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PHYS-E0421 Solid-State Physics (5cr), Spring 2019

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Lecture 3, 4/3/2019

Motivation

- Why are metals good electrical conductors and insulators not?
- Are all electrons the same?
- What limits electrical current microscopically?

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- Electrical conductivity = how electrons behave under electric field
- Remarks related to homeworks?

Today's topic – Semiclassical dynamics of electrons and electron scattering

- Semiclassical dynamics of Bloch electrons
- Electron band in an external field
  - Net current of an electron band in different cases
  - Displaced Fermi sphere, out-of-equilibrium distribution function (more details next week)
- Electron scattering processes limiting conductivity and restoring the system towards equilibrium
  - Electron-electron scattering
  - Electron-defect scattering
  - Electron-phonon scattering

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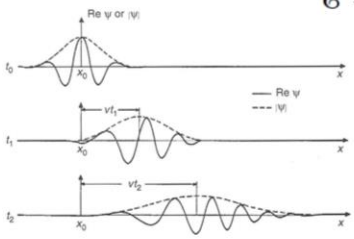
- Not yet conductivity! That's next lecture.

The motion and dynamics of Bloch electrons in a lattice

- In a defect-free static lattice the Bloch electrons do not scatter since the states are eigenfunctions of the time-independent Schrödinger equation and consistent with the lattice periodic potential
- Electrons moving in the lattice are described using wave packets written as linear combinations of Bloch waves
- The quantity describing the velocity of the wave packet is the group velocity

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) \cdot e^{-i\omega t}$$

$$\mathscr{E} = \hbar\omega$$



$$v_g = \frac{\partial \omega}{\partial k} \quad \text{or} \quad \mathbf{v}_g = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathscr{E}(\mathbf{k})$$

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Extra reading about wavepackets

- Bloch electrons are a good basis for considering real lattice
- Wave packet as a sum over Bloch states: sum_k c_k psi_k, Gaussian distribution c_k yields Gaussian wave packet envelope in real space
- Wave packet with well-defined k (and v_g) requires small delta k. Thus extended in real space and individual atoms are not important in their description.
- All the needed information from atomic level is included in the band structure (velocity, effective mass)
- In principle, electric field breaks the translational symmetry/periodicity of the lattice. Typically very small potential over the scale of unit cell.

Electron dynamics in k space

- The work done on electron by external electric field

$$\delta\mathcal{E} = -e\mathbf{E}\cdot\mathbf{d} = -e\mathbf{E}\cdot\mathbf{v}_g\delta t$$

- How is the evolution of the wave vector?

$$\frac{\delta\mathcal{E}}{\delta t} = \frac{\delta\mathcal{E}}{\delta k}\cdot\frac{\delta k}{\delta t}$$

$$v_g = \frac{\partial\omega}{\partial k} = \frac{1}{\hbar}\frac{\partial\mathcal{E}}{\partial k}$$

$$\hbar\frac{\partial k}{\partial t} = -eE \quad = -e(\mathbf{E}+\boldsymbol{v}\times\mathbf{B})$$

- Constant change in *k*!

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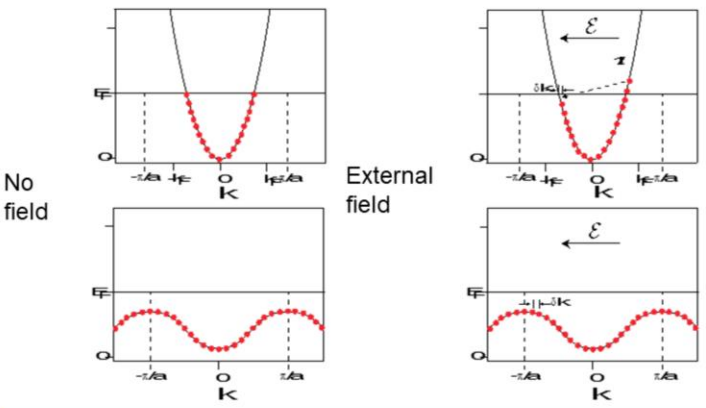
- Semiclassical picture, ”leap of faith”, justification from quantum mechanics is complicated
- Electric potential U = -Ed, d = v_g*t, units: potential in V => work in eV
- k moves parallel to E.
- With magnetic field F = -e(E+v x B), k moves perpendicular to v and B.

Parabolic vs sinusoidal band



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- In free electron model,”creeping up” the band structure corresponds to increased velocity (=classical picture). No interaction with the lattice.
- (Bloch) oscillations in partially filled band. Velocity and position oscillates due to scattering with the lattice.
- Full band: everything should be moving but nothing seems to change.

Electron dynamics in real space

- We already know velocity $v_g = \frac{\partial \omega}{\partial k} = \frac{1}{\hbar}\frac{\partial \mathscr{E}}{\partial k}$
- How about acceleration

$$a = \frac{\partial v_g}{\partial t} = \frac{1}{\hbar}\frac{\partial}{\partial t}\frac{\partial \mathscr{E}}{\partial k} = \frac{1}{\hbar}\frac{\partial^2 \mathscr{E}}{\partial k^2}\frac{\partial k}{\partial t} \quad \text{with} \quad \frac{1}{\hbar}\frac{\partial k}{\partial t} = -eE$$

$$\Rightarrow \quad a = -\frac{1}{\hbar}\frac{\partial^2 \mathscr{E}}{\partial k^2}eE$$

- Comparison with classical version

$$ma = -eE$$

- Allows us to identify "mass" $m^* = \hbar^2 \left(\frac{\partial^2 \mathscr{E}}{\partial k^2}\right)^{-1}$

3D:

$$\mathbf{v}_g = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k})$$

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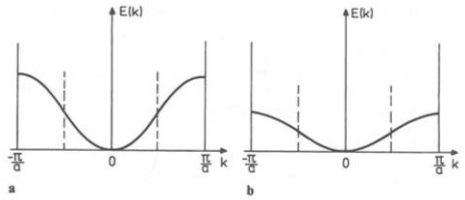
- Classically acceleration of electron by the field a = dv_g/dt = F/m = -eE/m
- With magnetic field F = -e(E+v x B)

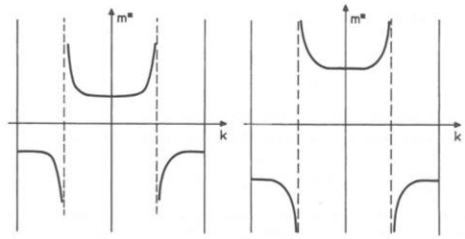
Effective mass

$$m^* = \hbar^2 \left(\frac{\partial^2 \mathscr{E}}{\partial k^2} \right)^{-1}$$



Effective mass tensor in 3D

$$(\boldsymbol{m}_e^*)_{ij} = \frac{\hbar^2}{\partial^2 \mathscr{E}(\boldsymbol{k}) / \partial k_i \partial k_j}$$



Ibach & Lüth, Fig 9.2, See also Elliott, Fig. 6.2

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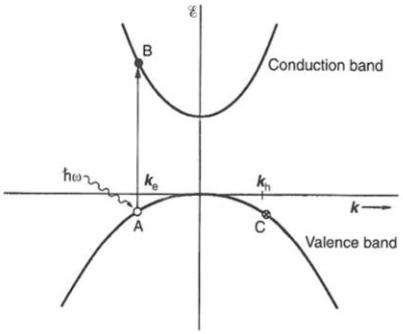
- As said, all the needed information from atomic level is included in the band structure (velocity, effective mass). They describe the interaction/scattering with the lattice.
- At the switch from positive to negative curvature/mass => zero curvature = infinite mass
- These affect how the acceleration under E-field is affected, i.e., F=ma, becomes deceleration
- Flat bands (or small bandwidth) => high effective mass. Localized electrons more difficult to move than delocalized ones (remember KCl from in-class exercise).

Electrons and holes

A hole is a positive "quasiparticle" describing an electron missing from an energy band.

$$k_\mathrm{h} = -k_\mathrm{e}$$
$$\mathscr{E}_\mathrm{h}(k_\mathrm{h}) = -\mathscr{E}_\mathrm{e}(k_\mathrm{e})$$
$$v_\mathrm{h}(k_\mathrm{h}) = v_\mathrm{e}(k_\mathrm{e})$$
$$m_\mathrm{h}^* = -m_\mathrm{e}^*$$



Elliott, Fig. 6.3

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- Properties given with respect to filled electron band
- v and m can be determined from energy and k

The current carried by band electrons

k space volume element d**k** at point **k**, element of particle flux:

$$\mathrm{d}\boldsymbol{J}(\boldsymbol{k}) = \boldsymbol{v}(\boldsymbol{k})\frac{\mathrm{d}\boldsymbol{k}}{4\pi^3} = \frac{\nabla_k(\mathscr{E}(\boldsymbol{k}))\mathrm{d}\boldsymbol{k}}{4\pi^3\hbar}$$

Net current (integral over the occupied part of the band):

$$\boldsymbol{j} = -\frac{e}{4\pi^3\hbar}\int_{1\mathrm{stB.Z}} \nabla_{\boldsymbol{k}}(\mathscr{E}(\boldsymbol{k}))\mathrm{d}\boldsymbol{k}$$

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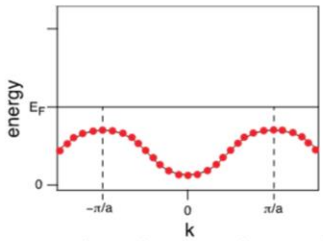
- dk/(4pi^3) gives the number of electronic states within dk and accounting for spin.
- [Integration of dk/(8pi^3) over Brillouin zone yields 1/(primitive cell volume).]

A full energy band

$$j = \frac{-e}{4\pi^3} \int_{k_{occ}} v(k)\mathrm{d}k = 0$$

A full band carries no net current!
(regardless of an external field)



$$E(\mathbf{k}\uparrow) = E(-\mathbf{k}\downarrow)$$
$$\Rightarrow v(-\mathbf{k}) = -v(\mathbf{k})$$

(assuming spin-degeneracy)

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- From time-reversal symmetry T psi(t) = psi^*(-t) => T psi_k = psi_-k
- Metals vs semiconductors
- Valence vs core electrons

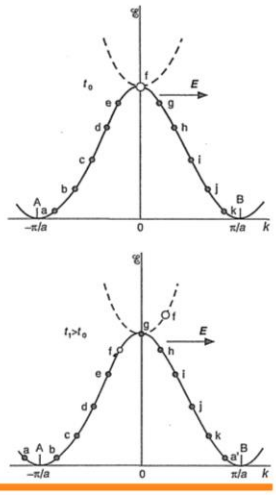
A partially filled band in an external field

$$\mathbf{j} \neq 0$$

$$j = \frac{-e}{4\pi^3}\int_{k_{occ}} v(k)\mathrm{d}k \qquad \text{(electrons)}$$

$$= \frac{-e}{4\pi^3}\int_{1stB.Z.} v(k)\mathrm{d}k - \frac{(-e)}{4\pi^3}\int_{k_{empty}} v(k)\mathrm{d}k$$

$$= 0 + \frac{e}{4\pi^3}\int_{k_{empty}} v(k)\mathrm{d}k. \qquad \text{(holes)}$$



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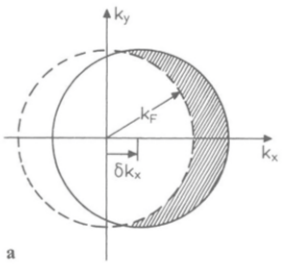
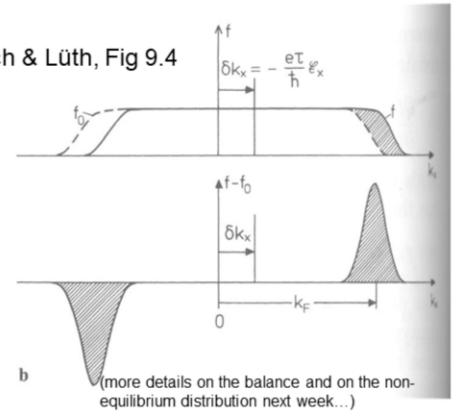
- All electrons in a partially filled band move in k-space concurrently (left), the hole as well
- Last form can be thought of as integral over missing electrons or integral over holes (positive charge, opposive wave vector)
- Due to opposite wave-vector it moves in real-space in same direction as electric field (as expected of positively charged particle)

A Fermi surface in an electric field, nonequilibrium electron distribution



Ibach & Lüth, Fig 9.4



$$\mathbf{k} \longrightarrow \mathbf{k} + \frac{e}{\hbar}\tau(\mathbf{k})\mathbf{E}$$

(more details on the balance and on the non-equilibrium distribution next week…)

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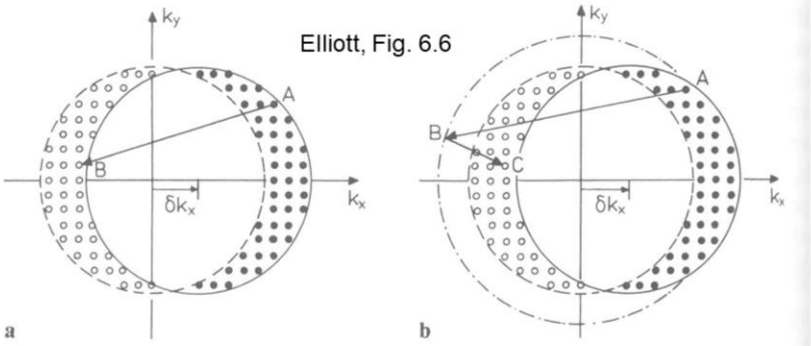
- Free electron model => spherical Fermi-surface
- Also from Drude model, eqn. (6.7,6.8), p = m*v = -e*tau*E = hbar*k, where tau is average time between collisions

Inelastic vs. elastic scattering processes



Only inelastic scattering events can bring the system closer to equilibrium.

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- Scattering only possible to unoccupied states

Scattering processes of electrons

A defect-free, static lattice would cause no scattering since the Bloch states are eigenfunctions of the time-independent Schrödinger equation. The current would persists even in zero field.

Possible scattering mechanisms / scattering centers:

1. Deviations from periodicity: lattice imperfections such as defects (point defects, dislocations, other extended defects), and lattice vibrations (phonons)
2. Electron-electron-scattering (turns out to be less important)

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- Wave packet broadens even if the momentum distribution remains the same.

Electron scattering from imperfections

- Perturbation theory approach: consider a lattice defect as a perturbation H' causing electron scattering from $\mathbf{k}$ to $\mathbf{k}'$

$$w_{\mathbf{k}'\mathbf{k}} \sim |\langle \mathbf{k}'|H'|\mathbf{k}\rangle|^2 = |\int d\mathbf{r}\, \psi^*_{\mathbf{k}'}(\mathbf{r}) H' \psi_{\mathbf{k}}(\mathbf{r})|^2$$

$$= |\int d\mathbf{r}\; u^*_{\mathbf{k}'}(\mathbf{r}) H' u_{\mathbf{k}}(\mathbf{r})\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}|^2$$

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- Rate of change in state occupation as a sum over probabilities to all final states k' => lifetime of state k
- Like Fermi's golden rule…
- Psi(t) = sum_k c_k(t) psi_k, nothing happens if we have just the unperturbed Hamiltonian (with eigenstates psi_k)
- Using time-dependent perturbation: c_k'(t) ~ sum_k w_k'k c_k(t), i.e., w corresponds to shift in amplitude

Static vs. time-dependent perturbation

- Static defect, $H' \neq H'(t)$

➔ Elastic scattering

- Time-dependent perturbation, lattice vibration *(phonon)*

$$H' = H'(\mathbf{r}, t)$$

➔ Inelastic scattering

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Electron-defect scattering

- Rate $R_\mathrm{d} = N_\mathrm{d}\Sigma_\mathrm{d}\nu_\mathrm{F}$
- N_d is density of defects, Σ_d cross section, and v velocity
- Independent of temperature
- Dominates at very low temperatures
- Elastic

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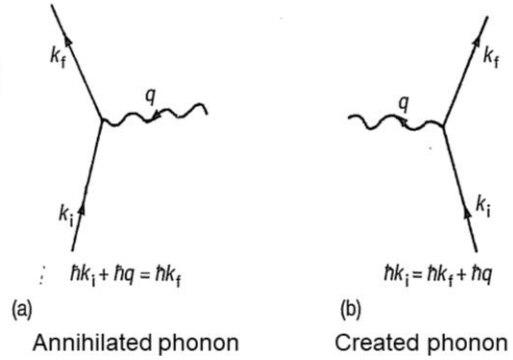
Scattering from phonons (1)

- Conservation of energy

$$\mathscr{E}(\boldsymbol{k}_\mathrm{f}) = \mathscr{E}(\boldsymbol{k}_\mathrm{i}) \pm \hbar\omega(\boldsymbol{q})$$

- Phonon energies small
  - Nearly elastic from electrons point-of-view



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- Annihilated phonon (left), created phonon (right)

Scattering from phonons (2)

- Matrix element for a vibrational mode, $H' \propto e^{i\mathbf{q}\cdot\mathbf{r}}$

$$\langle \mathbf{k}'|e^{i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k}\rangle = \int d\mathbf{r}\, u^*_{\mathbf{k}'}(\mathbf{r}) u_{\mathbf{k}}(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}'+\mathbf{q})\cdot\mathbf{r}}$$

- Since $u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r}+\mathbf{R})$, this differs from zero only if (left as an exercise)

$$\mathbf{k}' - \mathbf{k} = \mathbf{q} + \mathbf{G}$$

- Wave vector conservation, a condition similar to the conservation of momentum (modulo **G**)

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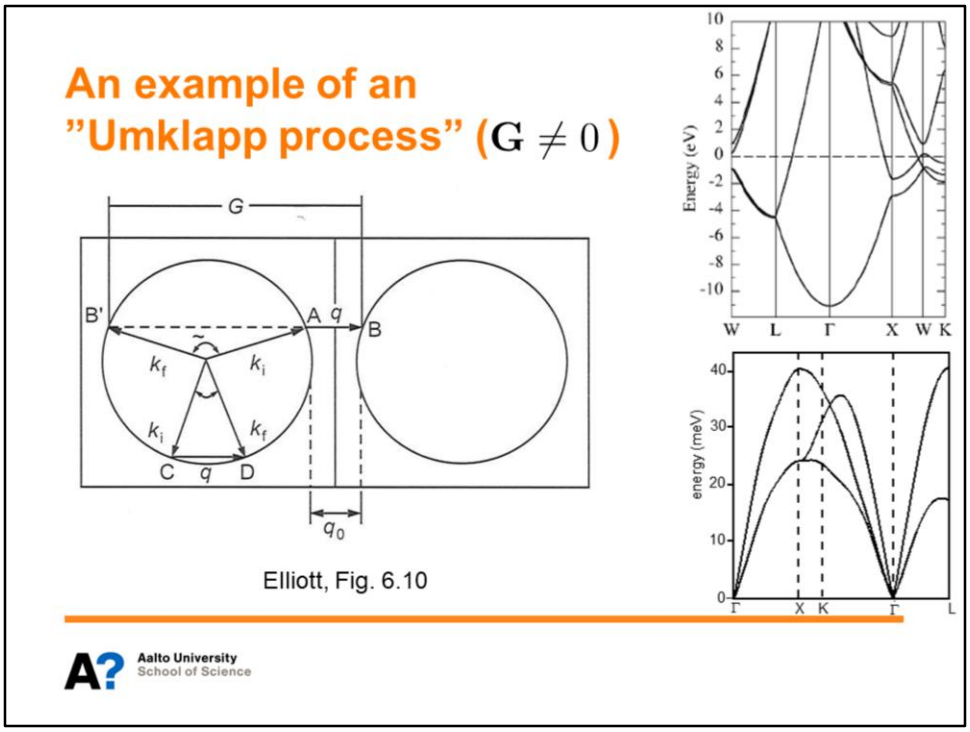
- I.e., exponent needs to be equal to G
- As shown in Elliott: H' ~ u.q, thus only longitudinal phonons couple to electrons
- Drawing D3.2 for understanding the dipolar potential perturbation and how electron feels it in transverse vs. longitudinal cases.



- Two Brillouin zones showing Fermi-surfaces
- A->B umklapp, C->D normal
- Everything happening close to Fermi-surface: occupied vs empty states, at low T small wave vector (and energy) of (acoustic) phonons. Room temp: kT about 26 meV
- See the example band structures and phonon dispersion of aluminum

The ”quasimomentum”

- The quantity $\hbar\mathbf{q}$ or $\hbar\mathbf{k}$ is conserved modulo $\hbar\mathbf{G}$
  - Often obtained from integral of planewaves over space
  - More generally from Noether’s theorem in lattice
- Resembles conservation of momentum
- But not a ”true” momentum.
- Like when momentum operators acts on plane wave
  - With Bloch wave, periodic part also contributes: consider e.g. momentum in free-electron model.
- Electronic states and phonons are solved with respect to lattice, motion in lab frame is unknown/ignored
- $\hbar k = m^* v_g$ only holds for parabolic band, not generally

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- Also called ”crystal momentum”
- Consider momentum in free-electron model in extended vs folded zone schemes: exp(ik.r) vs exp(i((k+G)-G).r)=exp(ik’.r)*exp(-iG.r)=exp(ik’.r)*u(r)
- Momentum conservation arises when Lagrangian is invariant under translation symmetry (continuous space). Also holds for (expectation value of) momentum in QM. And transforms to conservation of k when we consider simple wave packets.
- Here translation symmetry is discrete, constrained to lattice points.

Quasimomentum in infinite system vs. momentum in finite system

- Finite vs infinite systems:
  - Total momentum for electronic state in a piece of material is zero, or the electrons would fly out of it.
  - Schrödinger equation solutions for inside finite system look the same as from infinite system, only boundaries are different.
  - The total momentum of a lattice vibration is zero for any **q**:

$$\sum_i m_i \mathbf{v}_i = 0$$

- Internal vs external scattering:
  - In e.g. photoemission or inelastic neutron scattering "real" momentum is transferred to the sample

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- Illustrate potential well for electrons arising from Coulomb potentials of the nuclei…
- In infinite system we can still have nonzero momentum, since there are no boundaries, I think.
- Phonons solved from potential energy, no kinetic energy was considered.

Electron-phonon scattering

- Displays a temperature dependence since the number of populated phonon modes depends on temperature
- Dominates at higher temperatures
- Inelastic
- Only longitudinal phonons couple to electrons (in case of the so-called ”normal processes”, for which ***G***=0)
- LA phonons have lower energies than LO ones, therefore they are more easily excited and dominate electron-phonon processes

$$\frac{1}{\tau} = \frac{1}{\tau_{\mathrm{d}}} + \frac{1}{\tau_{\mathrm{ph}}}$$

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- High number of phonons per mode affects the amplitude and thus the scattering probability

Electron-electron scattering

- Conservation laws for a scattering process
  (1) + (2) ➔ (3) + (4) :

$$E_1 + E_2 = E_3 + E_4$$
$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4 + \mathbf{G}$$

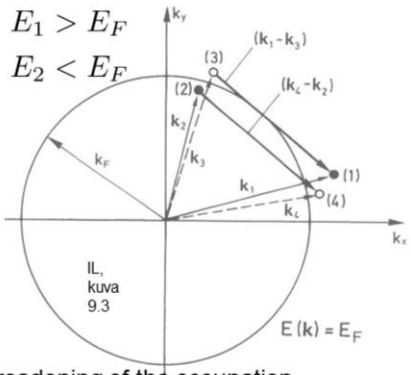
- The states involved must be consistent with the band structure
- Let's consider first just **G**=0

Conservation laws for electron-electron scattering

We assume

$E_1 > E_F$

$E_2 < E_F$



Broadening of the occupation function at Fermi level $\sim kT$

- According to the Pauli exclusion principle the scattering to an occupied state is not possible. At $T = 0$

$$E_3 > E_F, \; E_4 > E_F$$

- Conservation of **k**

$$\mathbf{k}_1 - \mathbf{k}_3 = \mathbf{k}_4 - \mathbf{k}_2$$

- Conservation of energy

$$E_1 + E_2 = E_3 + E_4 > 2E_F$$

$$(E_1 - E_F) + (E_2 - E_F) > 0$$

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- Only (E2-EF)/EF fraction of electrons 2 can scatter with electron 1
- Volume of spherical shell vs volume of sphere ~3(E1-EF)/EF. Alternatively consider some DOS profile, if flat then g*(E1-EF)/(g*EF). Or a fraction (k_1-k_F)/k_F
- States 3 and 4 should be empty states, but quasimomentum conservation forces them close to Fermi-surface

Effect of the Pauli exclusion principle on the e-e scattering

- Both the scatterer (2) and the the states for scattered electrons (3), (4) have to be close to the Fermi surface
- Only a fraction ~ $(E_1-E_F)/E_F$ is close enough
- The effect of the Pauli principle on scattering cross section,

$$\Sigma \propto \left(\frac{kT}{E_F}\right)^2 \Sigma_0$$

Probability to find (2) close to the Fermi surface x the probability to find (3) and (4) close enough, ~10^{-10} (T = 1 K)

Screened classical scattering cross section

Energy scales:

$$E_F \sim 5 - 10 \text{ eV}$$

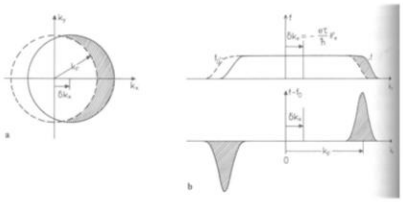
$$kT = 30 \text{ meV } (T = 300 \text{ K})$$

Summary and conclusions for electron scattering

- It is possible to describe the scattering of Bloch electrons similarly to as scattering of real particles by taking into account the conservation laws of lattice momentum **k** (modulo **G**) and energy.
- Scattering from a static lattice defect is elastic, whereas scattering from a time-dependent one, such as a phonon, is inelastic.
- Only inelastic scattering events are effective in restoring a non-equilibrium distribution of electrons towards equilibrium
- The Pauli exclusion principle has an important role when the importance of electron-electron scattering is considered
- Electron-electron scattering is very rare event compared to defect or phonon scattering. This is another justification for the model of non-interacting electrons. It is a good approximation to neglect this process.

Next Monday's program

- The new homework related mainly to Elliott chap. 6.3.2
- Lecture topics
  - Boltzmann equation and electrical conductivity
  - Thermal conductivity
  - Thermoelectric effects



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