FYS3410 - Vår 2016 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/v16/index.html

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

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2016 FYS3410 Lectures (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17,18,20)

Module I – Periodic Structures and Defects (Chapters 1-3, 20)

M18/1: 9-12 am	**Introduction. Crystal bonding. Periodicity and lattices, Brag diffraction and Laue condition, reciprocal space**	**3h**
W20/1 cancelled		
M25/1: 9-12 am	**Ewald construction, interpretation of a diffraction experiment , Brag planes, and Brillouin zones**	**3h**
W27/1 cancelled		
M01/2: 10-12 am	**Elastic strain and structural defects in crystals**	**2h**
W03/2: 9-10 am	**Atomic diffusion in solids**	**1h**
M08/2: 10-12 am	**Summary of Module I**	**2h**

Module II – Phonons (Chapters 4 and 5)

W10/2: 9-10 am	**Vibrations in monoatomic and diatomic chains of atoms**	**1h**
M15/2: 10-12am	**Periodic boundary conditions, phonons and density of states (DOS)**	**2h**
W17/2: 9-10 am	**Planck distribution**	**1h**
M22/2 : 10-12am	**Lattice heat capacity: Dulong-Petit, Einstein, and Debye models**	**2h**
W24/2 cancelled		
M29/2: 9-12am	**Comparison of different models for lattice heat capacity, thermal conductivity with phonons**	**3h**
W02/3: 9-10 am	**Thermal expansion**	**1h**
M07/3: 10-12am	**Summary of Module II.**	**2h**

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

W09/3: 9-10 am	**Free electron gas (FEG) versus free electron Fermi gas (FEFG)**	**1h**
M14/3: 10-12am	**DOS of FEFG in 3D. Effect of temperature – Fermi-Dirac distribution**	**2h**
W16/3: 9-10 am	**Heat capacity of FEFG in 3D**	**1h**
W30/3: 9-10 am	**DOS in 2D - quantum wells**	**1h**
M04/4: 10-12am	**DOS in 1D and 0D, i.e. quantum wires and quantum dots; transport properties of electrons**	**2h**
W06/4: 9-10 am	**Origin of the energy band gap**	
M11/4: 10-12am	**Nearly free electron model. Kronig-Penney model. Empty lattice approximation.**	**2h**
W13/4: 9-10 am	**Number of orbitals in a band**	**1h**
M18/4: 10-12am	**Summary of Module III.**	**2h**

Module IV – Semiconductors and interfaces (Chapters 8, 9-pp 223-231, 17)

W20/4: 9-10 am	**Metals versus semiconductors. Surfaces and interfaces.**	**1h**
M25/4: 9-12 am	**Effective mass method.**	**3h**
W27/4: 9-10 am	**Intrinsic carrier generation – elctrons and holes.**	**1h**
M02/5: 9-12 am	**Localized levels for hydrogen-like impurities – donors and acceptors. Doping.**	**3h**
W04/5: 9-10 am	**Carrier statistics in semiconductors**	**1h**
M09/5: 9-12 am	**p-n junctions**	**3h**
W11/5: 9-10 am	**Optoelectronic semiconductor properties and devices**	**1h**
M18/5: 9-12 am	**Device demonstrations. Summary of Module IV**	**3h**

Repetition

M23/5 9-12 am	**The course in a nutshell**	**2h**

W25/5, M30/5 and W1/6 cancelled

Exam during week 22 (tentatively 30-31/5)

Free electron Fermi gas (FEFG) at the ground state and T>0

- **Free electron Fermi gas (FEFG) – a gas of electrons subject to Pauli principle**
- **One electron system – wave functions – orbits; FEFG in 1D in ground state**
- **FEFG in 3D in ground state**
- **Fermi-Dirac distribution and electron occupancy at T>0**

Free electron Fermi gas – a gas of electrons subject to Pauli principle

- At low temperature, free mean path of a conduction electron in metal can be as long as 1 cm! Why is it not affected by ion cores or other conduction electrons? (30 seconds discussions)
  - Motion of electrons in crystal (matter wave) is not affected by periodic structure such as ion cores.
  - Electron is scattered infrequently by other conduction electrons due to the Pauli exclusion principle

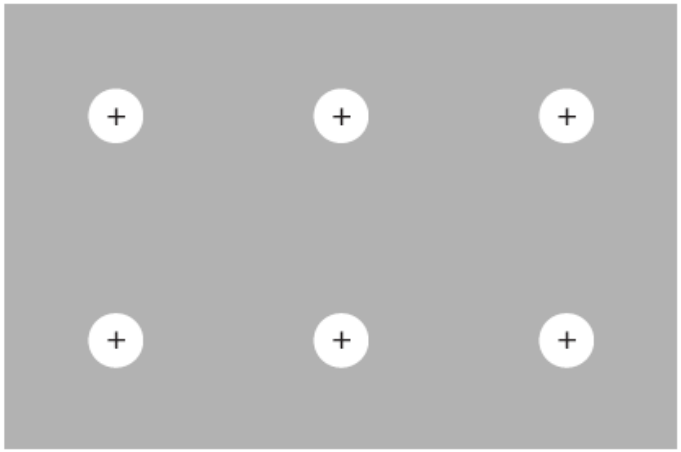

Figure 1 Schematic model of a crystal of sodium metal. The atomic cores are Na^+ ions: they are immersed in a sea of conduction electrons. The conduction electrons are derived from the 3*s* valence electrons of the free atoms. The atomic cores contain 10 electrons in the configuration $1s^2 2s^2 2p^6$. In an alkali metal the atomic cores occupy a relatively small part (~15 percent) of the total volume of the crystal, but in a noble metal (Cu, Ag, Au) the atomic cores are relatively larger and may be in contact with each other. The common crystal structure at room temperature is bcc for the alkali metals and fcc for the noble metals.

Free electron Fermi gas (FEFG) at the ground state and T>0

- Free electron Fermi gas (FEFG) – a gas of electrons subject to Pauli principle
- **One electron system – wave functions – orbits; FEFG in 1D in ground state**
- FEFG in 3D in ground state
- Fermi-Dirac distribution and electron occupancy at T>0
- Deriviation and estimate for the FEFG heat capacity

One electron system – wave functions - orbits

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

$$\psi_n = A \sin\left(\frac{2\pi}{\lambda_n}x\right) ; \qquad \tfrac{1}{2}n\lambda_n = L , \qquad \epsilon_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 .$$

Standing wave B. C.
n = 1, 2, …

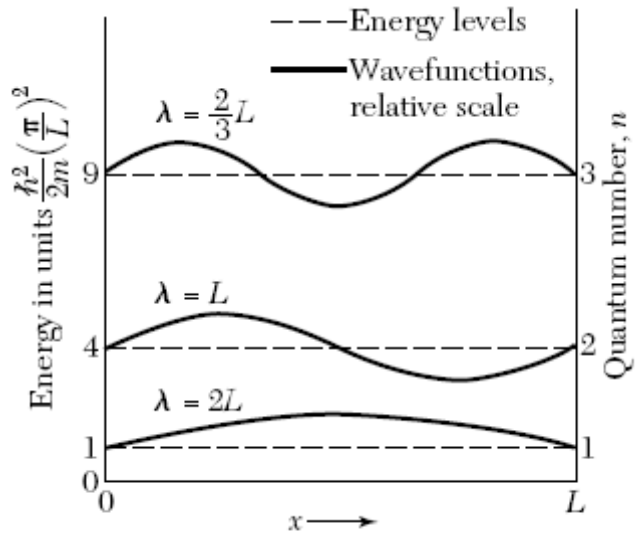

Figure 2 First three energy levels and wavefunctions of a free electron of mass m confined to a line of length L. The energy levels are labeled according to the quantum number n which gives the number of half-wavelengths in the wavefunction. The wavelengths are indicated on the wavefunctions. The energy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

- The Pauli exclusion principle
– n: quantum number
– m(=1/2 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 => $n_F = N/2$ ➔ 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!

Free electron Fermi gas (FEFG) at the ground state and T>0

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- One electron system – wave functions – orbits; FEFG in 1D in ground state
- **FEFG in 3D in ground state**
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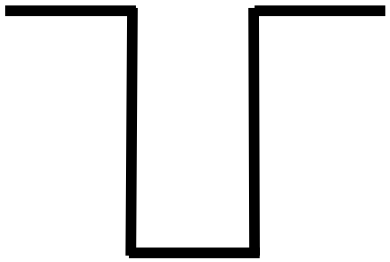
FEFG in 3D

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 $U(\mathbf{r})=0$

FEFG in 3D

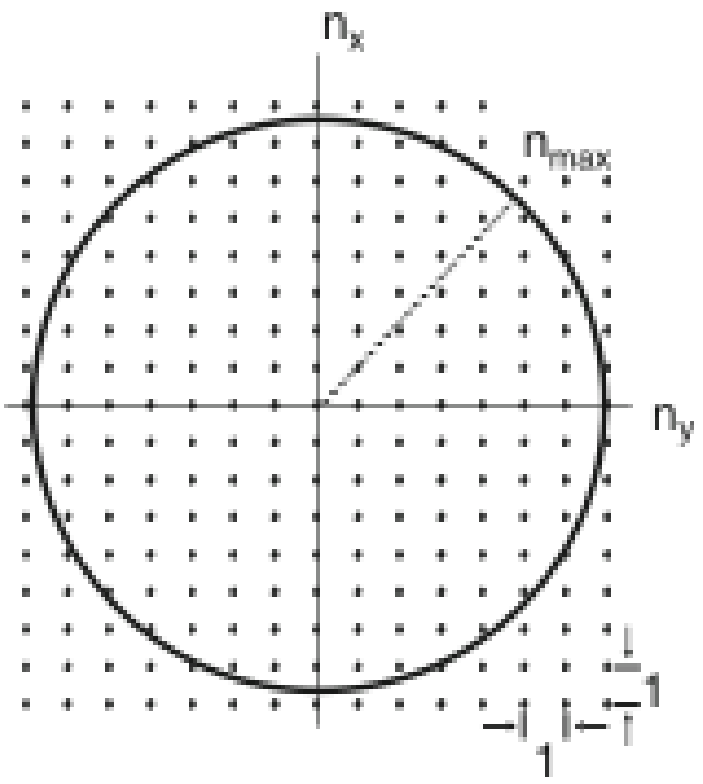
$$-\frac{\hbar^2\nabla^2}{2m_e}\psi(\mathbf{r}) = E\psi(\mathbf{r}) \qquad \psi(\mathbf{r}) \sim e^{i\mathbf{kr}}$$

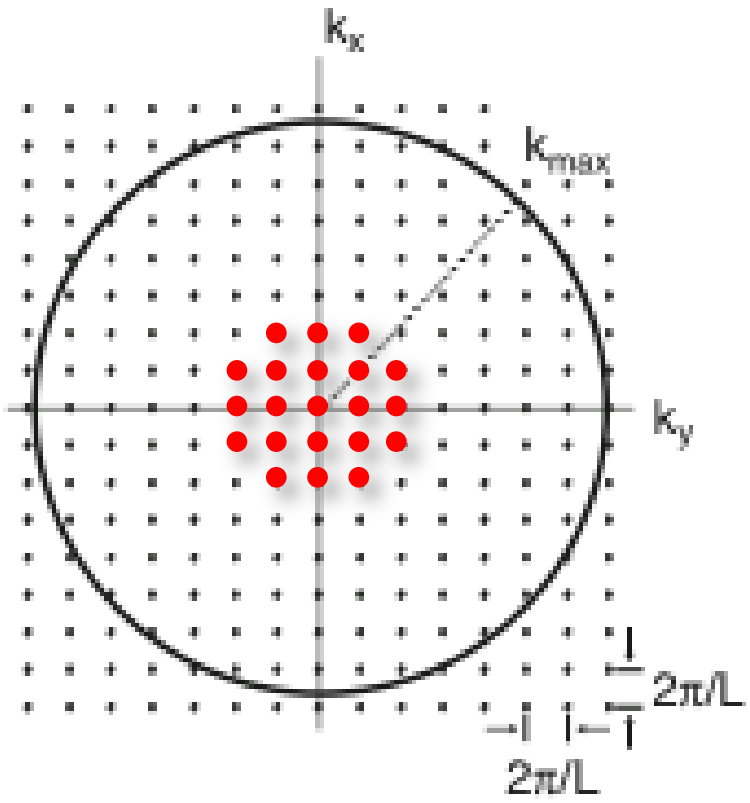
$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e}(k_x^2 + k_y^2 + k_z^2)$$

boundary conditions provide restrictions the wavevector k

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

FEFG in 3D





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

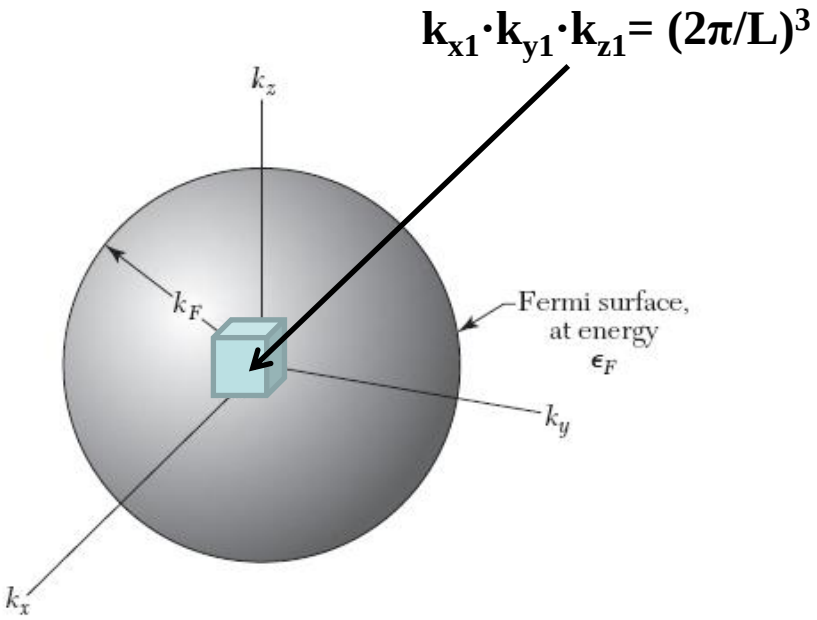
$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e}(k_x^2 + k_y^2 + k_z^2)$$

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

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!



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

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

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

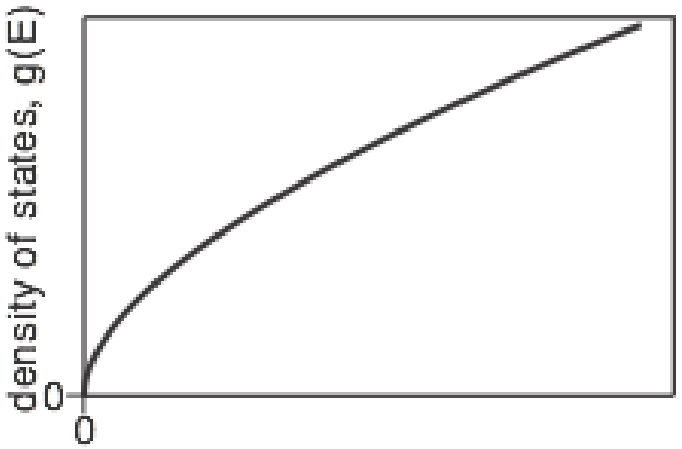
FEFG in 3D

For any E

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

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

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



FEFG in 3D

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{\mathbf{k}}(\mathbf{r})=\epsilon_{\mathbf{k}}\,\psi_{\mathbf{k}}(\mathbf{r})$$

- **Invoking periodic boundary condition instead of the infinite potential wall (standing wave) boundary condition, we get traveling waves as solutions:**

$$\psi(x+L,y,z)=\psi(x,y,z)$$

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r})=\exp\left(i\mathbf{k}\cdot\mathbf{r}\right)\ ,}$$

$$k_x=0\ ;\quad \pm\frac{2\pi}{L}\ ;\quad \pm\frac{4\pi}{L}\ ;\ \ldots\ ,$$

$$\epsilon_{\mathbf{k}}=\frac{\hbar^2}{2m}k^2=\frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)$$

$$k=2\pi/\lambda$$

Only if we know how much space one k point occupies ($\delta k_x \delta k_y \delta k_z = (2\pi/L)^3$)

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

Due to spin →

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

Fermi wave vector

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

Fermi energy

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

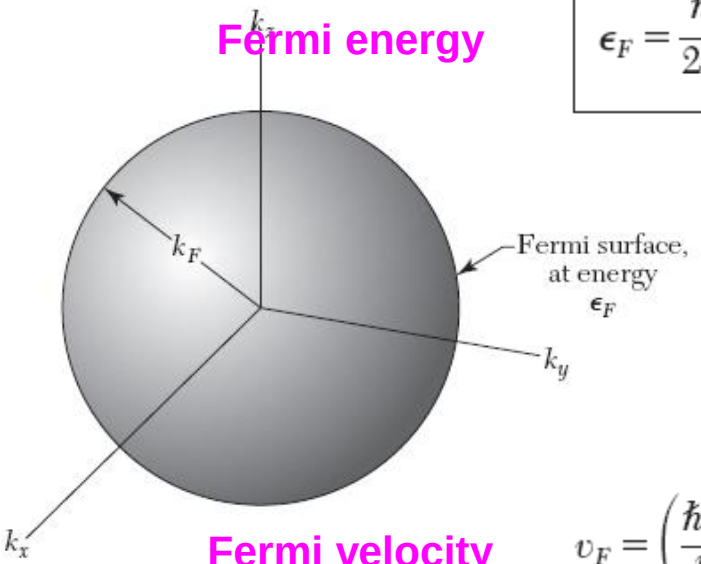


Figure 4 In the ground state of a system of N free electrons the occupied orbitals of the system fill a sphere of radius k_F, where $\epsilon_F = \hbar^2 k_F^2/2m$ is the energy of an electron having a wavevector k_F.

Fermi velocity

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

Table 1 Calculated free electron Fermi surface parameters for metals at room temperature

(Except for Na, K, Rb, Cs at 5 K and Li at 78 K)

Valency	Metal	Electron concentration, in cm^{-3}	Radius[a] parameter r_s	Fermi wavevector, in cm^{-1}	Fermi velocity, in $cm\ s^{-1}$	Fermi energy, in eV	Fermi temperature $T_F \equiv \epsilon_F/k_B$, in deg K
1	Li	4.70×10^{22}	3.25	1.11×10^{8}	1.29×10^{8}	4.72	5.48×10^{4}
	Na	2.65	3.93	0.92	1.07	3.23	3.75
	K	1.40	4.86	0.75	0.86	2.12	2.46
	Rb	1.15	5.20	0.70	0.81	1.85	2.15
	Cs	0.91	5.63	0.64	0.75	1.58	1.83
	Cu	8.45	2.67	1.36	1.57	7.00	8.12
	Ag	5.85	3.02	1.20	1.39	5.48	6.36
	Au	5.90	3.01	1.20	1.39	5.51	6.39
2	Be	24.2	1.88	1.93	2.23	14.14	16.41
	Mg	8.60	2.65	1.37	1.58	7.13	8.27
	Ca	4.60	3.27	1.11	1.28	4.68	5.43
	Sr	3.56	3.56	1.02	1.18	3.95	4.58
	Ba	3.20	3.69	0.98	1.13	3.65	4.24
	Zn	13.10	2.31	1.57	1.82	9.39	10.90
	Cd	9.28	2.59	1.40	1.62	7.46	8.66
3	Al	18.06	2.07	1.75	2.02	11.63	13.49
	Ga	15.30	2.19	1.65	1.91	10.35	12.01
	In	11.49	2.41	1.50	1.74	8.60	9.98
4	Pb	13.20	2.30	1.57	1.82	9.37	10.87
	Sn(w)	14.48	2.23	1.62	1.88	10.03	11.64

[a]The dimensionless radius parameter is defined as $r_s = r_0/a_H$, where a_H is the first Bohr radius and r_0 is the radius of a sphere that contains one electron.

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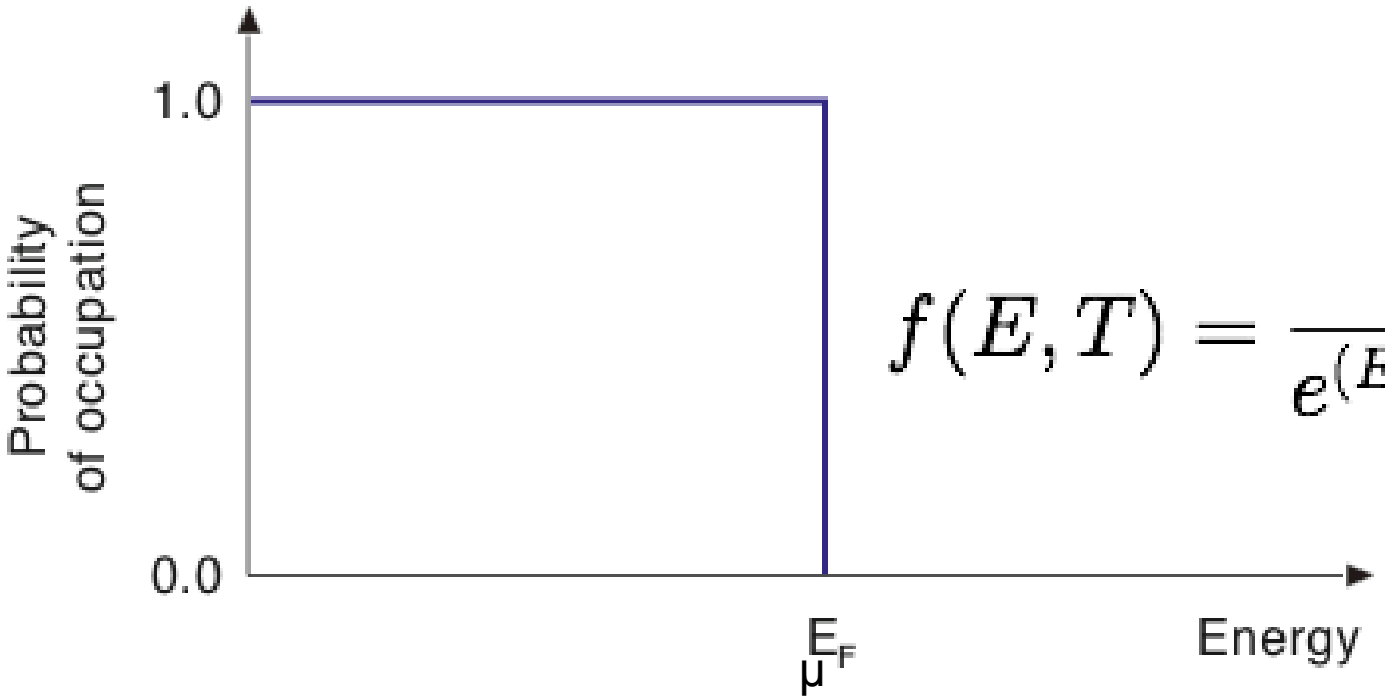
• One electron system – wave functions – orbits; FEFG in 1D in ground state

• FEFG in 3D in ground state

• Fermi-Dirac distribution and electron occupancy at T>0

•Deriviation and estimate for the FEFG heat capacity

Fermi-Dirac distribution

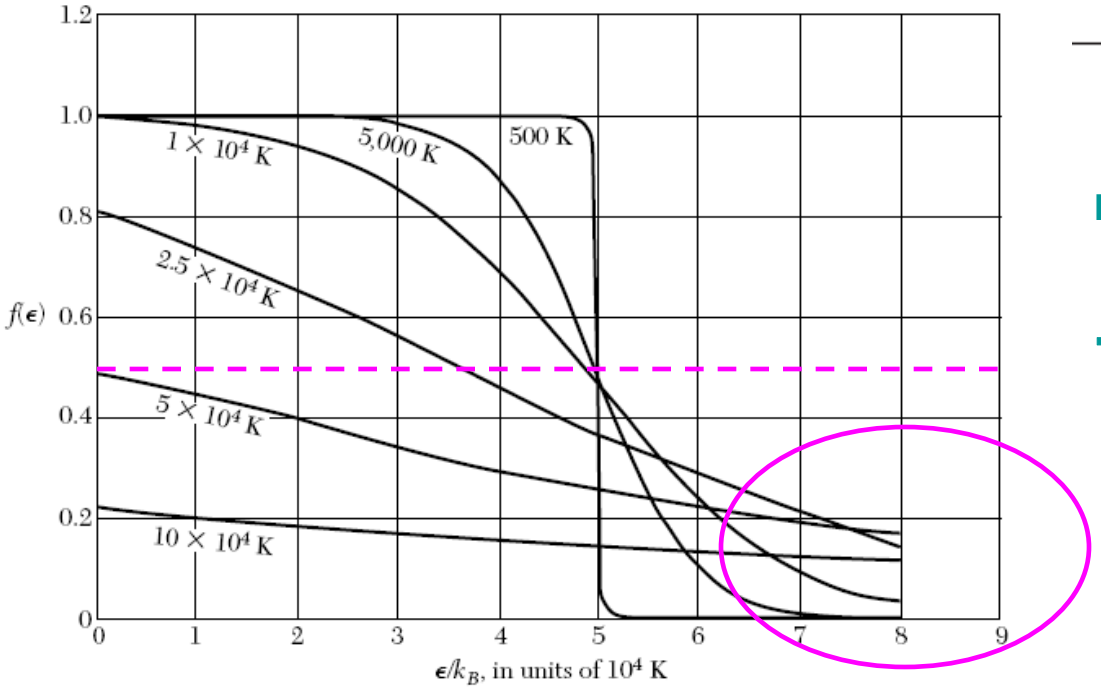


$$f(E,T) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

At T=0 all the states are filled up to the highest occupied state. This state is called the Fermi energy E_F. It is equal to the chemical potential μ at T=0.

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(** $\varepsilon = \mu$ **)=0.5; at 0K,** $\varepsilon_F = \mu$



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

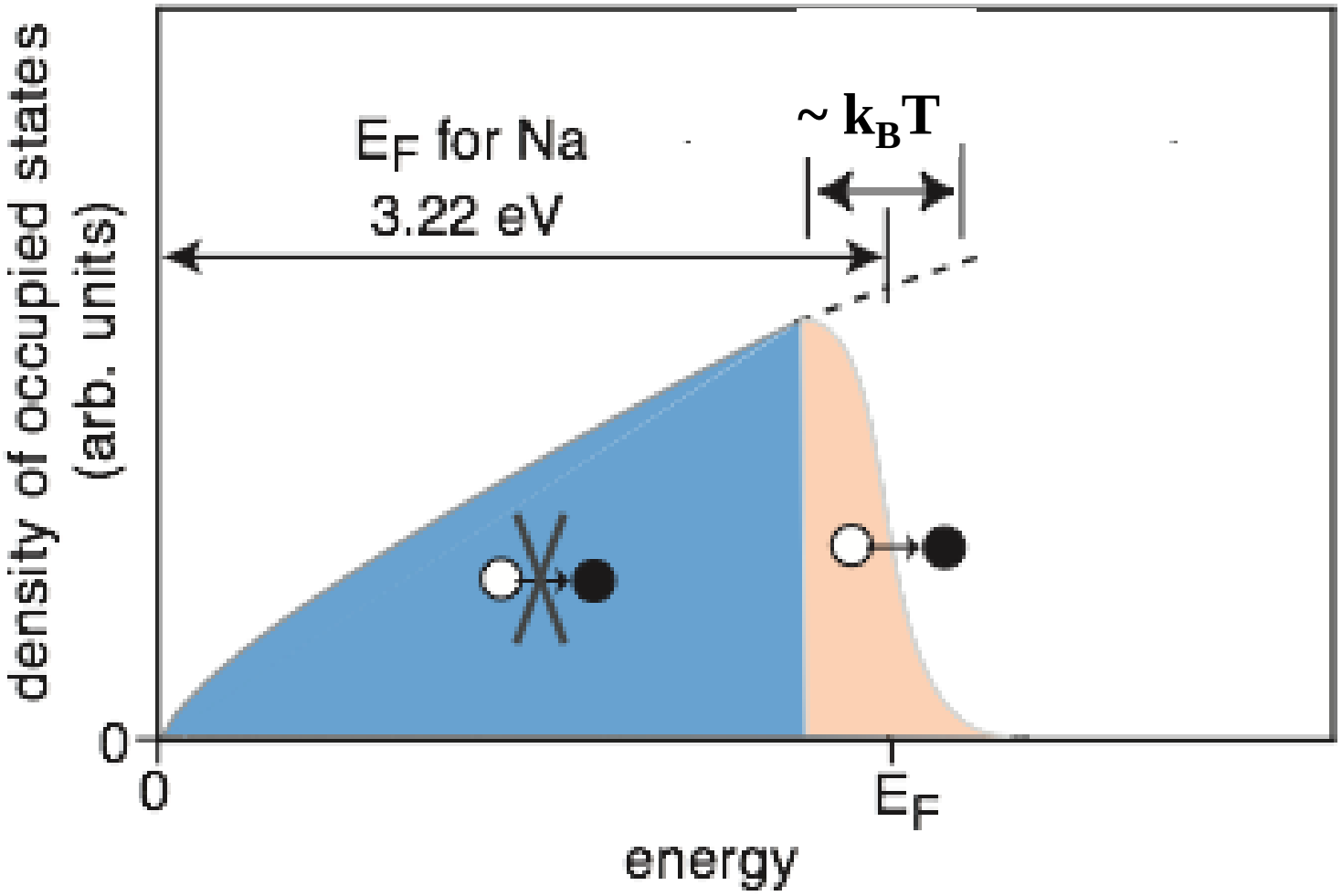
High energy tail – approximation

$$E - E_F > 3k_B T$$

➔ **Boltzmann-Maxwell distribution**

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

Fermi-Dirac distribution



Free electron Fermi gas (FEFG) at the ground state and T>0

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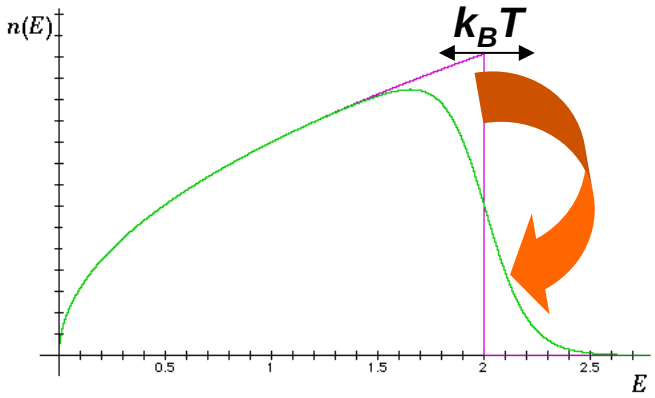
- **Deriviation and estimate for the FEFG heat capacity**

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.

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



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 ~ k_BT around E_F.

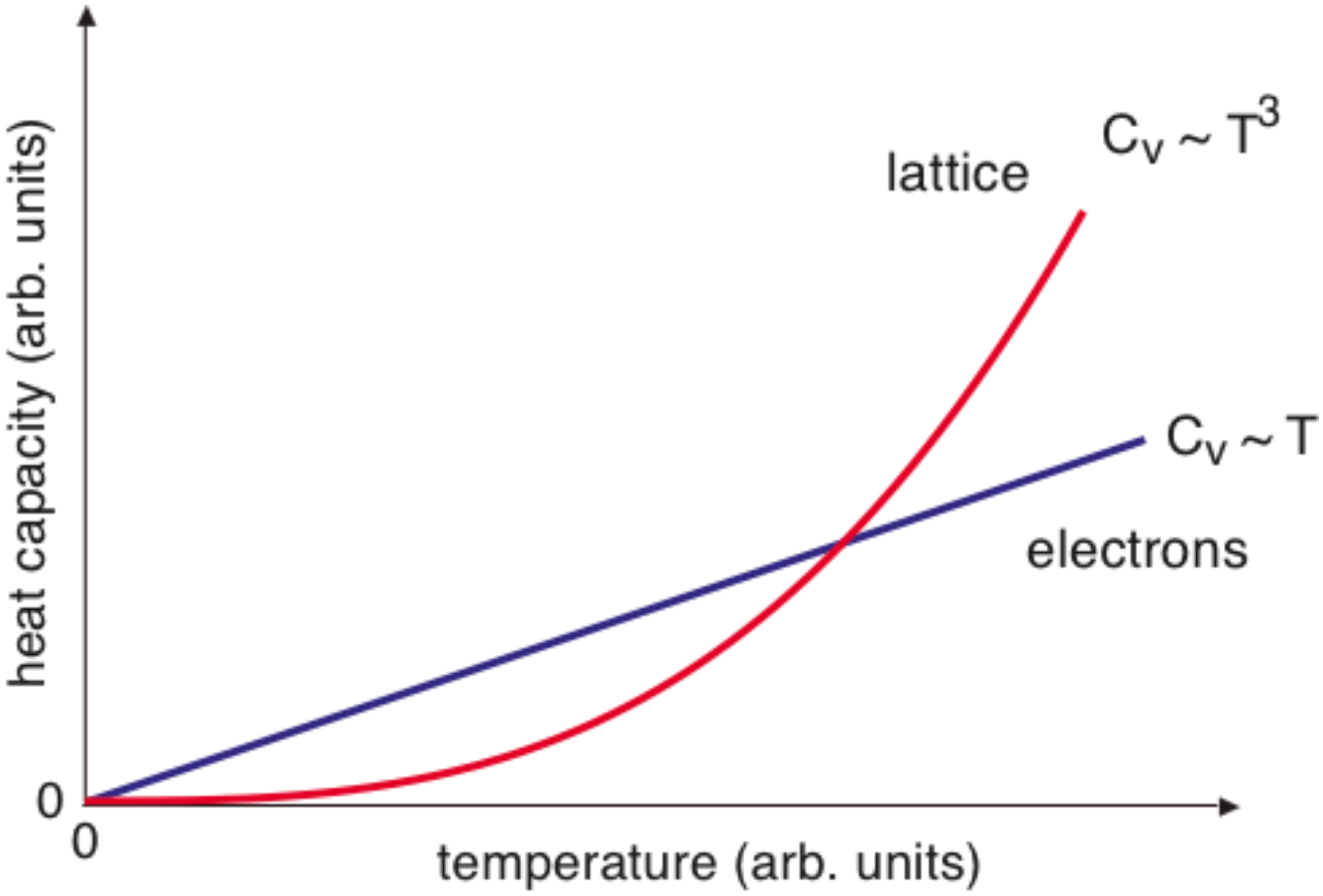
The fraction of electrons that we "transfer" to higher energies ~ k_BT/E_F, the energy increase for these electrons ~ k_BT. Thus, the increase of the internal energy with temperature is proportional to $n\times(k_BT/E_F)\times(k_BT) \sim n\,(k_BT)^2/E_F$. Note, $E_F = k_BT_F$

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

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

The Fermi gas heat capacity is much smaller (by $k_BT/E_F<<1$) 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_BT/E_F or T/T_F of the electrons are excited out of the ground state.

Heat capacity of a metal: lattice + electrons



- two contributions: lattice and electrons
- electrons unimportant at high T but dominating and sufficiently low T