3N \cdot \langle n \rangle \cdot \hbar\omega$$

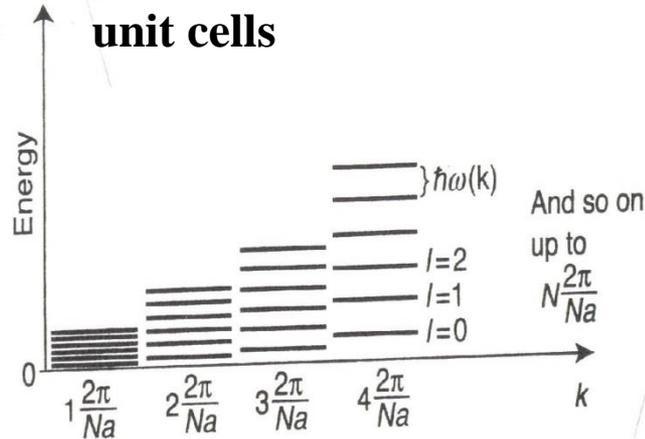
$$E = 3N \sum_{n=0}^{\infty} f(E_n) E_n = 3N \frac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_B T}}{\sum_{n=0}^{\infty} e^{-E_n/k_B T}} = 3N \frac{1}{e^{\hbar\omega/k_B T} - 1} \cdot \hbar\omega$$

Quantum oscillator versus phonon spectrum

Energy level diagram for one harmonic oscillator



Energy level diagram for a chain of atoms with one atom per unit cell and a length of N unit cells



$$E = 3N \cdot \langle n \rangle \cdot \hbar \omega$$

$$E = 3 \int_{\omega_{\min}}^{\omega_{\max}} d\omega D(\omega) \langle n \rangle \hbar \omega$$

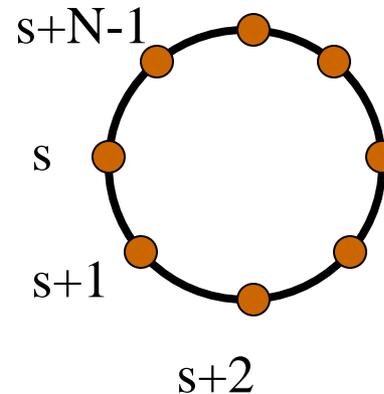
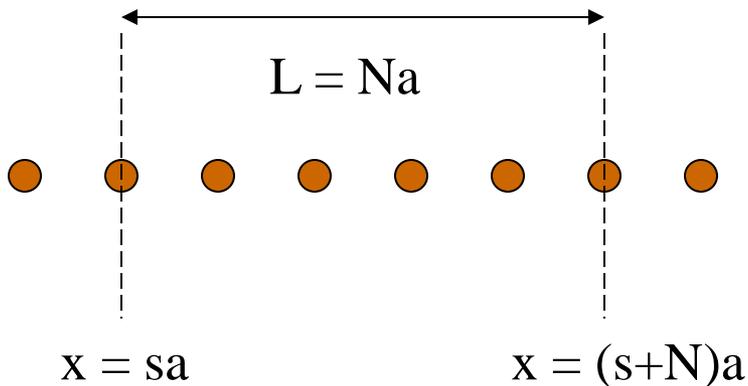
Calculating phonon density of states – DOS – in 1-D

A vibrational mode is a vibration of a given wave vector \vec{k} (and thus λ), frequency ω , and energy $E = \hbar\omega$. How many modes are found in the interval between (ω, E, \vec{k}) and $(\omega + d\omega, E + dE, \vec{k} + d\vec{k})$?

$$\# \text{ modes} \quad dN = N(\omega)d\omega = N(E)dE = N(k)d^3\vec{k}$$

We will first find $N(k)$ by examining allowed values of k . Then we will be able to calculate $N(\omega)$ and evaluate C_V in the Debye model.

First step: simplify problem by using periodic boundary conditions for the linear chain of atoms:



We assume atoms s and $s+N$ have the same displacement—the lattice has periodic behavior, where N is very large.

Calculating phonon density of states – DOS – in 1-D

Since atoms s and $s+N$ have the same displacement, we can write:

$$u_s = u_{s+N} \longrightarrow ue^{i(ksa-\omega t)} = ue^{i(k(s+N)a-\omega t)} \longrightarrow 1 = e^{ikNa}$$

This sets a condition on allowed k values:

$$kNa = 2\pi n \rightarrow k = \frac{2\pi n}{Na} \quad n = 1, 2, 3, \dots$$

So the separation between allowed solutions (k values) is:

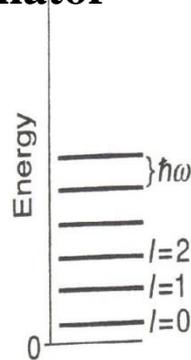
$$\Delta k = \frac{2\pi}{Na} \quad \Delta n = \frac{2\pi}{Na} \quad \text{independent of } k, \text{ so the density of modes in } k\text{-space is uniform}$$

Thus, in 1-D:

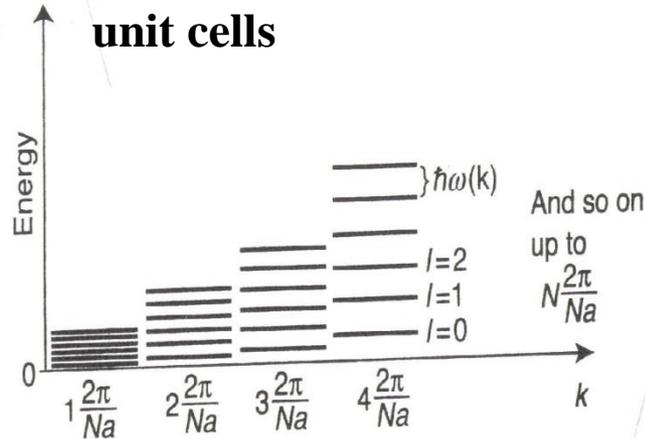
$$\frac{\# \text{ of modes}}{\text{interval of } k\text{-space}} = \frac{1}{\Delta k} = \frac{Na}{2\pi} = \frac{L}{2\pi}$$

Quantum oscillator versus phonon spectrum

Energy level diagram for one harmonic oscillator



Energy level diagram for a chain of atoms with one atom per unit cell and a length of N unit cells



$$E = 3N \cdot \langle n \rangle \cdot \hbar \omega$$

$$E = 3 \int_{\omega_{\min}}^{\omega_{\max}} d\omega D(\omega) \langle n \rangle \hbar \omega$$

Temperature dependence of thermal conductivity in terms of phonon properties

Mechanisms to affect the mean free pass (Λ) of phonons in periodic crystals:

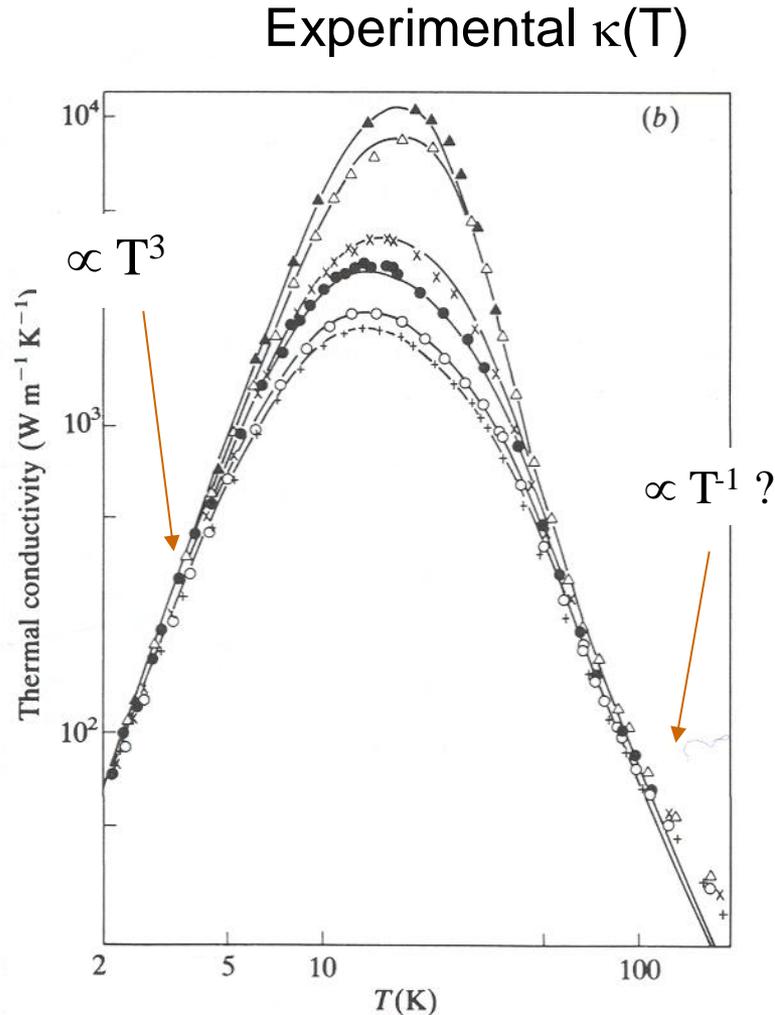
1. Interaction with impurities, defects, and/or isotopes
 2. Collision with sample boundaries (surfaces)
 3. Collision with other phonons
- } deviation from translation symmetry
- } deviation from harmonic behavior

To understand the experimental dependence $\kappa(T)$, consider limiting values of C_V and Λ (since v does not vary much with T).

$$C_V \begin{cases} \propto T^3 & \text{low } T \\ 3R & \text{high } T \end{cases} \quad \Lambda \propto \frac{1}{n_{ph}} = e^{\hbar\omega/kT} - 1 \begin{cases} \rightarrow \infty & \text{low } T \\ \frac{\hbar\omega}{kT} & \text{high } T \end{cases}$$

Temperature dependence of thermal conductivity in terms of phonon properties

T^3 estimation for κ the low temperature limit is fine!



However, T^{-1} estimation for κ in the high temperature limit has a problem. Indeed, κ drops much faster – see the data – and the origin of this disagreement is because – when estimating Λ – we accounted for all excited phonons, while a more correct approximation would be to consider “high” energetic phonons only. But what is “high” in this context?

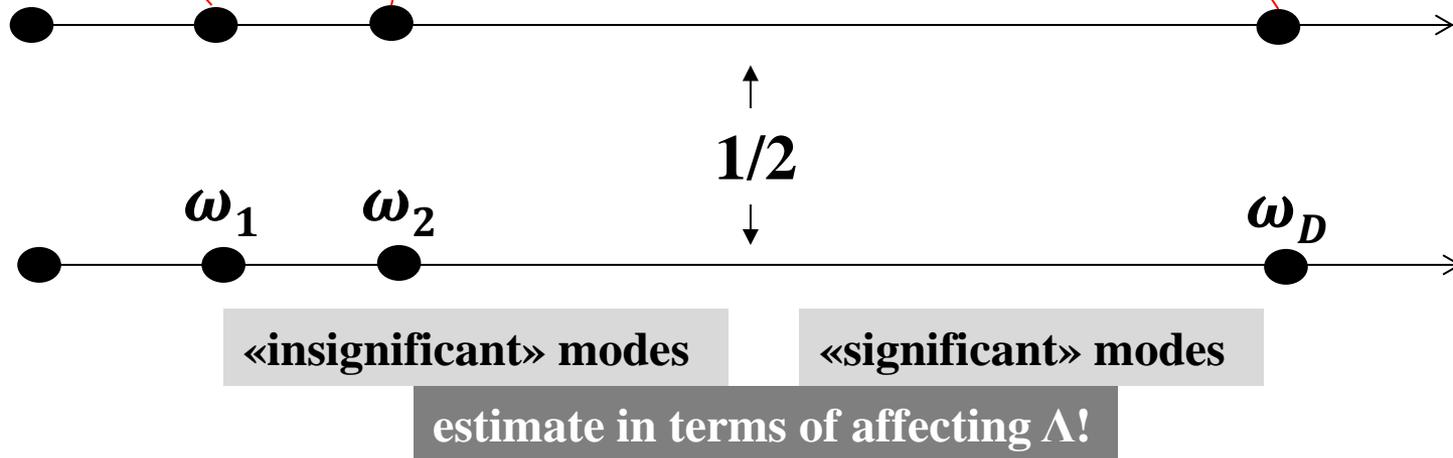
Figure 5.27 (a) The principal form for the variation of thermal conductivity. (b) Experimental data for LiF crystals containing different amounts of the isotope ${}^6\text{Li}$: \blacktriangle , 0.02% ${}^6\text{Li}$; \triangle , 0.01%; \times , 4.6%; \bullet , 9.4%; \circ , 25.4%; $+$, 50.1%. (After Berman and Brock 1965.)

Better estimation for Λ at the high temperature limit

$$k_1 = \frac{2\pi \cdot 1}{Na} = \frac{2\pi}{Na}$$

$$k_2 = \frac{2\pi \cdot 2}{Na} = \frac{4\pi}{Na}$$

$$k_N = \frac{2\pi \cdot N}{Na} = \frac{2\pi}{a}$$



The fact that «low energetic phonons» having k -values $\ll \pi/a$ do not participate in the energy transfer, can be understood by considering so called N- and U-phonon collisions readily visualized in the reciprocal space. Anyhow, we account for modes having energy $E_{1/2} = (1/2)\hbar\omega_D$ or higher. Using the definition of $\theta_D = \hbar\omega_D/k_B$, $E_{1/2}$ can be rewritten as $k_B\theta_D/2$. Ignoring more complex statistics, but using Boltzman factor only, the propability of $E_{1/2}$ would of the order of $\exp(-k_B\theta_D/2k_B T)$ or $\exp(-\theta_D/2T)$, resulting in $\Lambda \propto \exp(\theta_D/2T)$.

Temperature dependence of thermal conductivity in terms of phonon properties

Thus, considering defect free, isotopically clean sample having limited size D

	C_V	Λ	κ
low T	$\propto T^3$	$n_{\text{ph}} \rightarrow 0$, so $\Lambda \rightarrow \infty$, but then $\Lambda \rightarrow D$ (size)	$\propto T^3$
high T	$3R$	$\propto \exp(\theta_D/2T)$	$\propto \exp(\theta_D/2T)$

Thermal Expansion in 1-D

Evaluating this for the harmonic potential energy function $U(x) = cx^2$ gives:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x e^{-cx^2/kT} dx}{\int_{-\infty}^{+\infty} e^{-cx^2/kT} dx}$$

The numerator is zero!

$$\langle x \rangle = 0! \quad \text{independent of } T!$$

Thus any nonzero $\langle x \rangle$ must come from terms in $U(x)$ that go beyond x^2 . For HW you will evaluate the approximate value of $\langle x \rangle$ for the model function

$$U(x) = cx^2 - gx^3 + fx^4 - \dots \quad (c, g, f > 0 \quad \text{and} \quad gx^3, fx^4 \ll kT)$$

Why this form? On the next slide you can see that this function is a reasonable model for the kind of $U(r)$ we have discussed for molecules and solids.

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



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contribution to the heat capacity

Free electron gas (FEG) - Drude model

There could be different opinions what particular discovery was the main breakthrough for the acceleration of the condensed matter physics but a very prominent kick-off was by the discovery of the electron by J.J. Thompson in 1897. Soon afterwards (1900) P. Drude used the new concept to postulate a theory of electrical conductivity.

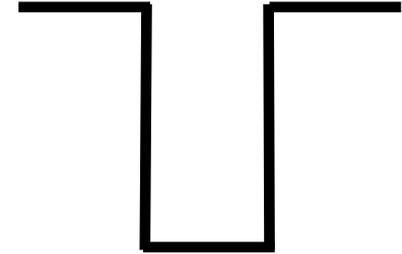
Drude was working prior to the development of quantum mechanics, so he began with a classical model, specifically:

- (i) positive ion cores within the electron gas that follows Maxwell-Boltzmann statistics;**
- (ii) following the kinetic theory of gases - the electrons are in form of free electron gas (FEG), so that individual electrons move in straight lines and make collisions only with the ion cores; electron-electron interactions are neglected;**
- (iii) Electrons lose energy gained from the electric field in collisions and the mean free path was approximately the inter-atomic spacing.**

Drude (or FEG) model successfully explained Ohm and Wiedemann-Franz laws, but failed to explain, e.g., electron heat capacity and the magnetic susceptibility of conduction electrons.

FEFG - Free Electron Fermi Gas

Consider electrons
as quantum particles in a box



$$-\frac{\hbar^2 \nabla^2}{2m_e} \psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

FEFG model means that $U(\mathbf{r}) = 0$.

One electron system – wave functions - orbits

- Neglect electron-electron interaction, infinite potential well, simple QM solution

$$\psi_n = A \sin\left(\frac{2\pi}{\lambda_n} x\right); \quad \frac{1}{2}n\lambda_n = L, \quad \epsilon_n = \frac{\hbar^2}{2m} \left(\frac{n\pi}{L}\right)^2. \quad \text{Standing wave B. C. } n = 1, 2, \dots$$

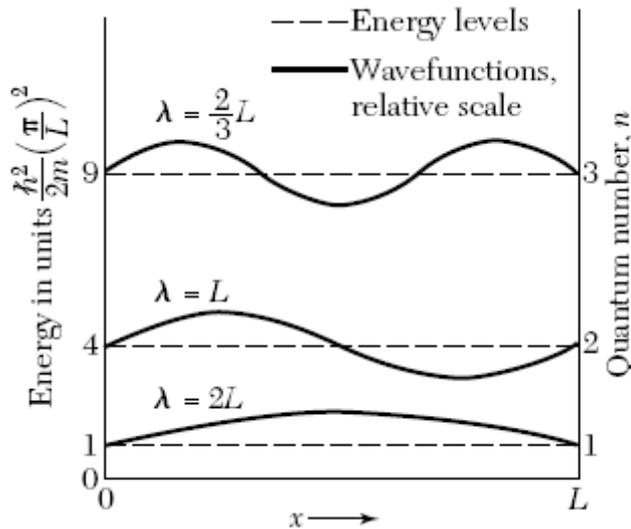


Figure 2 First three energy levels and wavefunctions of a free electron of mass m confined to a line of length L . The energy levels are labeled according to the quantum number n which gives the number of half-wavelengths in the wavefunction. The wavelengths are indicated on the wavefunctions. The energy ϵ_n of the level of quantum number n is equal to $(\hbar^2/2m)(n/2L)^2$.

- The Pauli exclusion principle
- n : quantum number
- $m(=1/2 \text{ and } -1/2)$: magnetic quantum number
- degeneracy: # of orbitals with the same energy
- Fermi energy (E_F): energy of the topmost filled level in the ground state of the N electron system

In this simple system, every quantum state holds 2 electrons $\Rightarrow n_F = N/2 \rightarrow$ Fermi energy:

$$\epsilon_F = \frac{\hbar^2}{2m} \left(\frac{n_F \pi}{L}\right)^2 = \frac{\hbar^2}{2m} \left(\frac{N \pi}{2L}\right)^2$$

Great, if we know the electron density, we know the Fermi energy!

FEFG in 3D

$$-\frac{\hbar^2 \nabla^2}{2m_e} \psi(\mathbf{r}) = E \psi(\mathbf{r}) \quad \psi(\mathbf{r}) \sim e^{i\mathbf{k}\mathbf{r}}$$

$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e} (k_x^2 + k_y^2 + k_z^2)$$

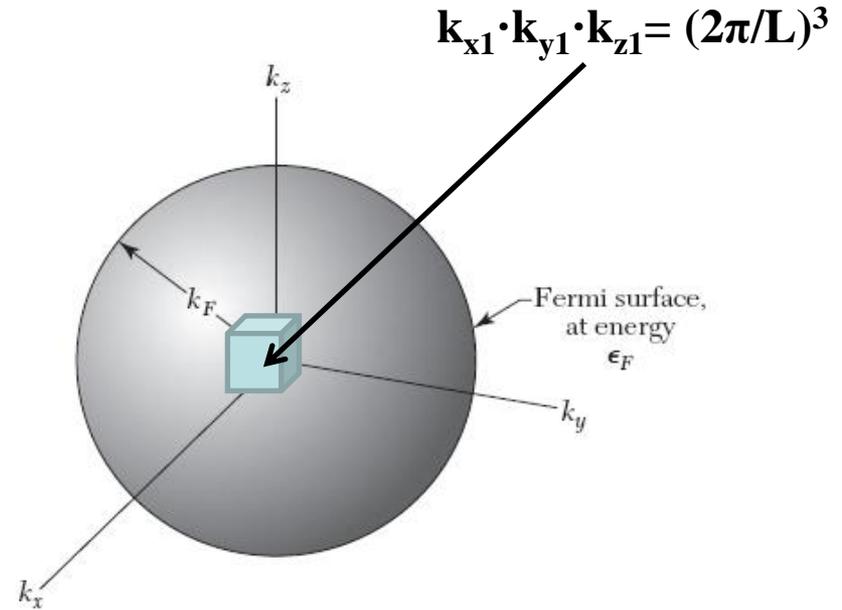
boundary conditions provide restrictions the wavevector \mathbf{k}

$$\mathbf{k} = (k_x, k_y, k_z) = \left(\frac{n_x 2\pi}{L}, \frac{n_y 2\pi}{L}, \frac{n_z 2\pi}{L} \right)$$

FEFG in 3D

The volume of $k_{x1} \cdot k_{y1} \cdot k_{z1} = (2\pi/L)^3$ corresponds to only one k-state, accommodating 2 electrons

While k_{\max} or k_F accommodate $N/2$!



$$2 \cdot \frac{4\pi k_F^3/3}{(2\pi/L)^3} = \frac{V}{3\pi^2} k_F^3 = N$$

$$k_F = \left(\frac{3\pi^2 N}{V} \right)^{1/3}$$

$$\epsilon_F = \frac{\hbar^2}{2m} k_F^2$$

$$\epsilon_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

$$v_F = \left(\frac{\hbar k_F}{m} \right) = \left(\frac{\hbar}{m} \right) \left(\frac{3\pi^2 N}{V} \right)^{1/3}$$

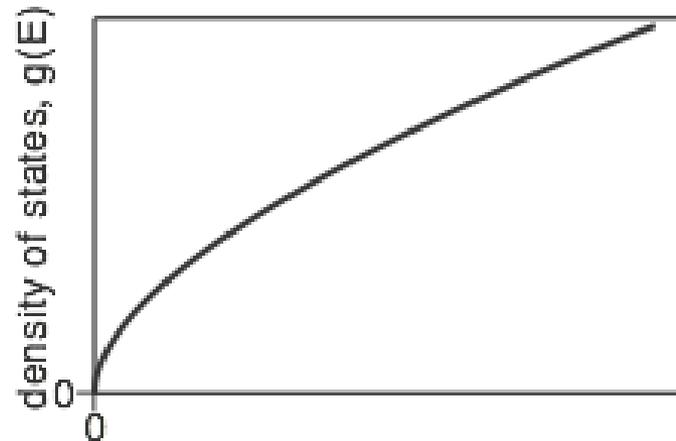
FEFG in 3D

For any E

$$E(N) = \frac{\hbar^2}{2m_e} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

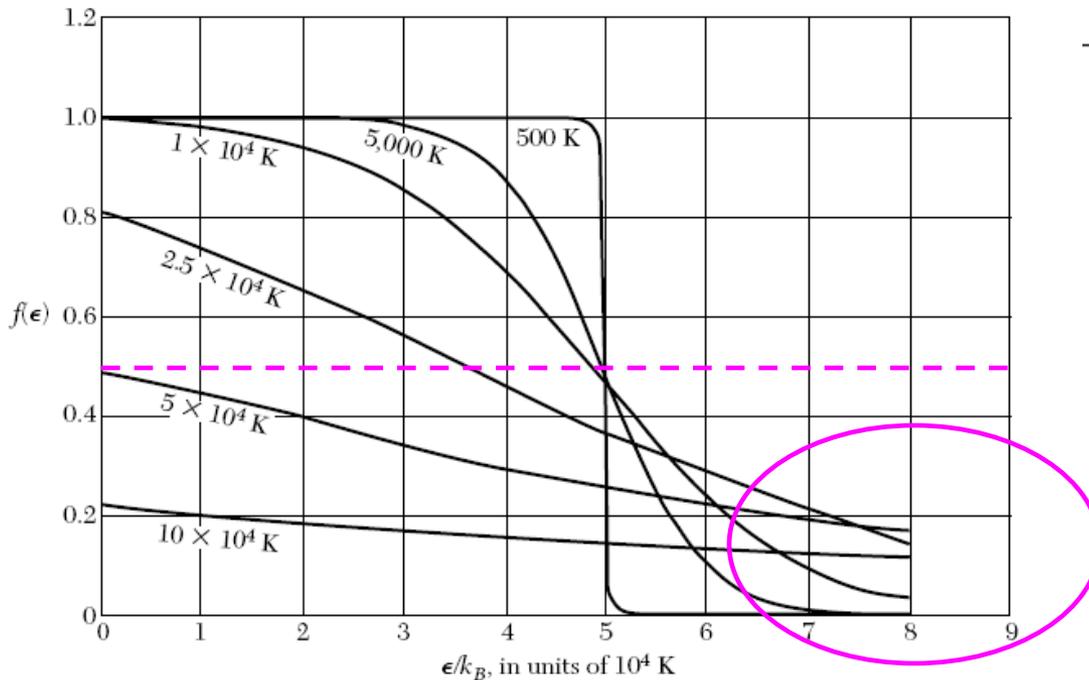
$$N(E) = \frac{V}{3\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{3/2} E^{3/2}$$

$$g(E)dE = \frac{dN}{dE}dE = \frac{V}{2\pi^2} \left(\frac{2m_e}{\hbar^2} \right)^{3/2} E^{1/2}dE$$



Fermi-Dirac distribution

- Describes the probability that an orbit at energy E will be occupied in an ideal electron gas under thermal equilibrium
- μ is chemical potential, $f(\epsilon = \mu) = 0.5$; at 0K, $\epsilon_F = \mu$



$$f(\epsilon) = \frac{1}{\exp[(\epsilon - \mu)/k_B T] + 1}$$

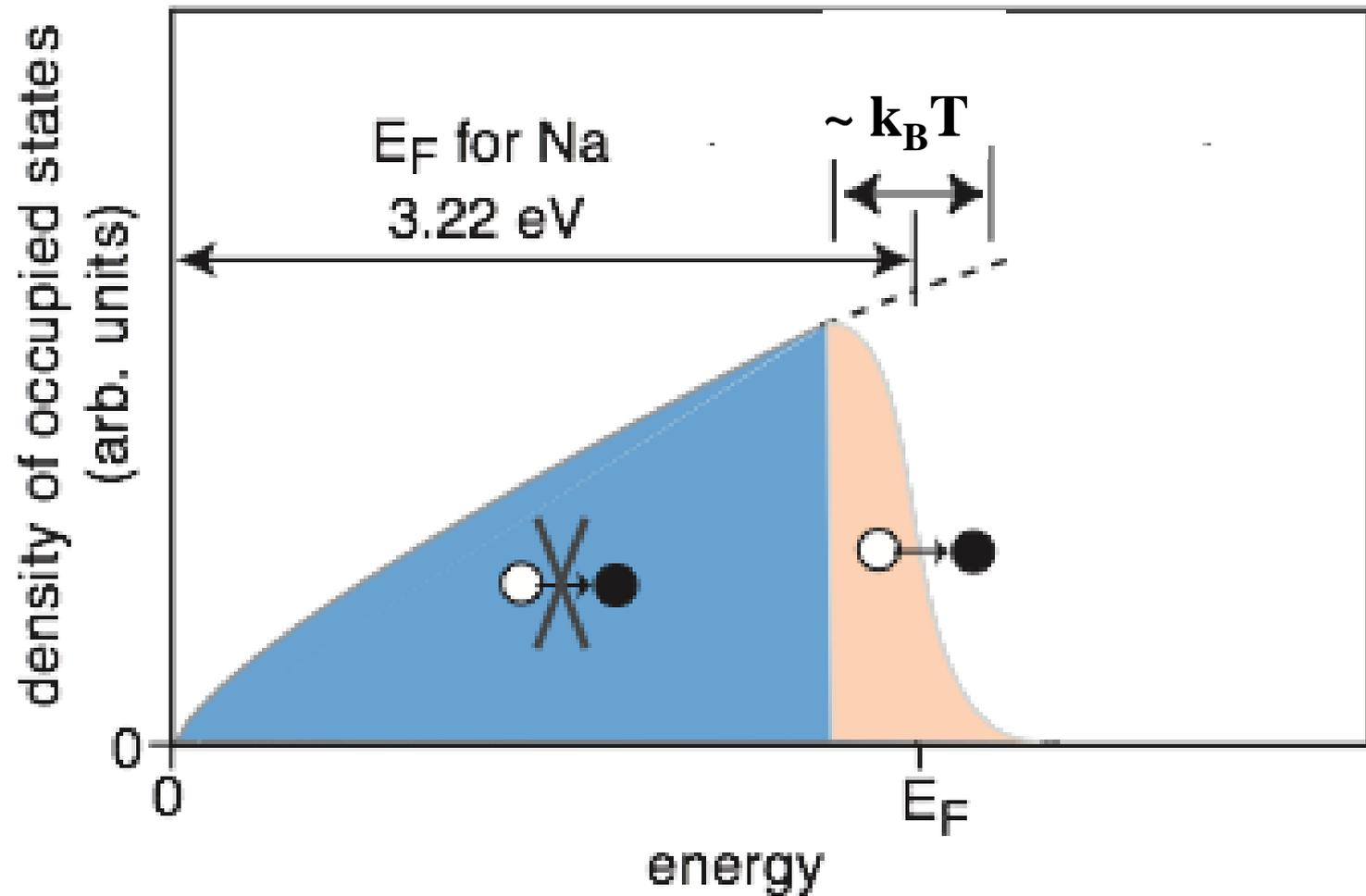
High energy tail – approximation

$$E - E_F > 3k_B T$$

→ Boltzmann-Maxwell distribution

$$f_{\text{Boltzmann-Maxwell}}(E) = \exp\left(-\frac{E - E_F}{k_B T}\right)$$

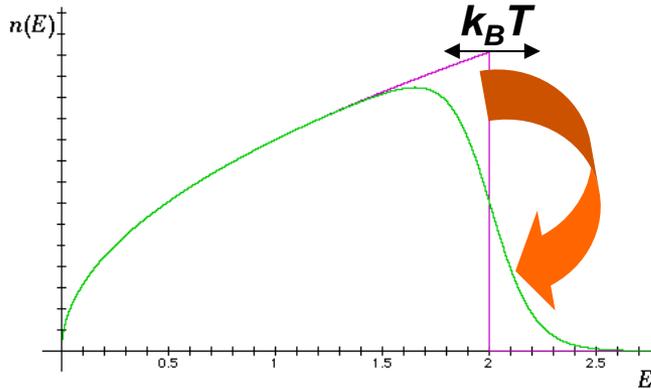
Fermi-Dirac distribution



Estimate for the heat capacity of FEFG

One of the greatest successes of the free electron model and FD statistics is the explanation of the T dependence of the heat capacity of a metal.

$$C_V \equiv \left. \frac{dQ(T)}{dT} \right|_{V=const} = \frac{dE_t(T)}{dT}$$



To calculate the heat capacity, we need to know how the internal energy of the Fermi gas, $E_t(T)$, depends on temperature. By heating a Fermi gas, we populate some states above the Fermi energy E_F and deplete some states below E_F . This modification is significant within a narrow energy range $\sim k_B T$ around E_F .

The fraction of electrons that we “transfer” to higher energies $\sim k_B T/E_F$, the energy increase for these electrons $\sim k_B T$. Thus, the increase of the internal energy with temperature is proportional to $n \times (k_B T/E_F) \times (k_B T) \sim n (k_B T)^2 / E_F$. Note, $E_F = k_B T_F$

$$C_V = \frac{dE_t(T)}{dT} \propto N \frac{k_B^2 T}{E_F}$$

$$\boxed{C_e = \frac{\pi^2}{2} n k_B \frac{k_B T}{E_F}} \quad \longleftrightarrow \quad \text{compare} \quad C_V = \frac{3}{2} n k_B \quad \text{for an ideal gas}$$

The Fermi gas heat capacity is much smaller (by $k_B T/E_F \ll 1$) than that of a classical ideal gas with the same energy and pressure. The small heat capacity is a direct consequence of the Pauli principle: most of the electrons cannot change their energy, only a small fraction $k_B T/E_F$ or T/T_F of the electrons are excited out of the ground state.

Condensed Matter Physics



Solid State Physics of Crystals



Properties of Waves in Periodic Lattices



Elastic waves in lattices

Vibrations

Phonon DOS

Planck distribution



Thermal properties:

heat capacity and conductance,
thermal expansion

Electron waves in lattices

Free electrons

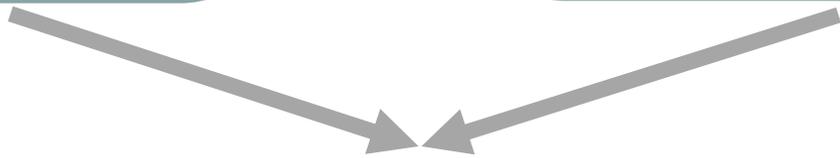
Electron DOS

Fermi-Dirac distribution



Electronic properties:

Electron concentration and transport,
contribution to the heat capacity



Advanced theory and novel materials properties

One electron approximation + periodic potential

$$-\frac{\hbar^2 \nabla^2}{2m_e} \psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

$$U(\mathbf{r}) = U(\mathbf{r} + \mathbf{R})$$

Bragg-reflection for nearly free electrons

consider only one direction (x)

free electron wave function

$$\psi(r) = e^{ikr}$$

with a de Broglie wavelength

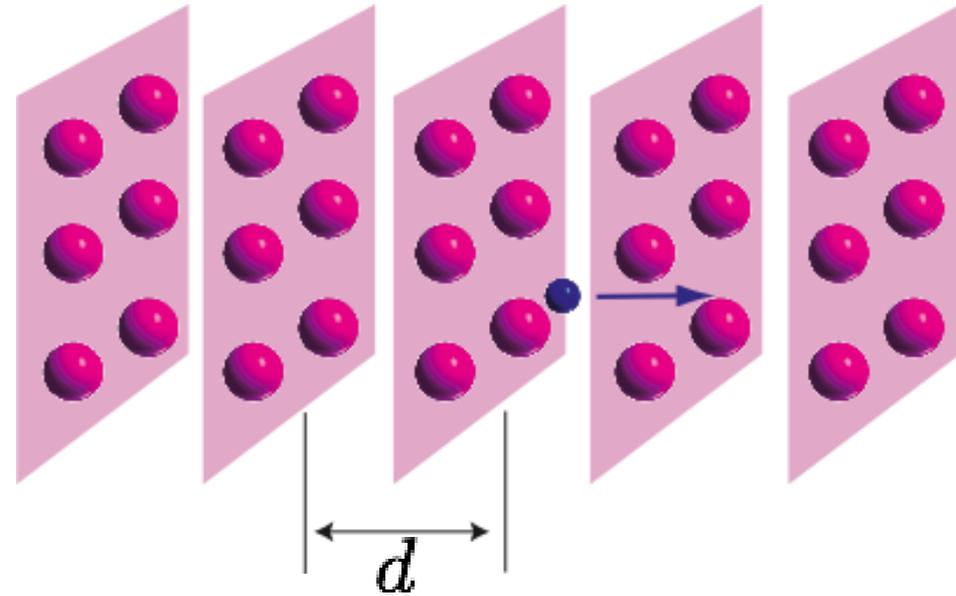
$$k = \frac{2\pi}{\lambda} \quad \lambda = \frac{2\pi}{k}$$

Bragg condition

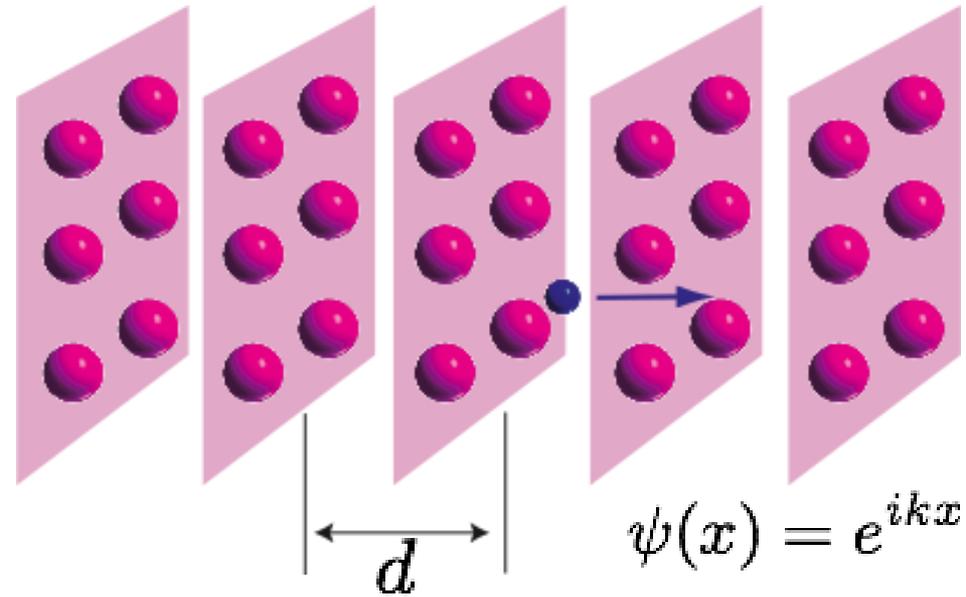
$$n\lambda = 2d \sin\theta \quad \text{with} \quad \theta = 90^\circ, -90^\circ$$

this gives a Bragg condition for electron waves:

$$k = \pm \frac{n\pi}{d}$$



Bragg-reflection for nearly free electrons



Bragg condition for electron waves:

$$k = \pm \frac{n\pi}{d}$$

Bragg reflection results in standing, not traveling electron waves

two possible linear combinations of $\exp(\pm i \frac{\pi}{d} x)$

$$\Psi(+)=\exp\left(i \frac{\pi}{d} x\right)+\exp\left(-i \frac{\pi}{d} x\right)=2 \cos\left(\frac{\pi}{d} x\right)$$

$$\Psi(-)=\exp\left(i \frac{\pi}{d} x\right)-\exp\left(-i \frac{\pi}{d} x\right)=2 i \sin\left(\frac{\pi}{d} x\right)$$

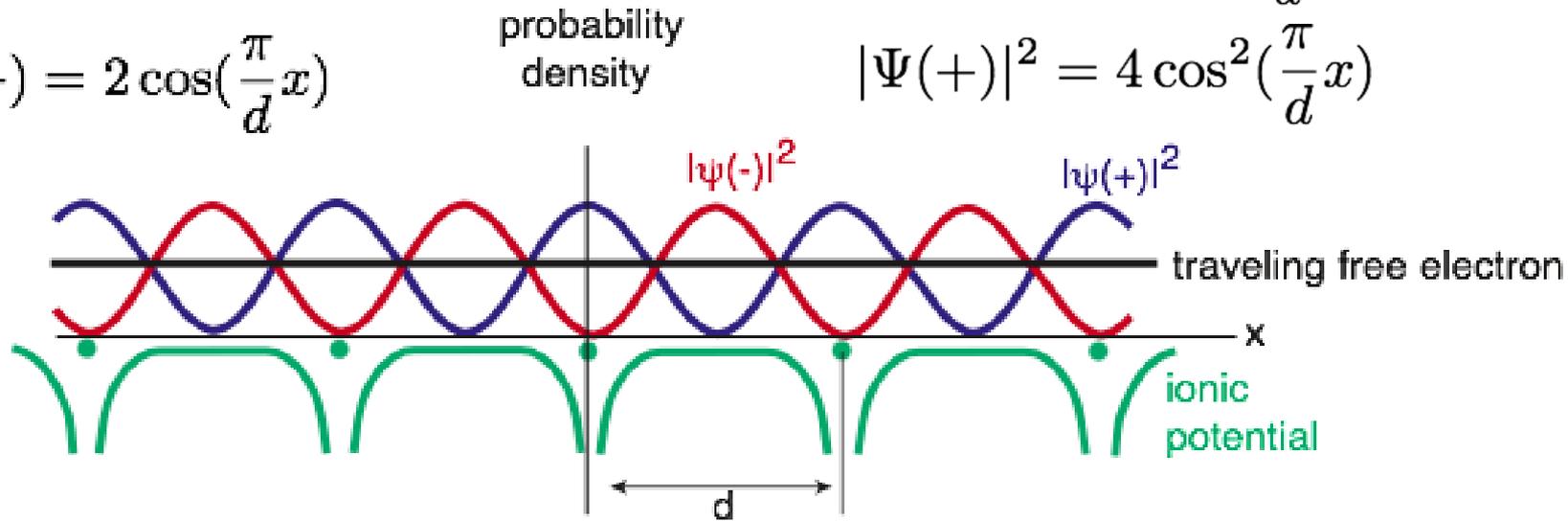
Gap opening for nearly free electrons

$$\Psi(-) = 2i \sin\left(\frac{\pi}{d}x\right)$$

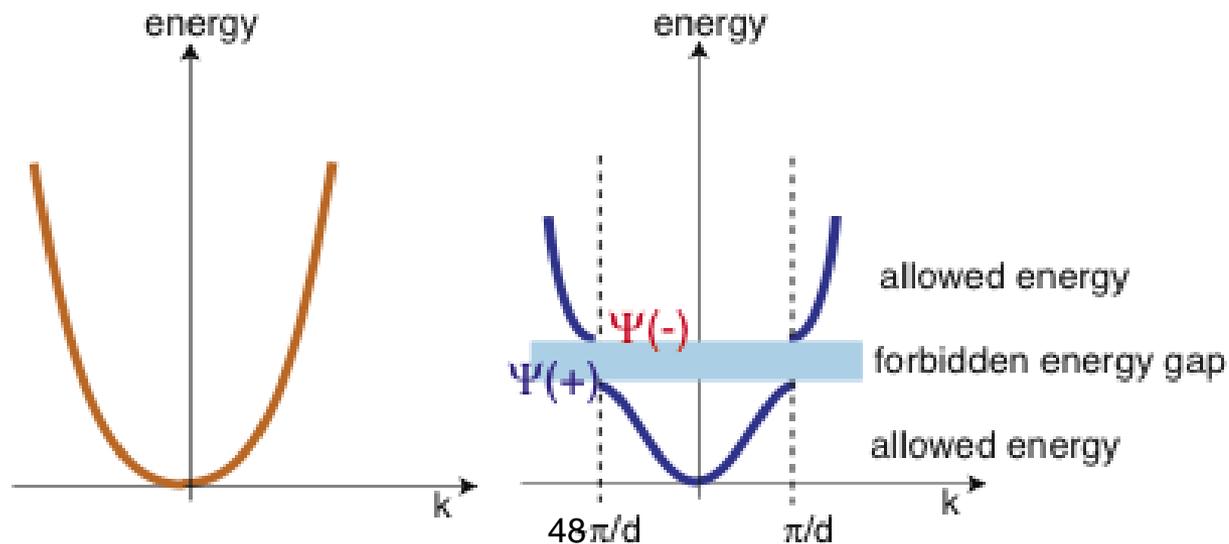
$$|\Psi(-)|^2 = 4 \sin^2\left(\frac{\pi}{d}x\right)$$

$$\Psi(+) = 2 \cos\left(\frac{\pi}{d}x\right)$$

$$|\Psi(+)|^2 = 4 \cos^2\left(\frac{\pi}{d}x\right)$$



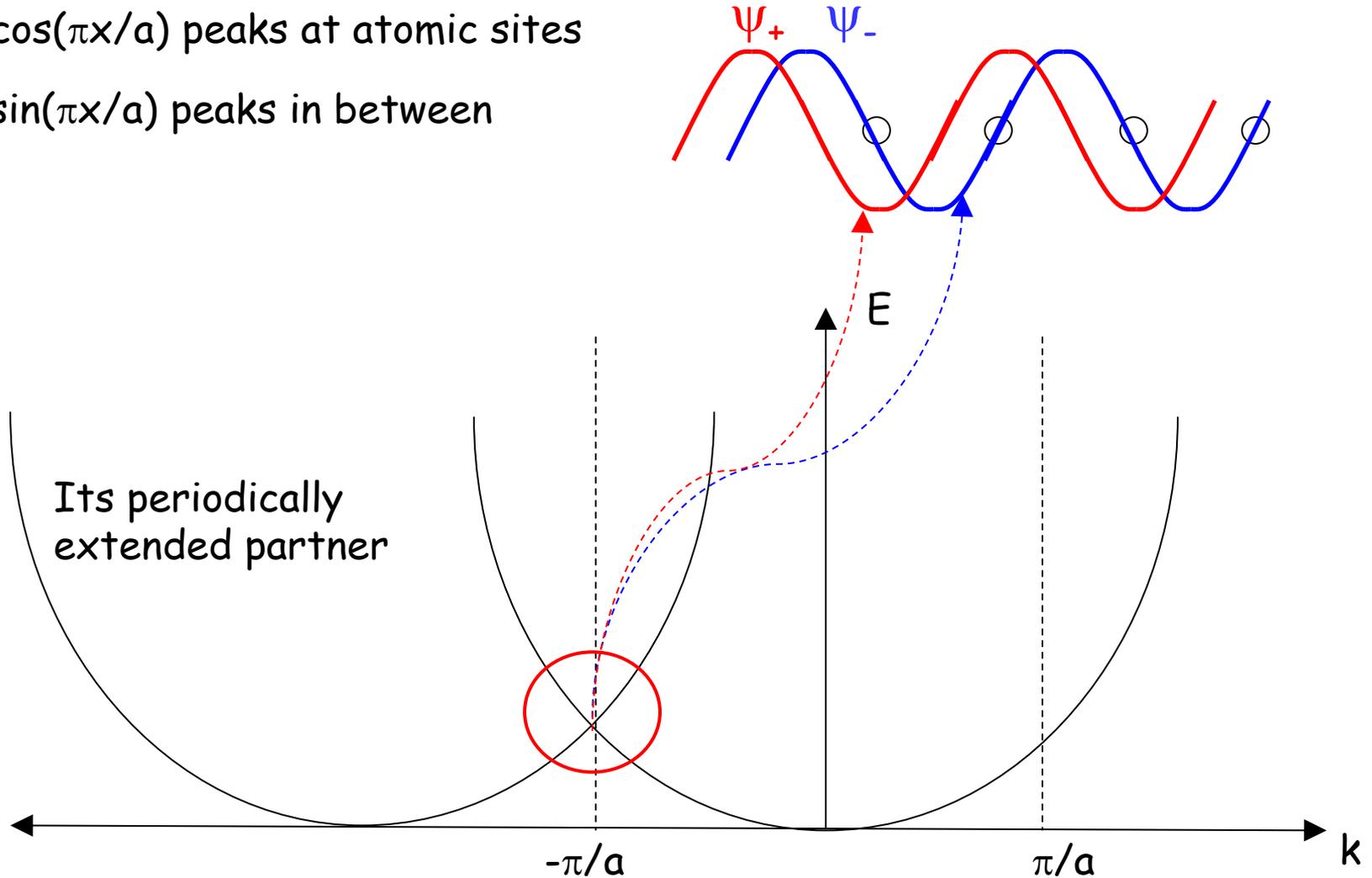
$$E = \frac{\hbar^2 k^2}{2m_e}$$



Why do we get a gap?

$\psi_+ \sim \cos(\pi x/a)$ peaks at atomic sites

$\psi_- \sim \sin(\pi x/a)$ peaks in between



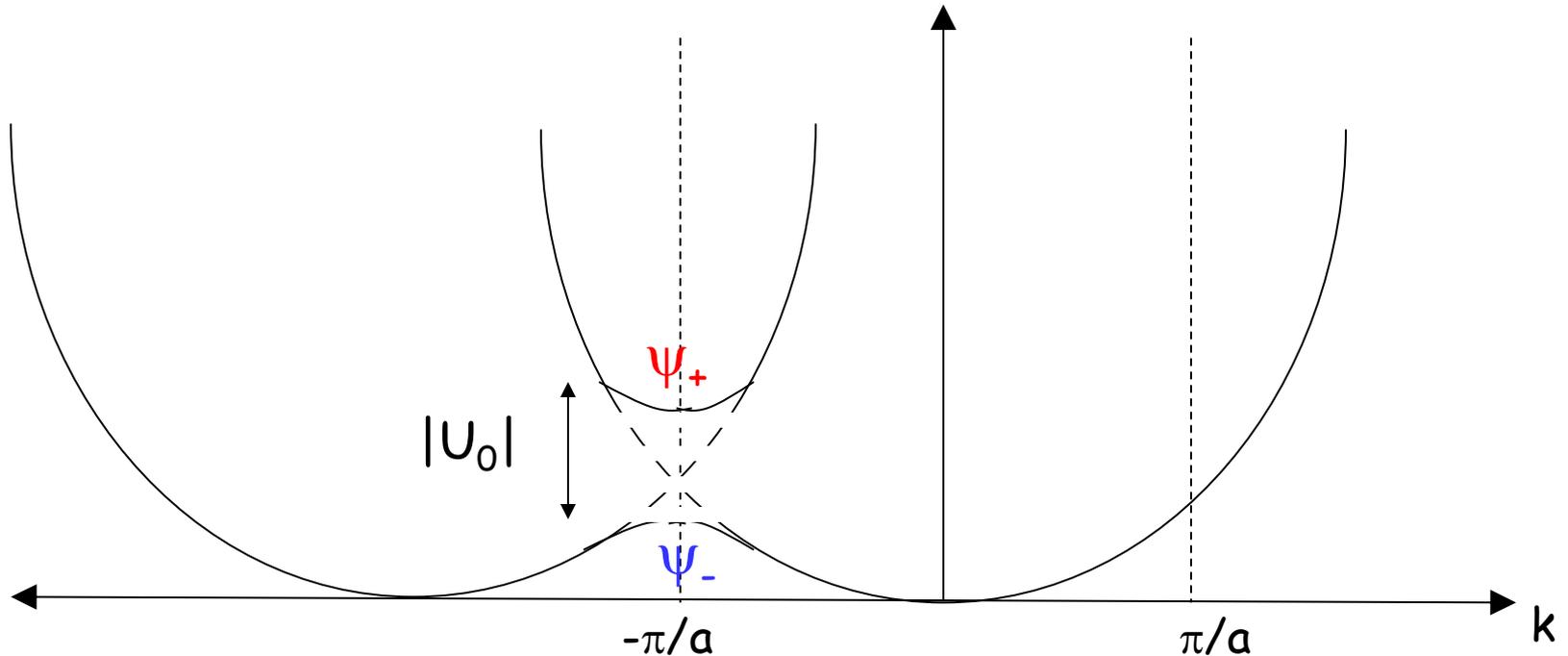
Let's now turn on the atomic potential

The ψ_+ solution sees the atomic potential and increases its energy

The ψ_- solution does not see this potential (as it lies between atoms)

Thus their energies separate and a gap appears at the BZ

This happens only at the BZ where we have standing waves



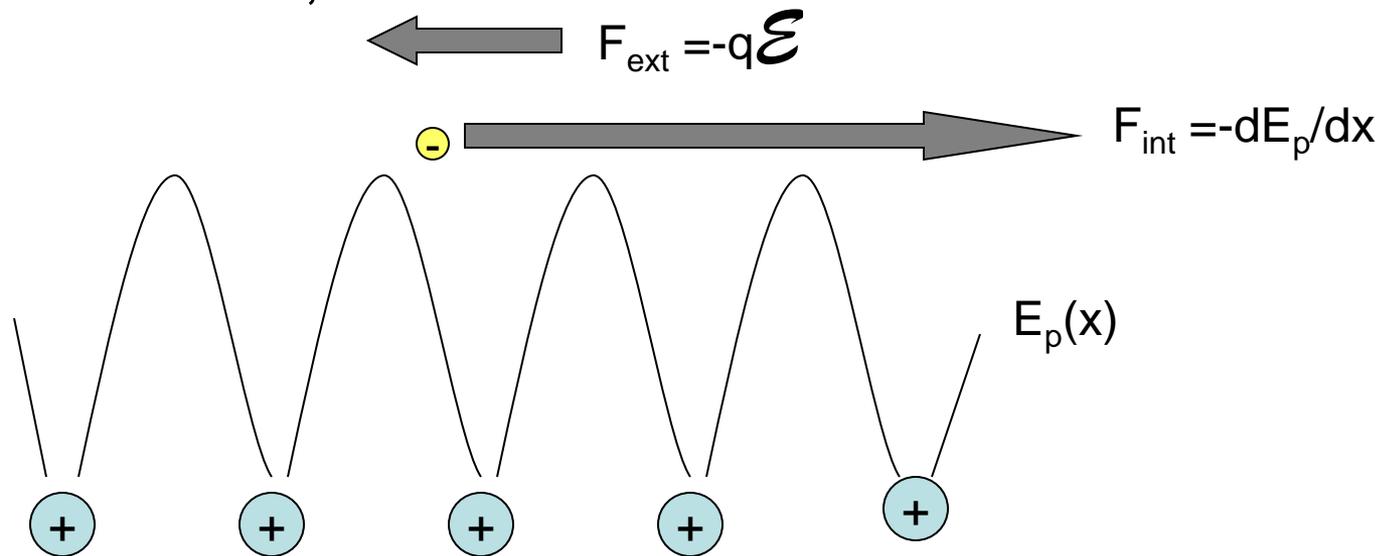
One electron approximation + periodic potential

$$-\frac{\hbar^2 \nabla^2}{2m_e} \psi(\mathbf{r}) + U(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

use of the effective mass method!!

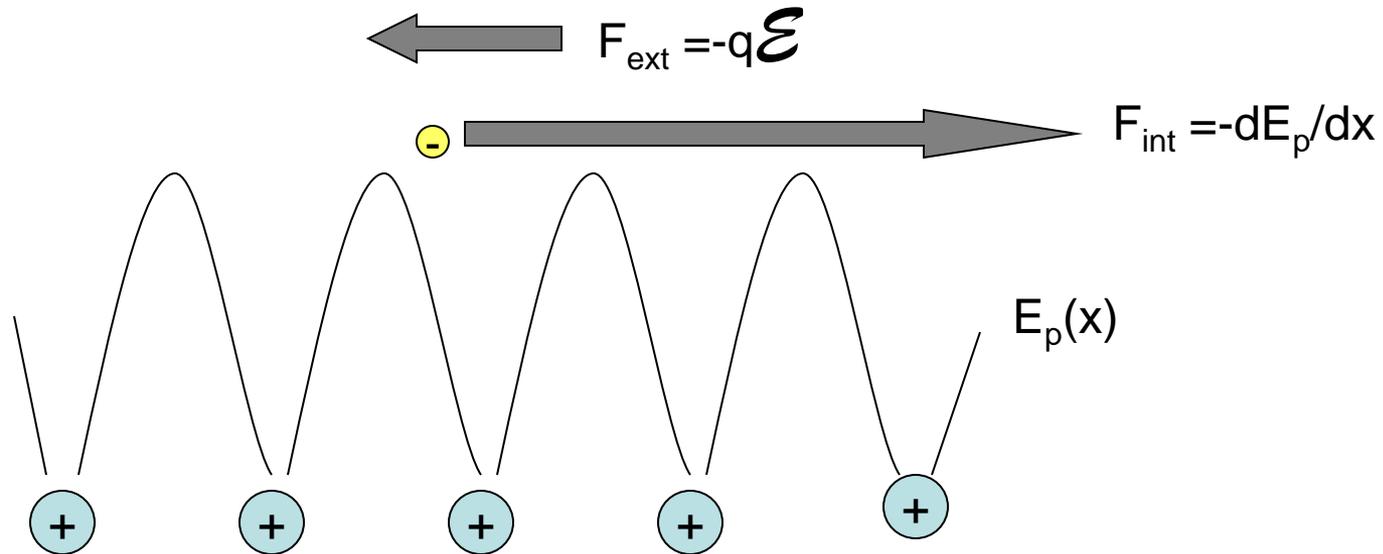
Internal and external forces affecting an electron in crystal

- The electron is subject to internal forces from the lattice (ions and core electrons) AND external forces such as electric fields
- In a crystal lattice, the net force may be opposite the external force, however:



Internal and external forces affecting an electron in crystal

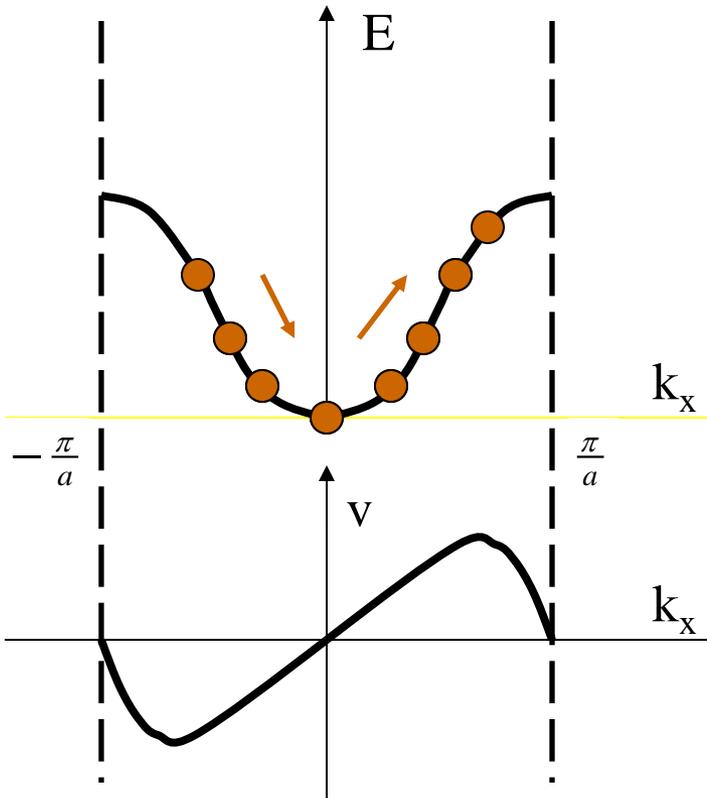
- electron acceleration is not equal to F_{ext}/m_e , but rather...
- $a = (F_{\text{ext}} + F_{\text{int}})/m_e == F_{\text{ext}}/m^*$
- The dispersion relation $E(K)$ compensates for the internal forces due to the crystal and allows us to use *classical* concepts for the electron as long as its mass is taken as m^*



Dynamics of electrons in a band

The external electric field causes a change in the k vectors of all electrons:

$$\vec{F} = \hbar \frac{d\vec{k}}{dt} = -e\vec{E} \quad \longrightarrow \quad \frac{d\vec{k}}{dt} = \frac{-e\vec{E}}{\hbar}$$

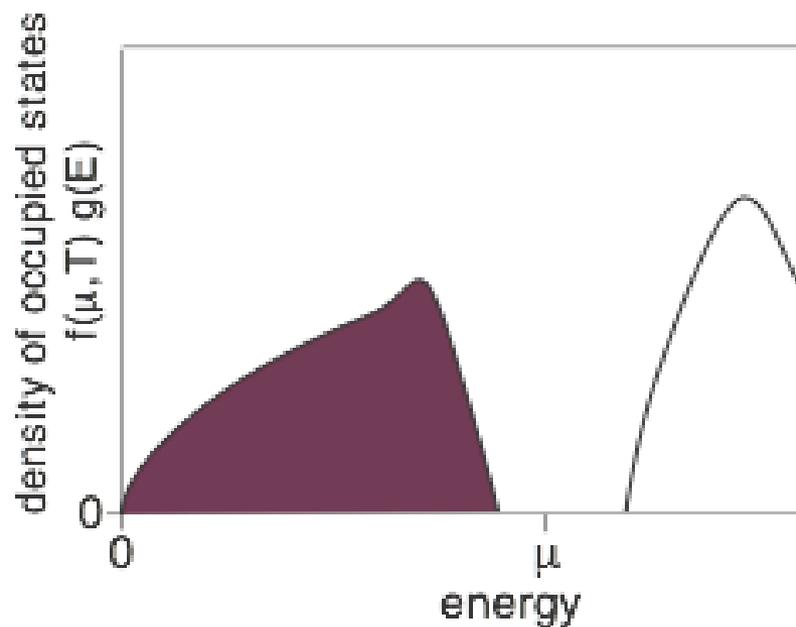
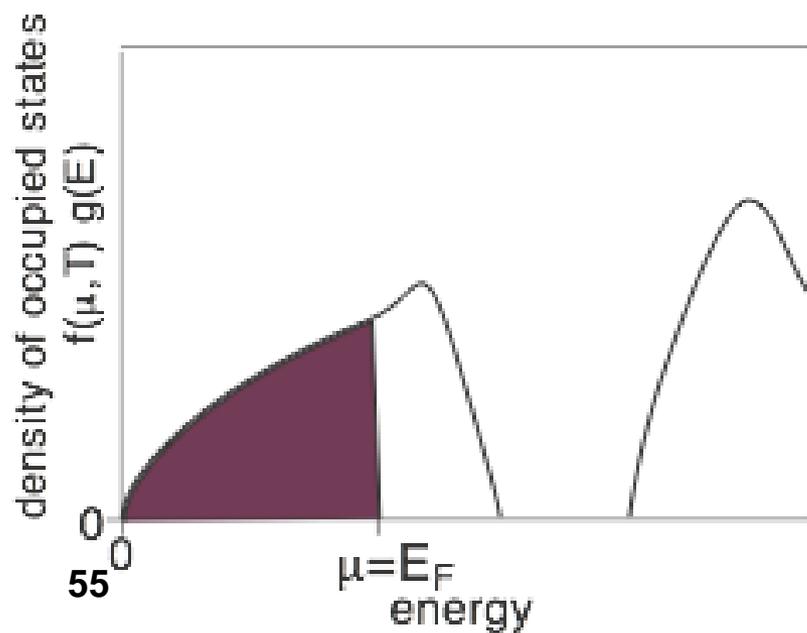
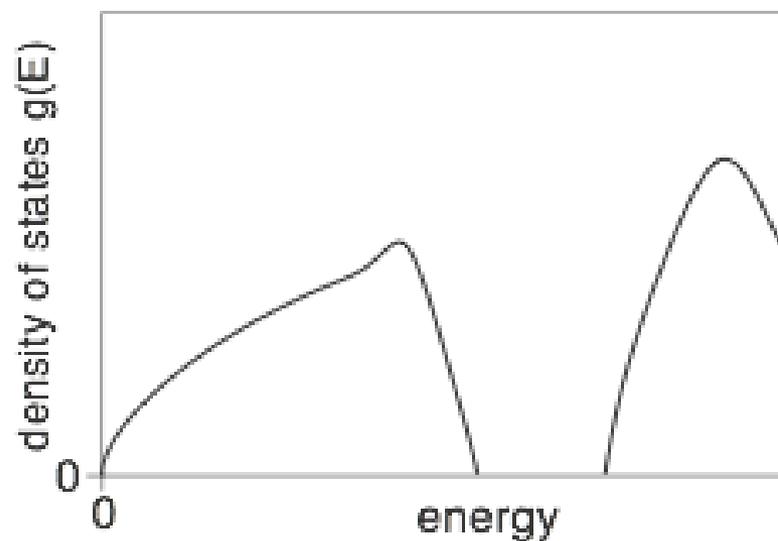
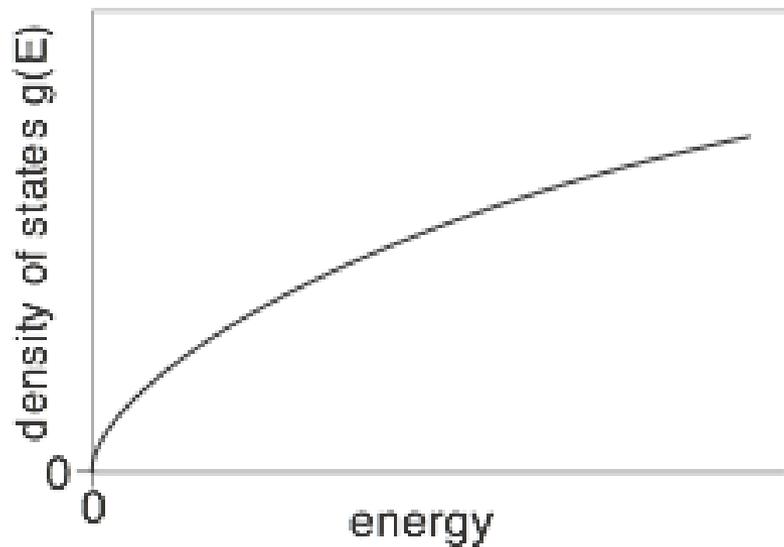


If the electrons are in a partially filled band, this will break the symmetry of electron states in the 1st BZ and produce a net current. But if they are in a filled band, even though all electrons change k vectors, the symmetry remains, so $J = 0$.

When an electron reaches the 1st BZ edge (at $k = \pi/a$) it immediately reappears at the opposite edge ($k = -\pi/a$) and continues to increase its k value.

As an electron's k value increases, its velocity increases, then decreases to zero and then becomes negative when it re-emerges at $k = -\pi/a$!!

Band-to-band transitions



Band-to-band transitions

electrons in the conduction band (CB)

$$n = \frac{1}{V} \int_{E_C}^{\infty} g_C(E) f(E, T) dE$$

missing electrons (holes) in the valence band (VB)

$$p = \frac{1}{V} \int_{-\infty}^{E_V} g_V(E) [1 - f(E, T)] dE$$

Band-to-band transitions

for the conduction band

$$(E - \mu) \gg k_B T$$

$$f(E, T) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \approx e^{-(E-\mu)/k_B T}$$

for the valence band

$$-(E - \mu) \gg k_B T$$

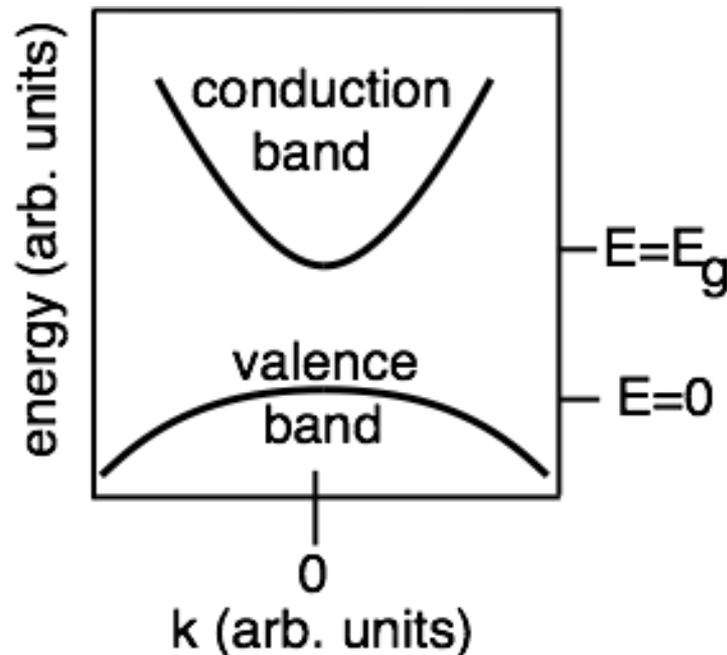
$$1 - f(E, T) = 1 - \frac{1}{e^{(E-\mu)/k_B T} + 1} = \frac{e^{(E-\mu)/k_B T} + 1}{e^{(E-\mu)/k_B T} + 1} - \frac{1}{e^{(E-\mu)/k_B T} + 1} \approx e^{(E-\mu)/k_B T}$$

Both are Boltzmann distributions!

This is called the non-degenerate case.

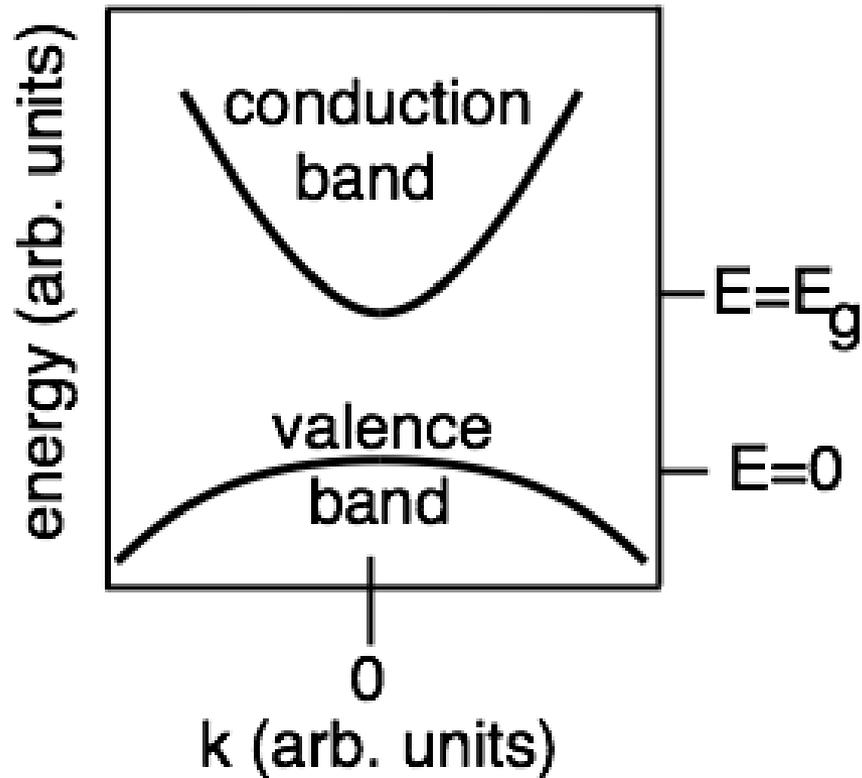
Band-to-band transitions

$$n = 2 \left(\frac{2\pi m_e^* k_B T}{h^2} \right)^{3/2} e^{-(E_g - \mu)/k_B T} = N_{\text{eff}}^C e^{-(E_g - \mu)/k_B T}$$



$$p = 2 \left(\frac{2\pi m_h^* k_B T}{h^2} \right)^{3/2} e^{-\mu/k_B T} = N_{\text{eff}}^V e^{-\mu/k_B T}$$

Band-to-band transitions



$$n = N_{\text{eff}}^C e^{-(E_g - \mu)/k_B T}$$

conduction band

CBM

μ

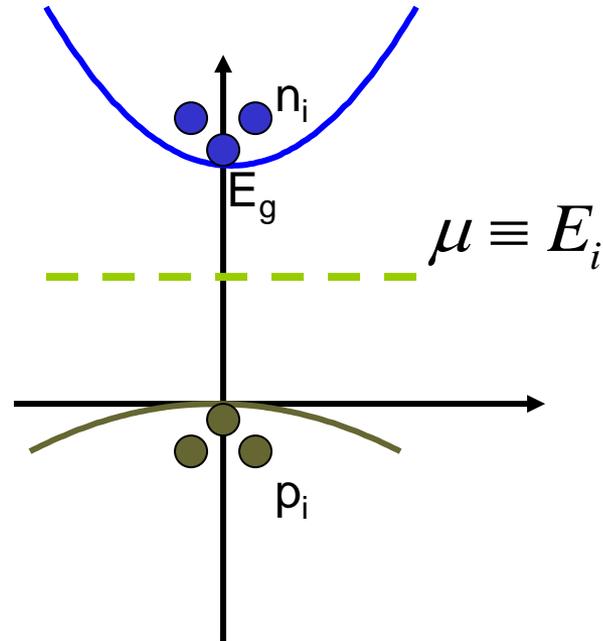
VBM

valence band

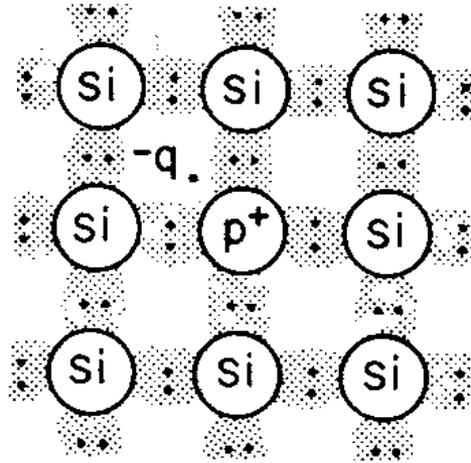
$$p = N_{\text{eff}}^V e^{-\mu/k_B T}$$

Detailed description: A schematic energy level diagram. It shows three horizontal lines. The top line is labeled 'conduction band' and has a hatched area above it. The middle line is labeled 'CBM' (Conduction Band Minimum) and has a red vertical bar on it. The bottom line is labeled 'valence band' and has a hatched area below it. The middle line is also labeled ' μ ' (chemical potential) and has a red vertical bar on it. The top line is also labeled 'VBM' (Valence Band Maximum). Blue arrows point from the red bars to the circled terms in the equations above and below. The equation above is $n = N_{\text{eff}}^C e^{-(E_g - \mu)/k_B T}$ and the equation below is $p = N_{\text{eff}}^V e^{-\mu/k_B T}$.

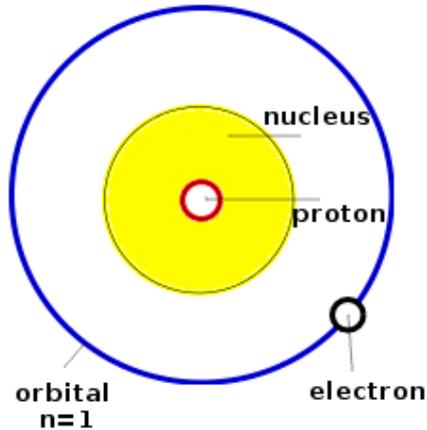
Carrier concentration in the bands



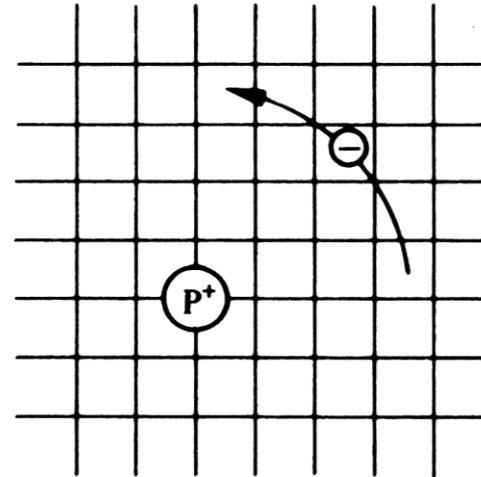
Hydrogen like impurities in semiconductors



P donor in Si can be modeled as hydrogen-like atom

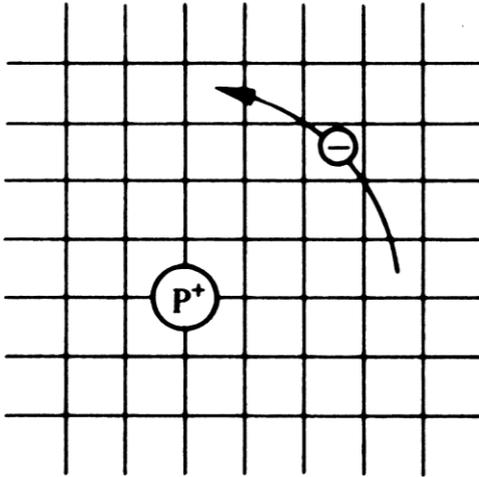


Hydrogen atom



Hydrogen-like donor

Hydrogen like impurities in semiconductors



Instead of m_0 , we have to use m_n^* .
Instead of ϵ_0 , we have to use $K_s \epsilon_0$.

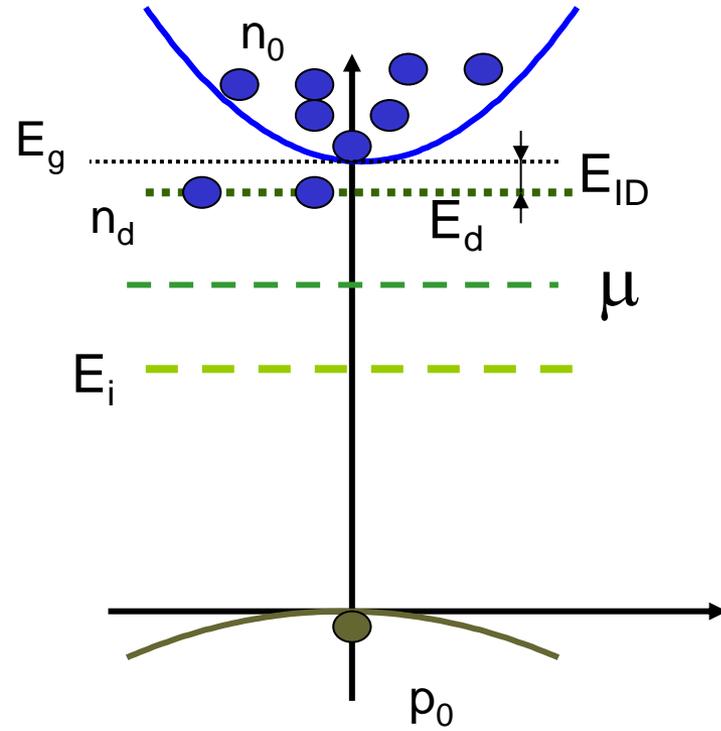
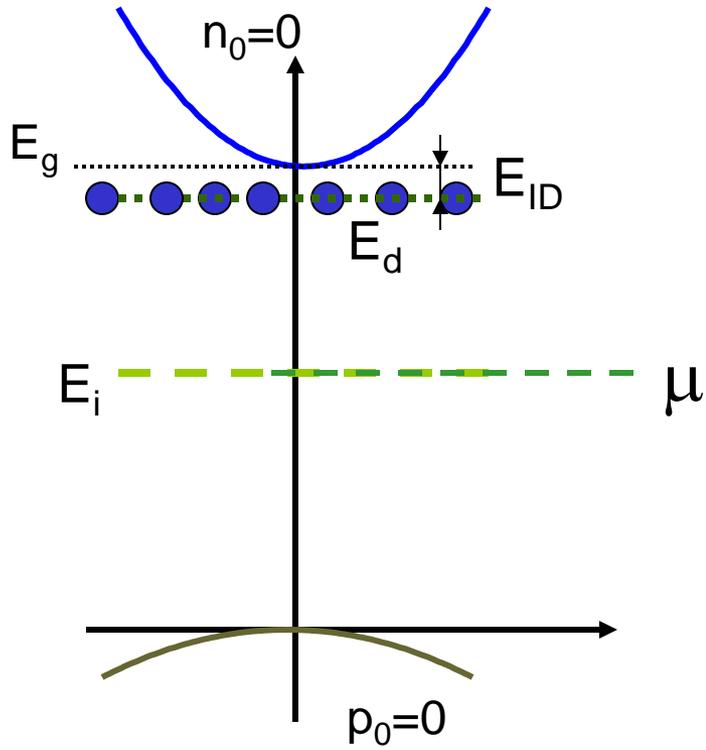
K_s is the relative dielectric constant
of Si ($K_{s, Si} = 11.8$).

Hydrogen-like donor

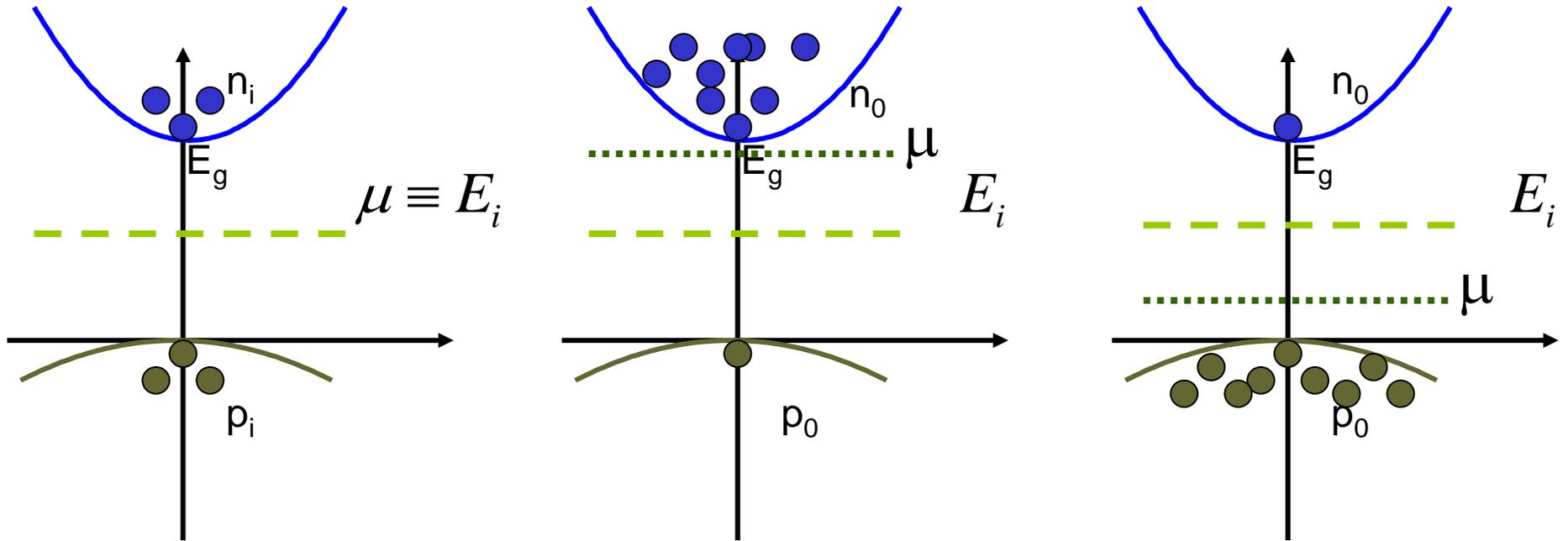
$$E_H = -\frac{m_0 q^4}{2(4\pi\epsilon_0\hbar)^2} = -13.6 \text{ eV}$$

$$E_d = -\frac{m_n^* q^4}{2(4\pi K_s \epsilon_0 \hbar)^2} = -13.6 \text{ eV} \frac{m_n^*}{m_0} \left(\frac{\epsilon_0}{K_s \epsilon_0} \right)^2 \approx -0.05 \text{ eV}$$

Hydrogen like impurities in semiconductors

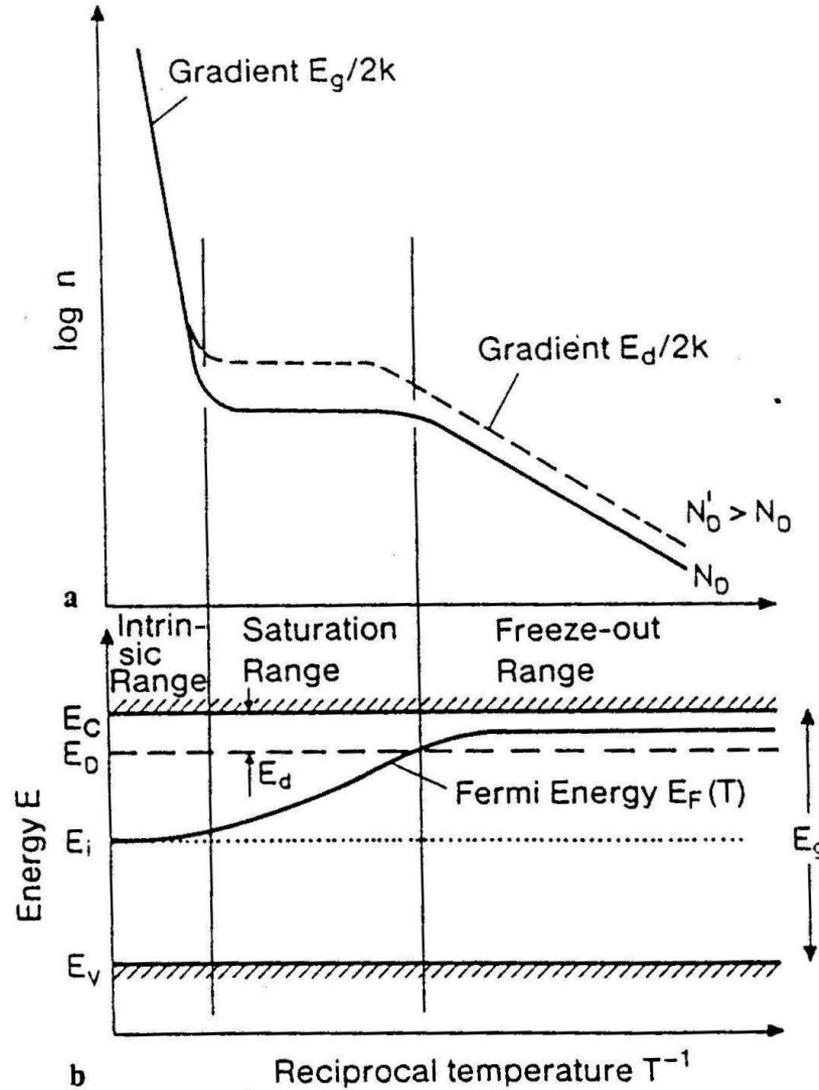


Intrinsic and extrinsic semiconductors



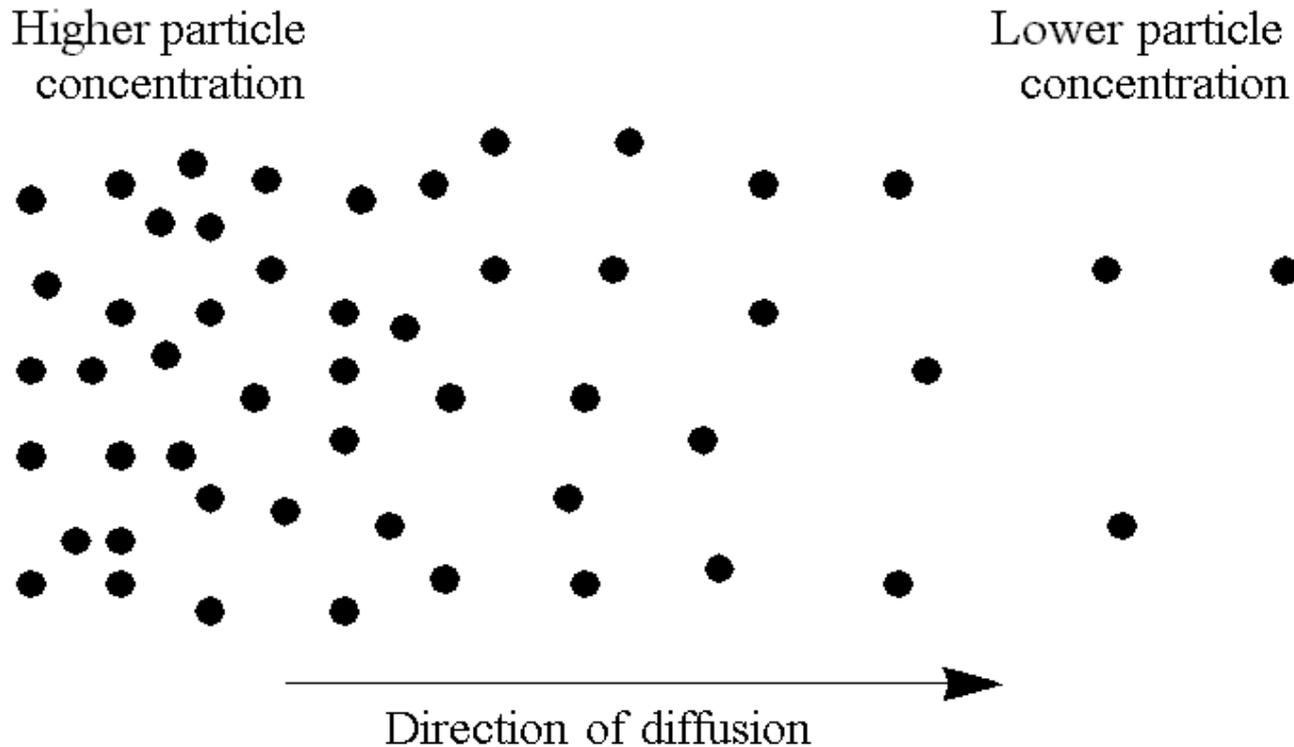
Equilibrium charge carrier concentration in semiconductors

$$n_0 + N_a^- = p_0 + N_d^+$$



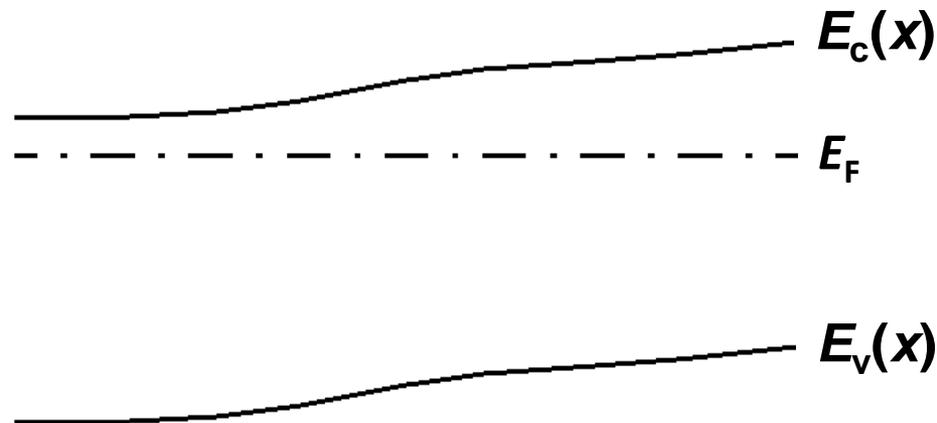
Charge carriers in non-equilibrium conditions

Particles diffuse from regions of higher concentration to regions of lower concentration region, due to random thermal motion.



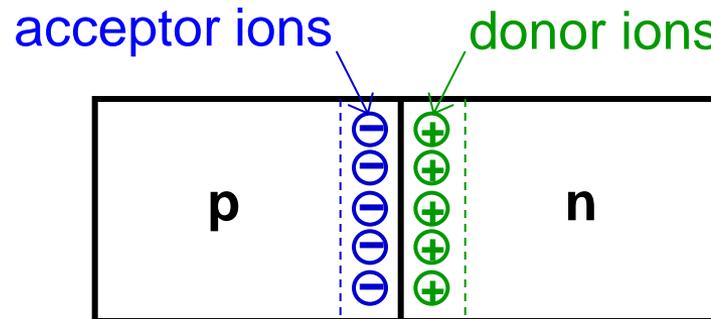
Charge carriers in non-equilibrium conditions

- The position of E_F relative to the band edges is determined by the carrier concentrations, which is determined by the net dopant concentration.
- **In equilibrium E_F is constant**; therefore, the band-edge energies vary with position in a non-uniformly doped semiconductor:



P-N junctions in equilibrium

- When the junction is first formed, mobile carriers **diffuse** across the junction (due to the concentration gradients)
 - Holes diffuse from the **p side** to the n side, leaving behind **negatively charged immobile acceptor ions**
 - Electrons diffuse from the **n side** to the p side, leaving behind **positively charged immobile donor ions**



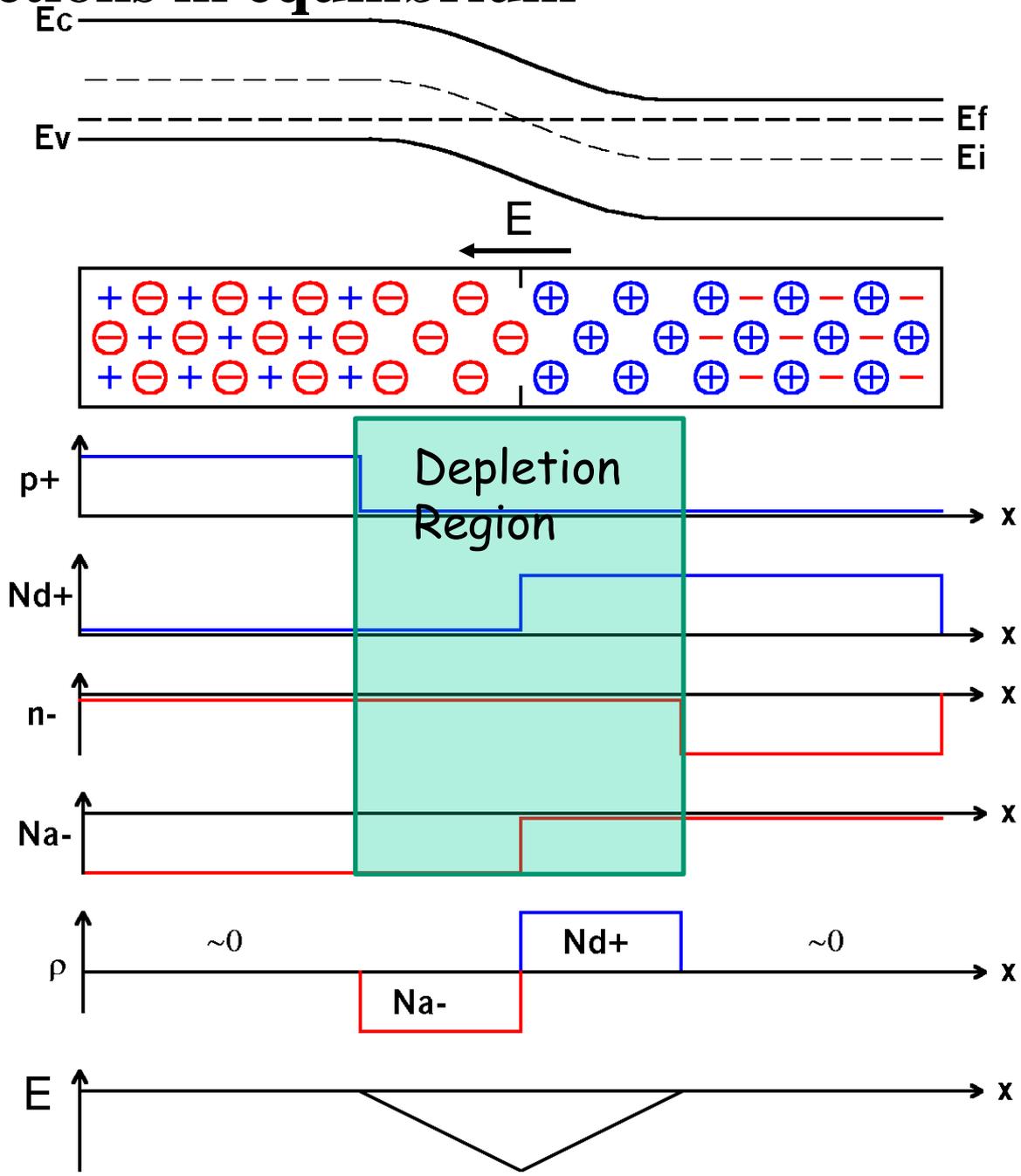
→ A region depleted of mobile carriers is formed at the junction.

- The space charge due to immobile ions in the depletion region establishes an electric field that opposes carrier diffusion.

P-N junctions in equilibrium



P-N junctions in equilibrium



Condensed Matter Physics

Solid State Physics of Crystals

Disordered systems

Properties of Waves in Periodic Lattices

Elastic waves in lattices
Vibrations
Phonon DOS
Planck distribution

Disordered systems

Thermal properties:
heat capacity and conductance,
thermal expansion

Electron waves in lattices
Free electrons
Electron DOS
Fermi-Dirac distribution

Disordered system

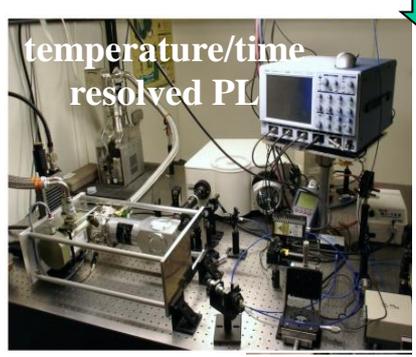
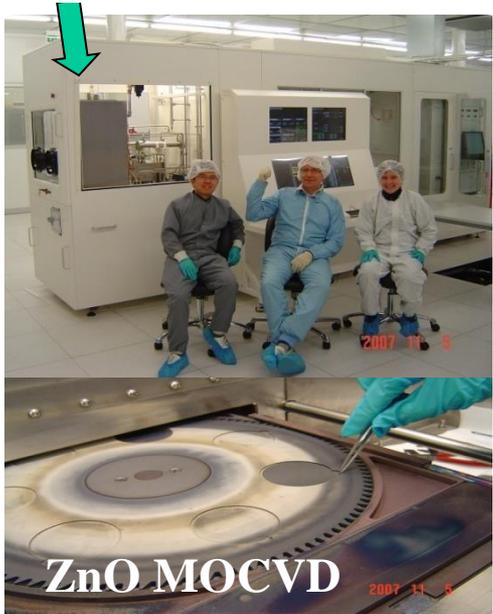
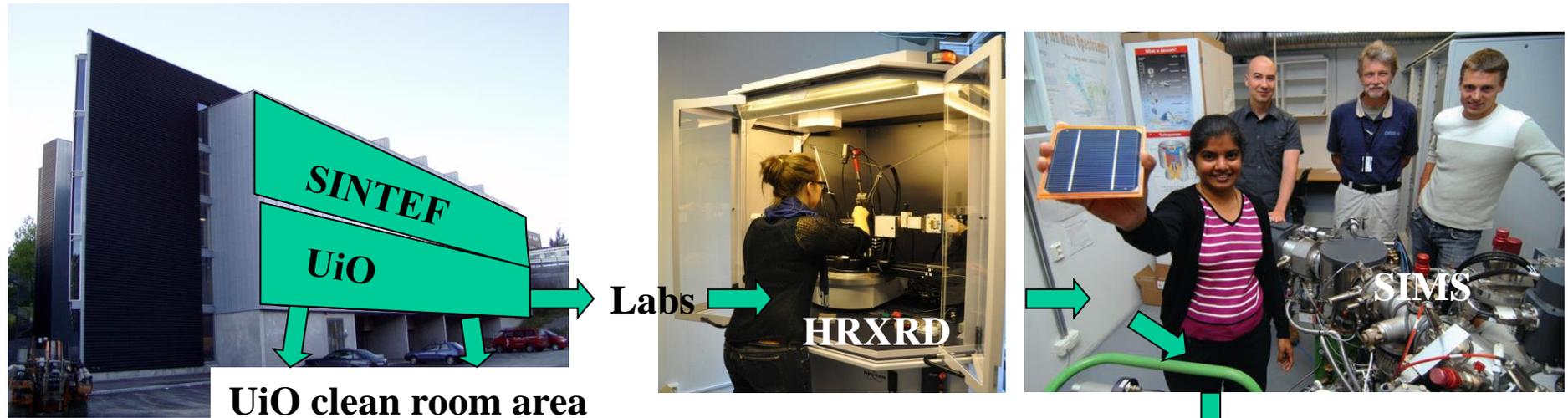
Electronic properties:
Electron concentration and transport,
contribution to the heat capacity

Advanced theory and novel materials properties

Disordered systems

Semiconductor physics at UiO

Micro- and Nanotechnology Laboratory (MiNaLab)



Halvlederfysikk ved UiO / MiNa-Lab

- 4 Professors
- 4 Adm/technical staff
- ~ 10 Post docs
- ~ 15 PhD students and ~ 10 Msc students

Semiconductor physics at UiO

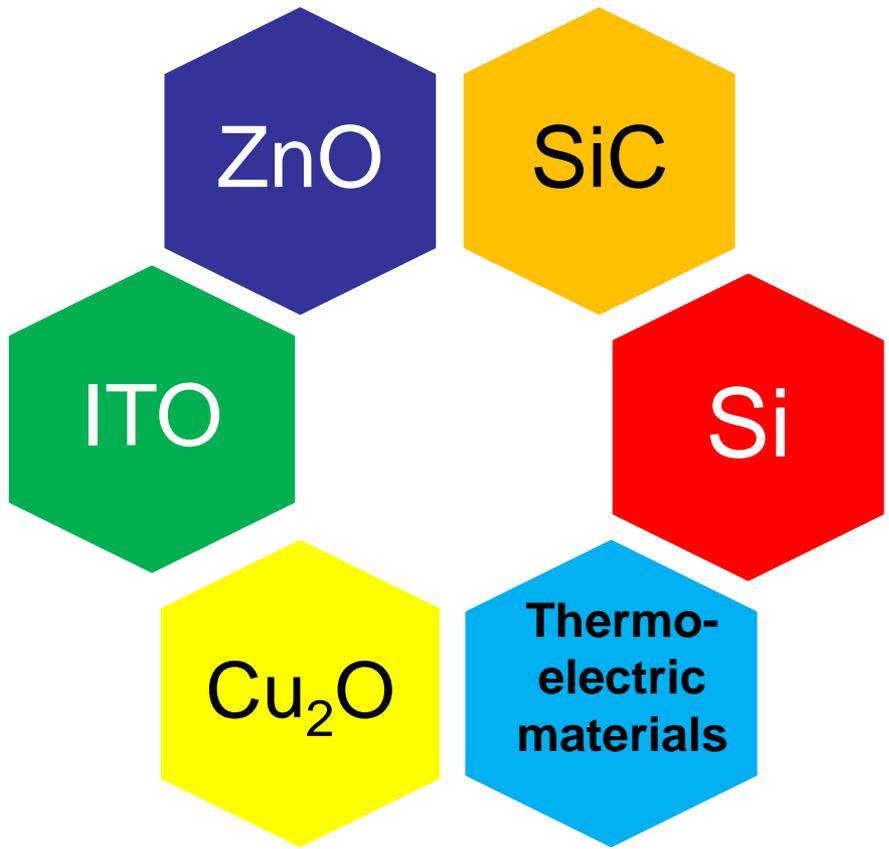
- LED's
- Transparent electronics



- Displays
- Electronic ink



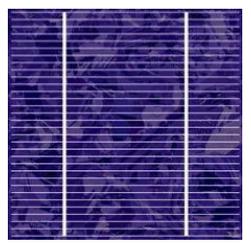
- Optical cavities
- Multi-junction solar cells



- Power electronics
- High temperature sensors



- Solar cells
- Detectors
- IC's



- Thermoelectric generators
- Thermoelectric cooling