FYS3400 - Vår 2020 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/v17/index.html

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

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2020 FYS3400 Lecture Plan (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17-20 + guest lectutes)

		calender week
Module I – Periodity and Disorder (Chapters 1-3, 19, 20)		
To 16/1 12-13	Introduction.	
On 22/1 10-12	Crystal bonding. Periodicity and lattices. Lattice planes and Miller indices. Reciprocal space.	4
To 23/1 12-13	Bragg diffraction and Laue condition	
On 29/1 10-12	Ewald construction, interpretation of a diffraction experiment, Bragg planes and Brillouin zones	5
To 30/1 12-13	Surfaces and interfaces. Disorder. Defects crystals. Equilibrium concentration of vacancies	
On 5/2 10-12	Mechanical properties of solids. Diffusion phenomena in solids; Summary of Module I	6
Module II – Phonons (Chapters 4, 5, and 18 pp.557-561)		
To 6/2 12-13	Vibrations in monoatomic and diatomic chains of atoms; examples of dispersion relations in 3D	
On 12/2 10-12	Lattice heat capacity: Dulong-Petit and Einstein models	7
To 13/2 12-13	Effect of temperature - Planck distribution;	
On 19/2 10-12	canceled	8
To 20/2 12-13	Periodic boundary conditions (Born – von Karman); phonons and its density of states (DOS); Debye models	
On 26/2 10-12	Comparison of different lattice heat capacity models; Thermal conductivity.	9
To 27/2 12-13	Thermal expansion	
On 4/3 10-12	Summary of Module II	10
Module III – Electrons I (Chapters 6, 7, 11 - pp 315-317, 18 - pp.528-530, 19, and Appendix D)		
To 5/3 12-13	Free electron gas (FEG) versus free electron Fermi gas (FEFG);	
On 11/3 10-12	DOS of FEFG in 3D; Effect of temperature – Fermi-Dirac distribution.	11
To 12/3 12-13	canceled	
	teaching free week	12
Module IV – Disordered systems (guest lecture slides)		
On 25/3 10-12	Thermal properties of glasses: Model of two level systems (Joakim Bergli)	13
To 26/3 12-13	Experiments in porous media (Gaute Linga)	
On 1/4 10-12	Electron transport in disordered solids: wave localization and hopping (Joakim Bergli)	14
To 2/4 12-13	Theory of porous media (Gaute Linga)	
	Easter	15
Module V – Electrons II (Chapters 8, 9 pp 223-231, and 17, 19)		
On 15/4 10-12	After Easter repetition; Heat capacity of FEFG in 3D	16
To 16/4 12-13	DOS of FEFG in 2D - quantum well, DOS in 1D – quantum wire, and in 0D – quantum dot	
On 22/4 10-12	Origin of the band gap; Nearly free electron model; Kronig-Penney model	17
To 23/4 12-13	Effective mass method for calculating localized energy levels for defects in crystals	
On 29/4 10-12	Intrinsic and extrinsic electrons and holes in semiconductors	18
To 30/4 12-13	Carrier statistics in semiconductors; p-n junction	
On 06/5 10-12	Optoelectronic properties of semiconductors I (Inhwan Lee)	19
To 07/5 12-13	Optoelectronic properties of semiconductors II (Inhwan Lee)	
On 13/5 10-12	Summary of Modules III and V	
To 14/5 12-13	Repetition - course in a nutshell	

Exam: oral examination

May 28th – 29th

Condensed Matter Physics

Condensed Matter Physics

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Solid State Physics of Crystals

Condensed Matter Physics

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Solid State Physics of Crystals

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Properties of Waves in Periodic Lattices

Condensed Matter Physics

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Solid State Physics of Crystals

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Properties of Waves in Periodic Lattices

Condensed Matter Physics

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Solid State Physics of Crystals

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Properties of Waves in Periodic Lattices

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Elastic waves in lattices
Vibrations
Phonon DOS
Planck distribution

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Thermal properties:
heat capacity and conductance, thermal expansion

Condensed Matter Physics

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Solid State Physics of Crystals

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Properties of Waves in Periodic Lattices

Elastic waves in lattices
Vibrations
Phonon DOS
Planck distribution

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Thermal properties:

heat capacity and conductance, thermal expansion

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

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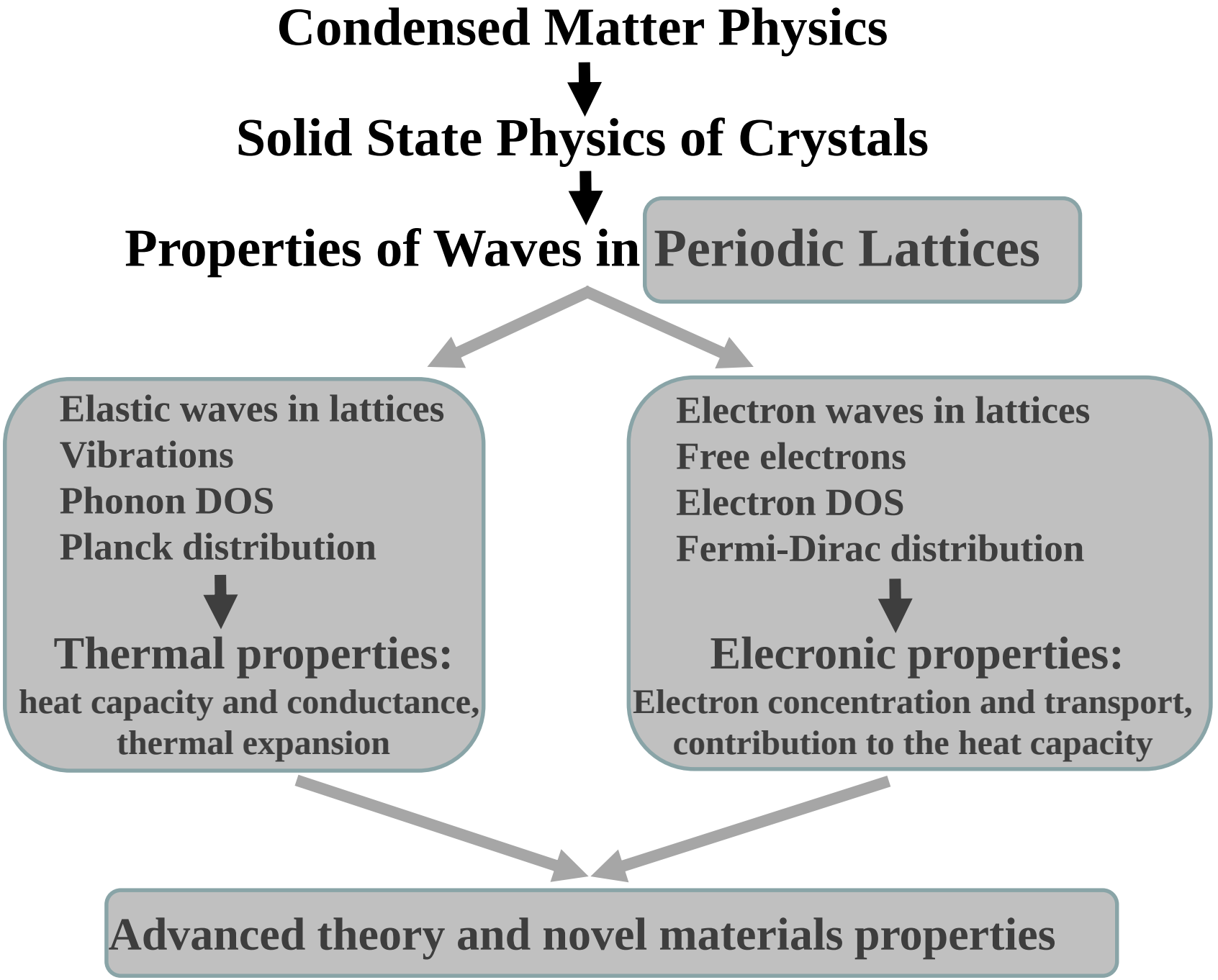
Elecronic properties:

Electron concentration and transport, contribution to the heat capacity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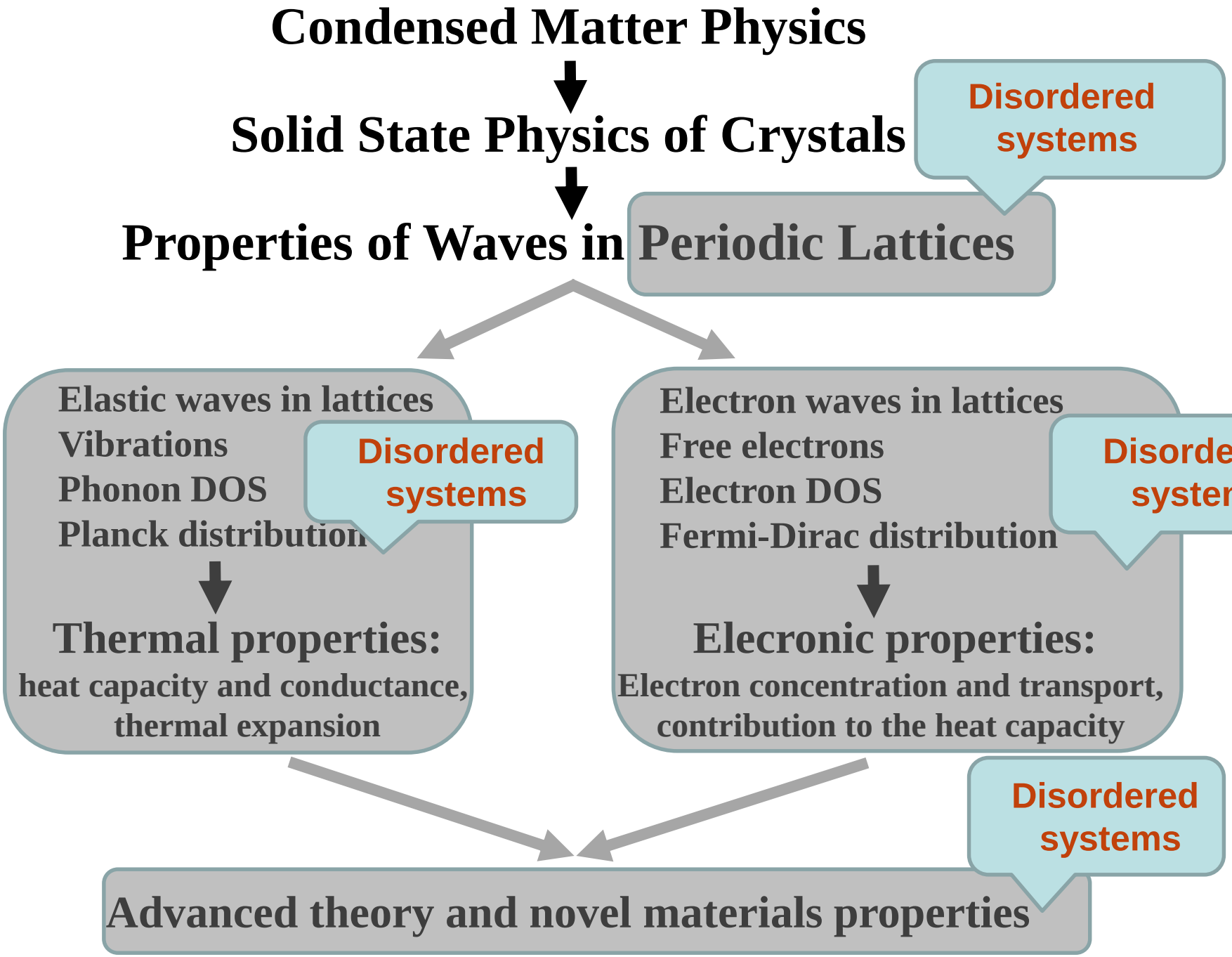
Elecronic properties:
Electron concentration and transport, contribution to the heat capacity
Advanced theory and novel materials properties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After Easter repetition: FEG vs FEFG

- **Free electron gas (FEG) - Drude model**
- **Free electron Fermi gas (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**

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 considering why resistivity in different materials ranges from 10^{-8} Ω·m (Ag) to 10^{20} Ω·m (polystyrene)?

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

(i) positive ion cores within an electron gas that follows Maxwell-Boltzmann statistics;

(ii) following the kinetic theory of gases - the electrons ae 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 colisions and the mean free path was approximately the inter-atomic spacing.

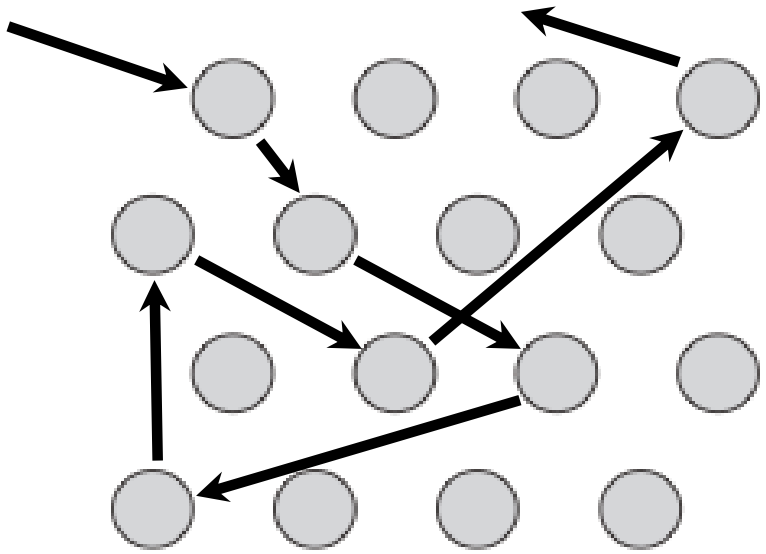
Drude (or FEG) model successfully exlpained Ohm amd Wiedemann-Franz laws, but failed to explain, e.g., electron heat capacity and the magnetic susceptibility of conduction electrons.

Free electron gas (FEG) - Drude model

Velocity of electrons in FEG
e.g. at room temperature

$$\frac{1}{2}mv_t^2 = \frac{3}{2}k_BT$$

$$v_t = \sqrt{\frac{3k_BT}{m}}$$



$$v_t \approx 10^5 \mathrm{ms}^{-1} \qquad \lambda = \tau v_t$$

$$\lambda \approx 1\mathrm{nm}$$

$$v_t \approx 10^5 \mathrm{ms}^{-1}$$

$$\tau \approx 1 \times 10^{-14}\ \mathrm{s}$$

FEG heat capacity

- **an average thermal energy of an ideal gas particle, e.g. an electron from FEG, moving in 3D at some temperature *T* is:**

$$E = \tfrac{3}{2} k_B T$$

- **Then for a total nr of N electrons the total energy is:**

$$U = \tfrac{3}{2} N k_B T$$

- **And the electronic heat capacity would then be:**

$$C_{el} = \frac{dU}{dT} = \tfrac{3}{2} N k_B$$

- **If FEG approximation is correct this C_{el} should be added to phonon-related heat capacitance, however, if we go out and measure, we find the electronic contribution is only around one percent of this, specifically at high temperature is still Dulong-Petit value, $3N_A k_B$, that is valid.**

FEG explaining Wiedemann-Franz law

Wiedemann and Franz found in 1853 that the ratio of thermal and electrical conductivity for ALL METALS is constant at a given temperature (for room temperature and above).

$$\frac{\kappa}{\sigma} = constant$$

Later it was found by L. Lorenz that this constant is proportional to temperature

$$\frac{\kappa}{\sigma} = LT$$

FEG explaining Wiedemann-Franz law

estimated thermal conductivity
(from a classical ideal gas)

$$\kappa = \frac{1}{3} v_t^2 \tau c_v$$

$$\sigma = \frac{n e^2 \tau}{m_e}$$

$$\frac{\kappa}{\sigma} = \frac{3}{2}\frac{k_B^2}{e^2} T = LT$$

the actual quantum mechanical result is

$$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\frac{k_B^2}{e^2} T = LT$$

this is 3, more or less....

Free electron gas (FEG) - Drude model

- **Why does the Drude model work so relatively well when many of its assumptions seem so wrong?**
- **In particular, the electrons don’t seem to be scattered by each other. Why?**
- **How do the electrons sneak by the atoms of the lattice?**
- **What are mysterious ”positive” charges realed by Hall effect measuremt in semiconductors?**
- **Why do the electrons not seem to contribute to the heat capacity?**

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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

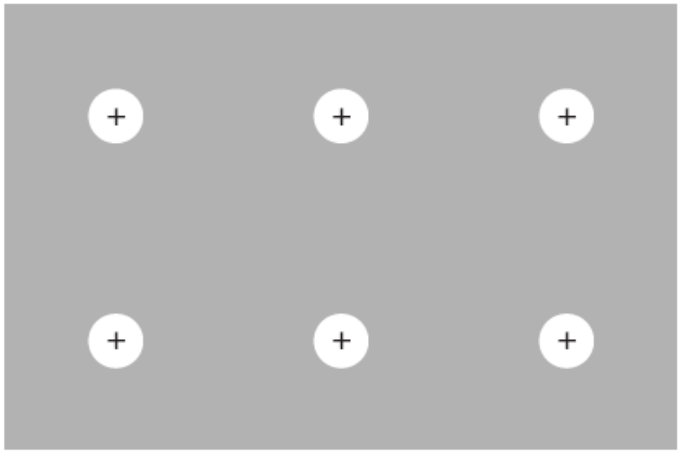

Figure 1 Schematic model of a crystal of sodium metal. The atomic cores are Na^+ ions: they are immersed in a sea of conduction electrons. The conduction electrons are derived from the 3*s* valence electrons of the free atoms. The atomic cores contain 10 electrons in the configuration $1s^2 2s^2 2p^6$. 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.

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, …

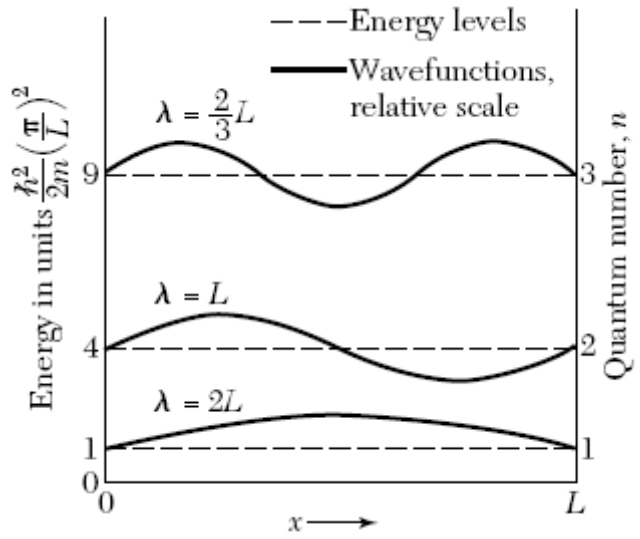

Figure 2 First three energy levels and wavefunctions of a free electron of mass m confined to a line of length L. The energy levels are labeled according to the quantum number n which gives the number of half-wavelengths in the wavefunction. The wavelengths are indicated on the wavefunctions. The energy 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!

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- Free electron Fermi gas (FEFG) in 1D in ground state
- **FEFG in 3D in ground state**
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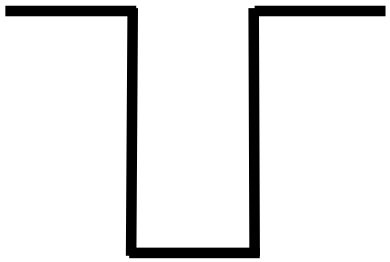
FEFG in 3D

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

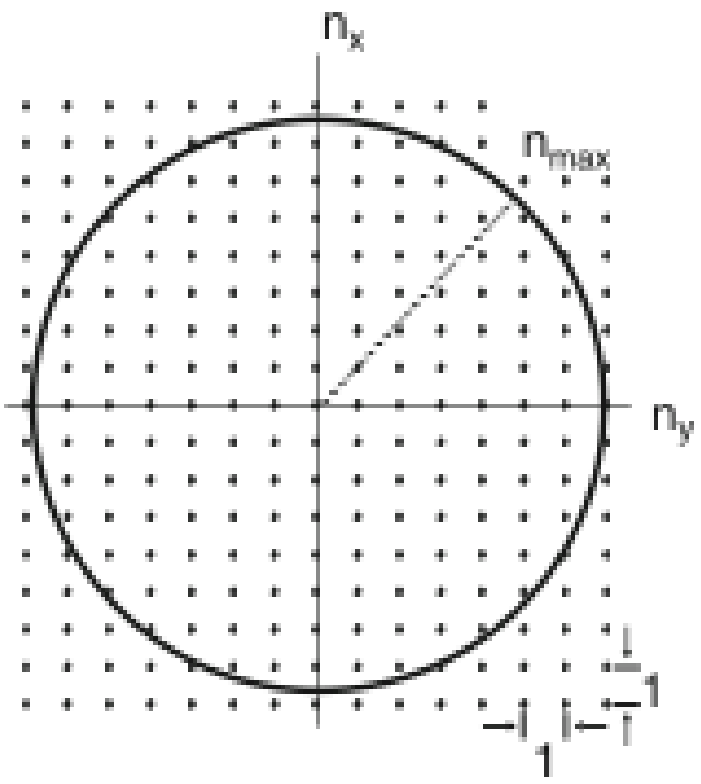
$$-\frac{\hbar^2\nabla^2}{2m_e}\psi(\mathbf{r}) = E\psi(\mathbf{r}) \qquad \psi(\mathbf{r}) \sim e^{i\mathbf{kr}}$$

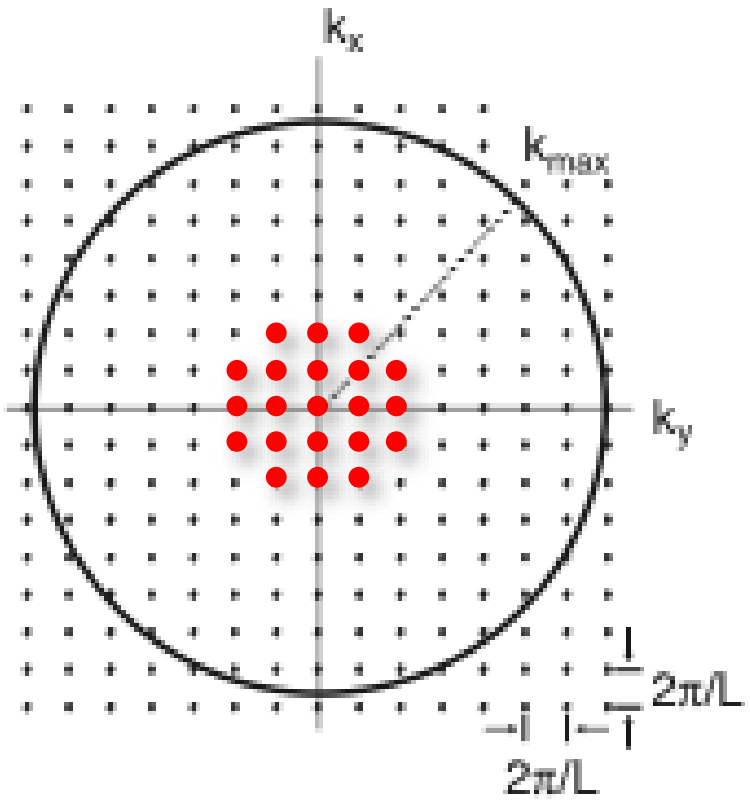
$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e}(k_x^2 + k_y^2 + k_z^2)$$

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





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

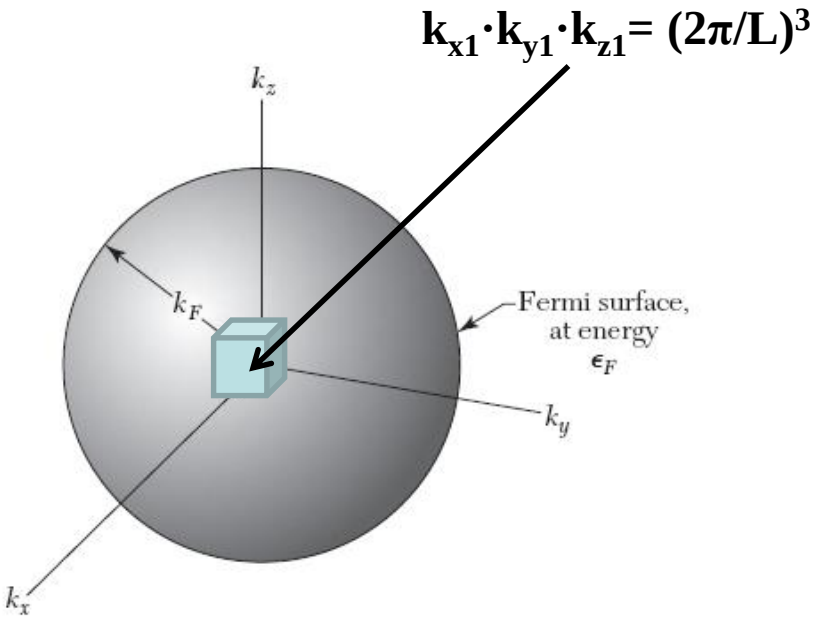
$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e}(k_x^2 + k_y^2 + k_z^2)$$

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

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!



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

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

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

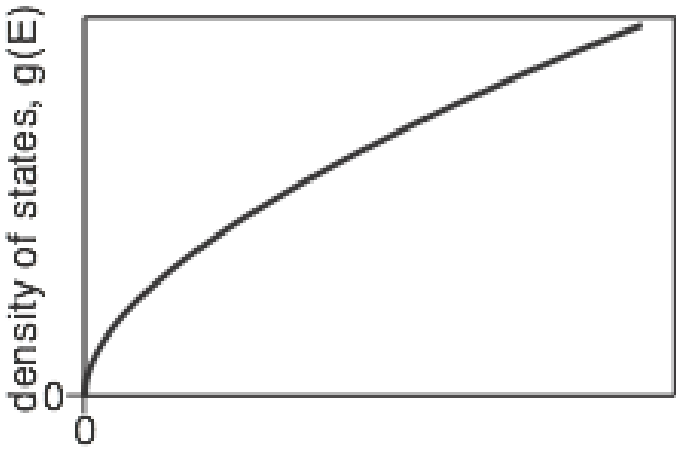
FEFG in 3D

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

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

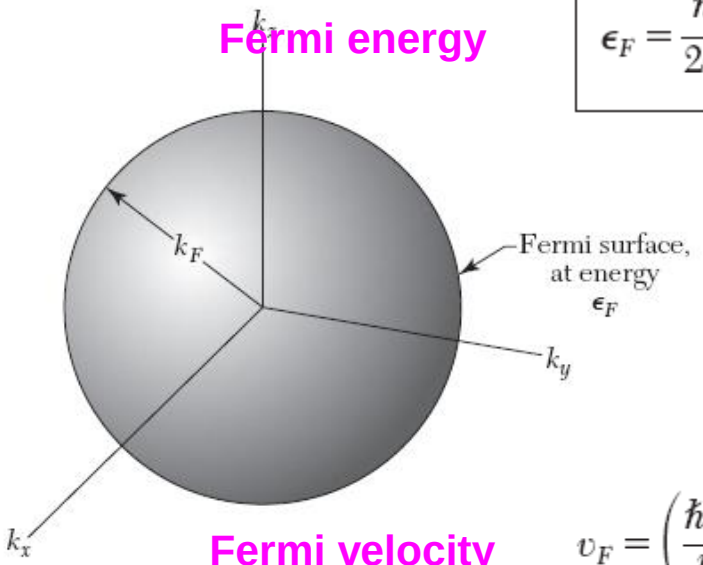


Figure 4 In the ground state of a system of N free electrons the occupied orbitals of the system fill a sphere of radius k_F, where $\epsilon_F = \hbar^2 k_F^2/2m$ is the energy of an electron having a wavevector k_F.

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.

After Easter repetition: FEG vs FEFG

- Free electron gas (FEG) - Drude model
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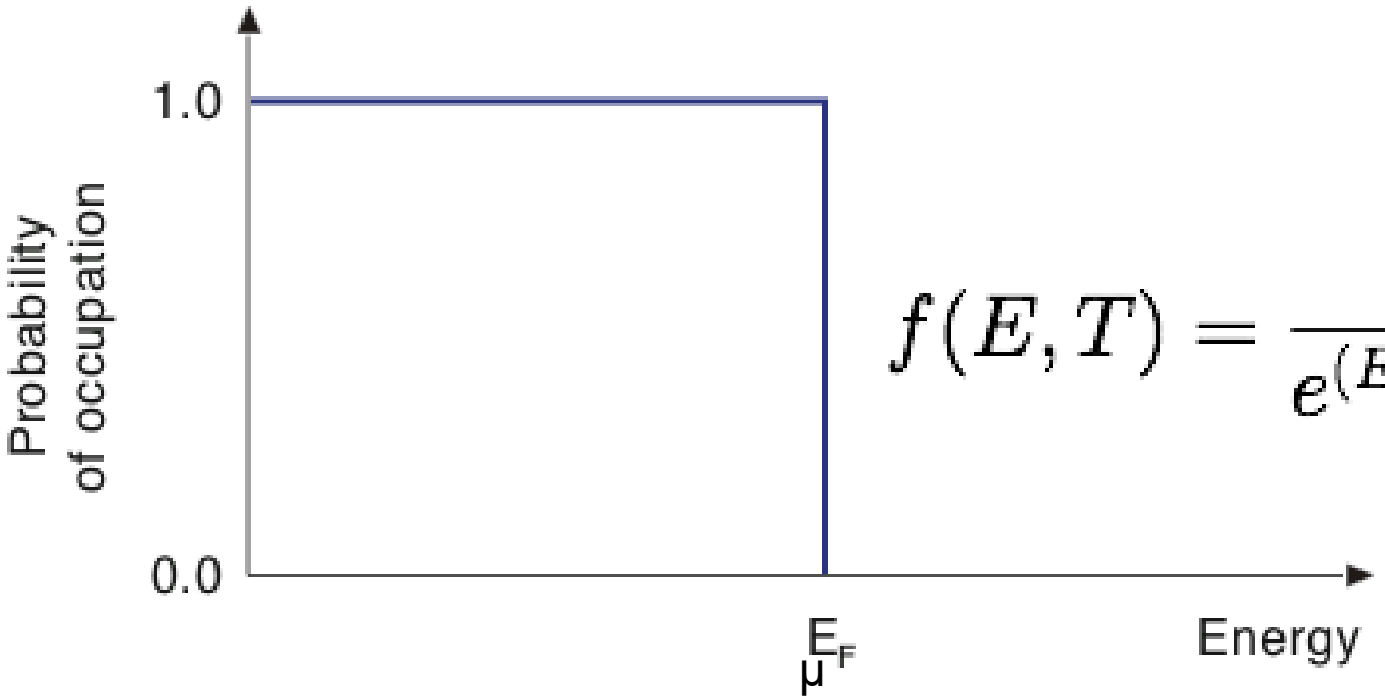
Fermi-Dirac distribution



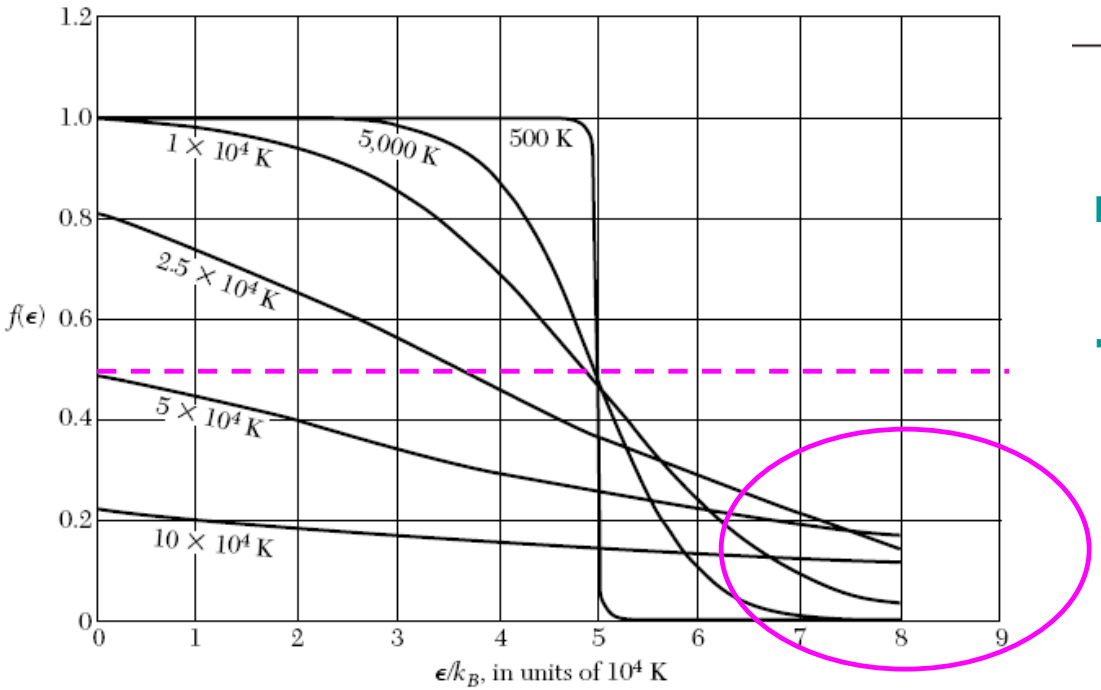
$$f(E,T) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

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,** $\varepsilon_F = \mu$

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



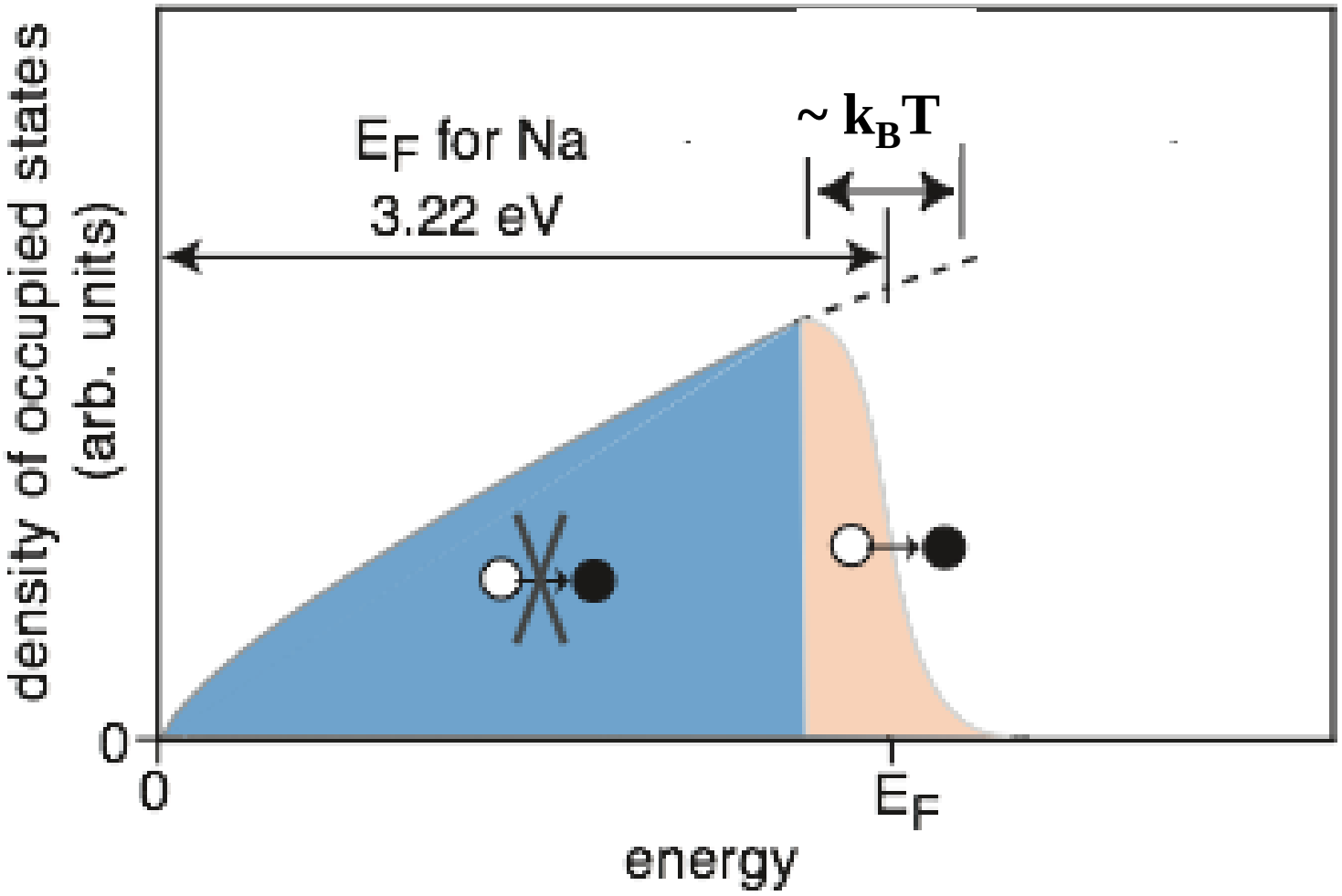
High energy tail – approximation

$$E - E_F > 3k_B T$$

➔ **Boltzmann-Maxwell distribution**

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

Fermi-Dirac distribution



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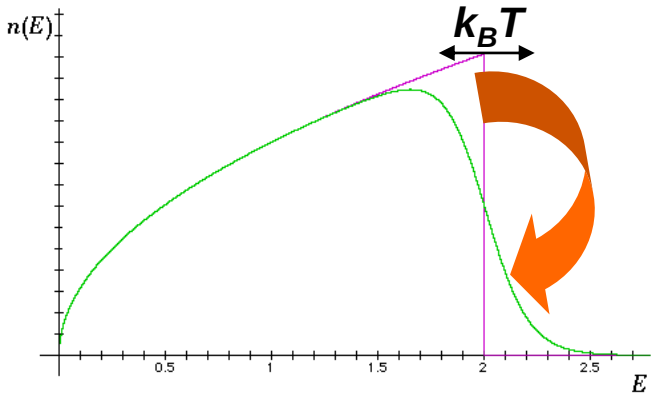
Estimate for the heat capacity of FEFG

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.

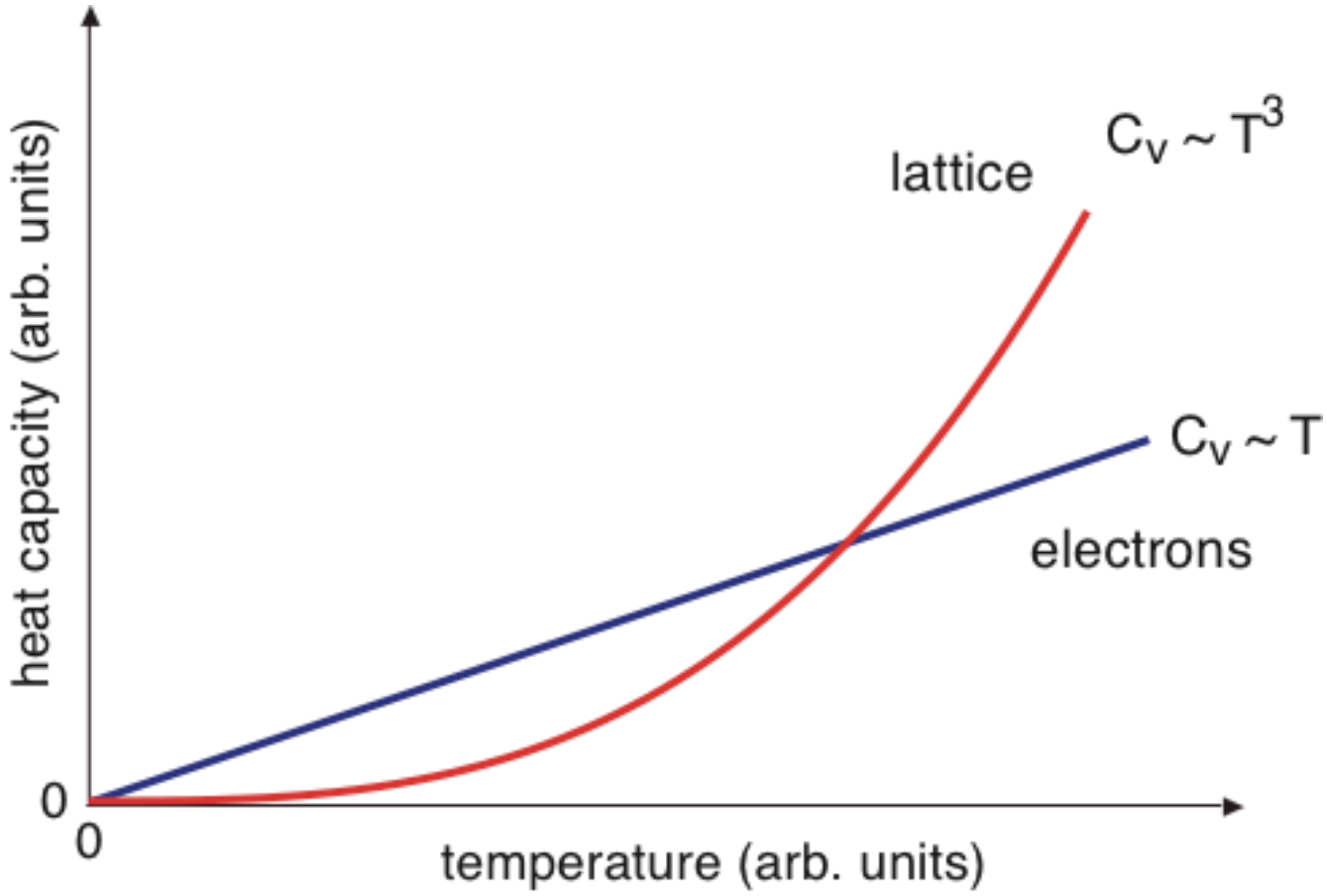
The fraction of electrons that we "transfer" to higher energies ~ k_BT/E_F, the energy increase for these electrons ~ k_BT. Thus, the increase of the internal energy with temperature is proportional to $n\times(k_BT/E_F)\times(k_BT) \sim n\,(k_BT)^2/E_F$. Note, $E_F = k_BT_F$

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

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

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