IMPRS Course May 2017 M. Seutef

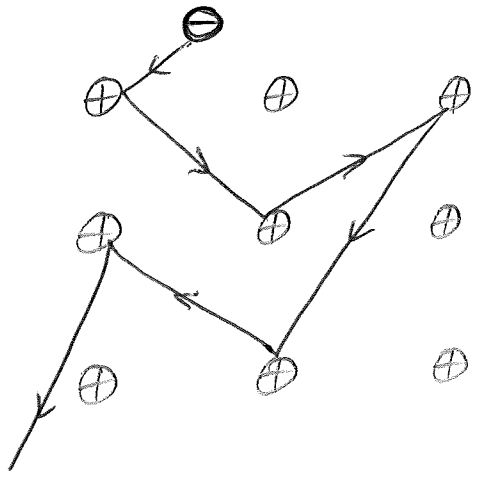
Solid State Physics (in a nutshell)

Topics

1) Drude model
2) Band theory
3) Screening in dielectrics & metals
4) Phonons
5) Peierls transition
6) Ginzburg-Landau theory
7) Magnetism

1) The Drude Model

- kinetic gas theory concepts applied to electrons in a solid that scatter with fixed ions
- one of the first microscopic models for solids ($\sim$ 1900 ... discovery of electron: 1897)



- motion between collisions:

$$\dot{\vec{p}} = \vec{F}_L = -e\left(\vec{E} + \frac{1}{c}\frac{\vec{p}}{m} \times \vec{B}\right)$$

Lorentz force

- Collision probability in $[t, t+dt]$:

$\frac{dt}{\tau}$, $\tau \equiv$ relaxation time

- after collisions: equilibrium Maxwell-Boltzmann distribution

$$\Rightarrow \boxed{\left\langle \frac{d\vec{p}}{dt} \right\rangle = + \vec{F}_L - \frac{\langle \vec{p} \rangle}{\tau}}$$

EOM (eq. of motion) for average momentum

$\Rightarrow$ can be used to compute various transport properties, e.g., conductivity:

$$\vec{j} = -en\frac{\vec{p}}{m}$$

$\vec{j}$: current density
n: density of electrons

$$\vec{E} = \vec{E}(\omega)\, e^{-i\omega t} \Longrightarrow \vec{j}(\omega) = \sigma(\omega)\,\vec{E}(\omega)$$

$$\boxed{\sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau}, \quad \sigma_0 = \frac{n e^2 \tau}{m}}$$ ← DC conductivity

Drude conductivity

- phenomenological model → useful
- <u>but!</u> severe problems with microscopic foundations

(i) Scattering rate $\frac{1}{\tau}$ cannot be related to <u>scattering with ions</u>: σ_{dc}^{-1} decreases $\searrow 0$ in perfect crystal (no defects) at $T \searrow 0$

$\Rightarrow$ electrons can move almost freely in a perfect periodic crystal

$\Rightarrow$ Bloch theorem (Chap. 2) with <u>quasi-momentum conservation</u>

(ii) kinetic gas theory makes some wrong predictions, e.g., specific heat $C_V = \frac{3}{2} n k_B = \text{const.}$, but in reality $C_V \propto T$

$\Rightarrow$ electrons in crystal have fermionic quantum statistics rather than classical Maxwell-Boltzmann

- rough argument for when quantum statistics must be used:

$r_s \simeq n^{-1/3}$ $\lesssim$ $\frac{2\pi\hbar}{\sqrt{3 m k_B T}}$

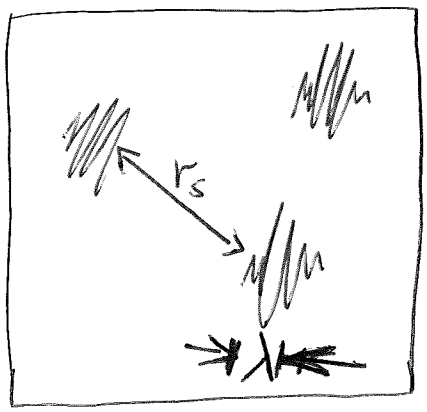
interparticle distance

average de Broglie wavelength $\lambda = \frac{2\pi\hbar}{\langle p \rangle}$

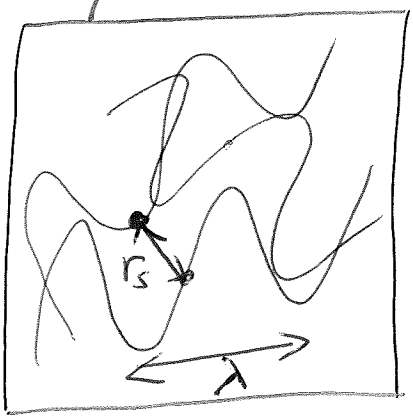
in ideal gas:

$$\left\langle \frac{m}{2} v^2 \right\rangle = \left\langle \frac{p^2}{2m} \right\rangle = \frac{3}{2} k_B T$$

classical



quantum



wave function overlap!

check: $r_s \lesssim \langle \lambda \rangle$ up to constant $E_F \gtrsim T$,

where E_F is Fermi energy of free electrons with density n: $E_F = (3\pi^2 n)^{2/3} \frac{\hbar^2}{2m}$

typical value for metals:

$$E_F \sim 1\text{–}20 \text{ eV} \gg k_B T \simeq 0.01 \text{ eV}$$

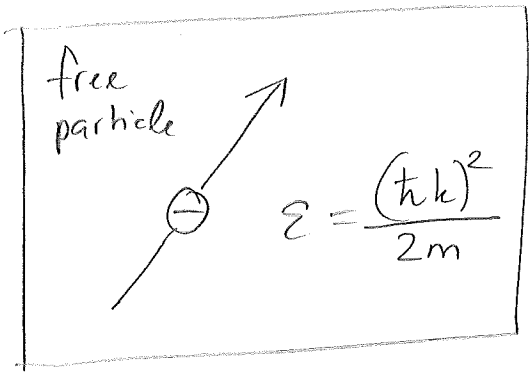
$$k_B T = 1 \text{ eV} \hat{=} 11604 \text{ K}$$

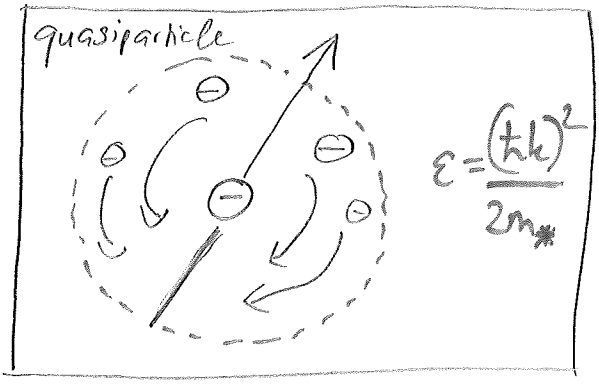
Materials under normal conditions always require quantum description of electrons!

(iii) In real materials, $\frac{e}{m}$ can take a whole range of values (as if there are many kinds of electrons, even with positive charge!).

On the other hand, the success of the Drude model shows that "scattering of something with something else" is not so wrong.

In reality: "particles" are <u>excitations of the ground state with fixed energy-momentum relation</u> $\Rightarrow$ <u>quasiparticles</u>

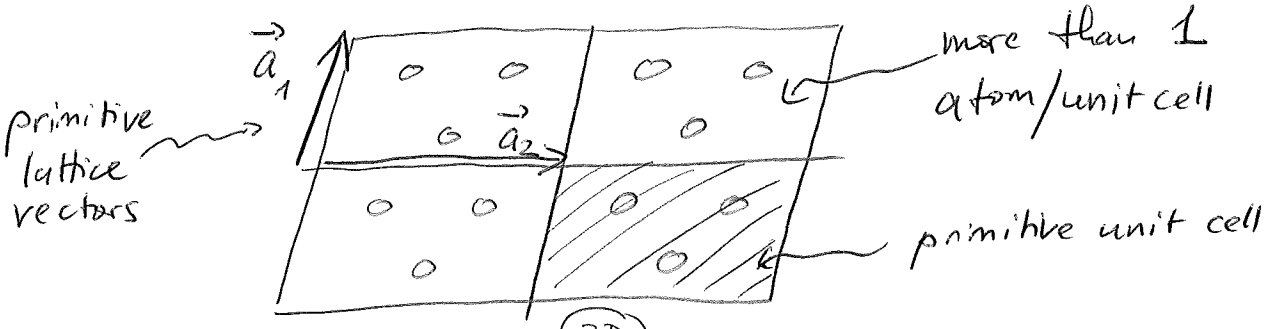




$\Rightarrow$ many different groundstates: Fermi liquid, Superconductor, magnetic order, (fractional) Quantum Hall liquid, with different excitations: quasi-electrons, Bogoliubov fermions, magnons / spinons, (fractionally) charged (bosons!) fermions, ...

2) Band theory = Electrons in a periodic potential

- periodic structures : crystal symmetries



3D

$$\{\vec{R}: \vec{R} = \sum_{i=1}^{3} n_i \vec{a}_i \quad n_i \in \mathbb{Z}\}$$

$\{0, \pm 1, \pm 2, \ldots\}$

is called Bravais lattice

- classification of lattice by symmetry

Point group: symmetry operations which leave at least one point fixed

Space group: full symmetry group

$\vec{r} \longrightarrow \underline{\underline{D}}\vec{r} + \vec{a}$: $\underline{\underline{D}}$: point group

$\vec{a}$: translation

Examples: - Bravais lattices in 2D

- Honeycomb lattice is not a Bravais lattice

- in 3D: Bravais lattice can have 7 point groups (crystal systems) and 14 space groups (Bravais ~1850)
- in 2D: space groups $\hat{=}$ wallpaper groups (see Wikipedia)

- Importance of symmetry for description of solids:
  - quantum number (quasi-momentum $\vec{k}$) → see below
  - symmetry determines response functions.

  Example: Conductivity

$$j_\alpha = \sum_{\alpha'} \sigma_{\alpha\alpha'} E_{\alpha'} \qquad \alpha, \alpha' = x, y, z$$

$\underline{\underline{D}}\,\underline{\underline{\sigma}}\,\underline{\underline{D}}^{-1} \stackrel{!}{=} \underline{\underline{\sigma}}$ invariance for all point group operations $\underline{\underline{D}}$

e.g., rotations about 180° around $\hat{z}$ axis:

$$\underline{\underline{D}} = \begin{pmatrix} -1 & & \\ & -1 & \\ & & +1 \end{pmatrix}$$

$$\underline{\underline{D}} \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \underline{\underline{D}}^{-1} = \begin{pmatrix} +\sigma_{11} & +\sigma_{12} & -\sigma_{13} \\ +\sigma_{21} & +\sigma_{22} & -\sigma_{23} \\ -\sigma_{31} & -\sigma_{32} & +\sigma_{33} \end{pmatrix} \stackrel{!}{=} \underline{\underline{\sigma}}$$

$$\Rightarrow \quad \sigma_{13} = \sigma_{23} = \sigma_{31} = \sigma_{32} = 0$$

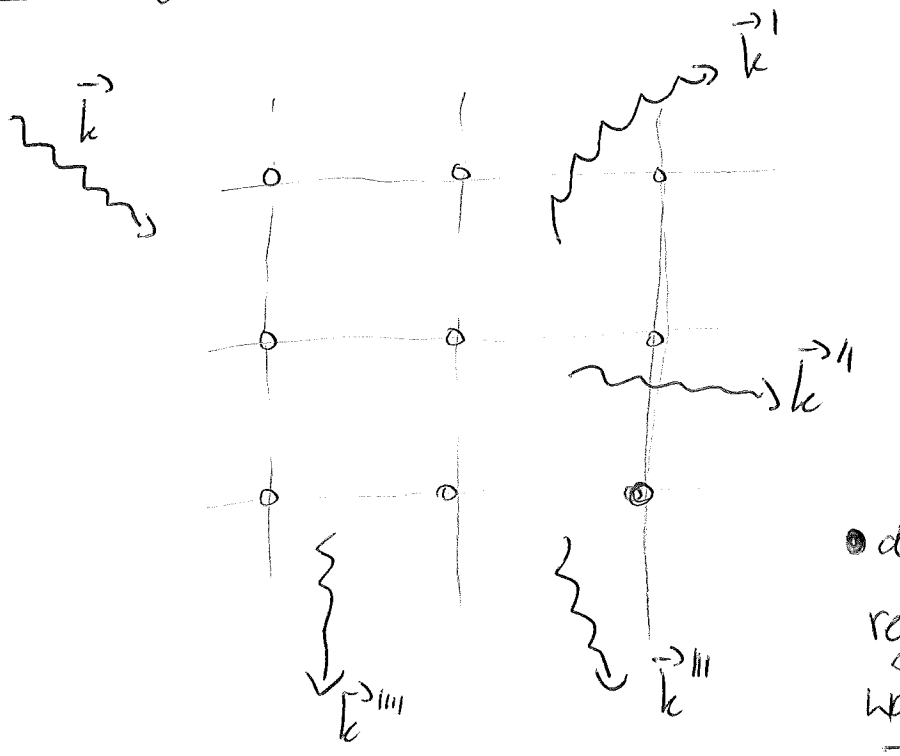
similarly: rotations around $\hat{x}, \hat{y} \Rightarrow \underline{\underline{\sigma}}$ diagonal

rotations about 120° around body diagonal

$\Rightarrow$ permutations of $\hat{x}, \hat{y}, \hat{z} \Rightarrow \underline{\underline{\sigma}} = \sigma \mathbb{1}$

isotropic

Scattering waves off periodic structures (diffraction)



- discrete Bragg reflexes with wave vectors $\vec{k}', \vec{k}'', \ldots$

- condition for constructive interference of scattered wave in direction $\vec{k}'$:

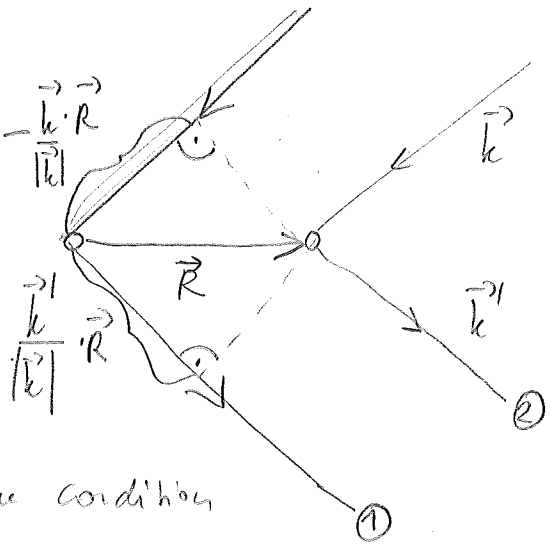
$$\left(\vec{k} - \vec{k}'\right) \cdot \vec{R} = 2\pi n \quad , \; n \in \mathbb{Z}$$

for all $\vec{R} \in$ Lattice (von Laue)

Proof:

path difference ① – ②:

$$\left(\frac{\vec{k}}{|\vec{k}|} - \frac{\vec{k}'}{|\vec{k}'|}\right) \cdot \vec{R} \stackrel{!}{=} n \cdot \lambda$$



for constructive interference

$$\lambda = \frac{2\pi}{|\vec{k}^{(n)}|} \Rightarrow \text{Von Laue condition}$$

(elastic scattering)

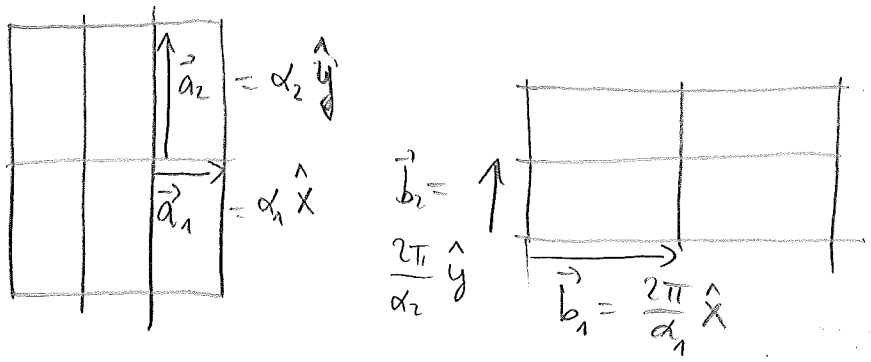
The reciprocal lattice

For a lattice $\{\vec{R}\}$, the reciprocal lattice is given by $\{\vec{G}\}$ with $\vec{G}\cdot\vec{R} = 2\pi n$, $n \in \mathbb{Z}$ for all $\vec{R} \in \{\vec{R}\}$, i.e., $e^{i\vec{G}\cdot\vec{R}} = 1$

If $\{\vec{R}\}$ (Bravais lattice) has primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$, then the reciprocal lattice is a Bravais lattice with primitive vectors $\vec{b}_i$ such that $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$.

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{|\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|} \qquad 1,2,3 \text{ cyclic}$$

Example: rectangular lattice



- reformulation of von Laue condition:

Constructive interference $\Leftrightarrow$ $\vec{k} - \vec{k}' \in$ reciprocal lattice

- technical remark: reciprocal lattice also defines Fourier components of a function which is periodic on the lattice: $f(\vec{r}+\vec{R}) = f(\vec{r}) \Rightarrow$

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

$$f_{\vec{G}} = \frac{1}{\text{vol}} \int_{\text{unit cell}} d^3r\, e^{-i\vec{G}\cdot\vec{r}} f(\vec{r})$$

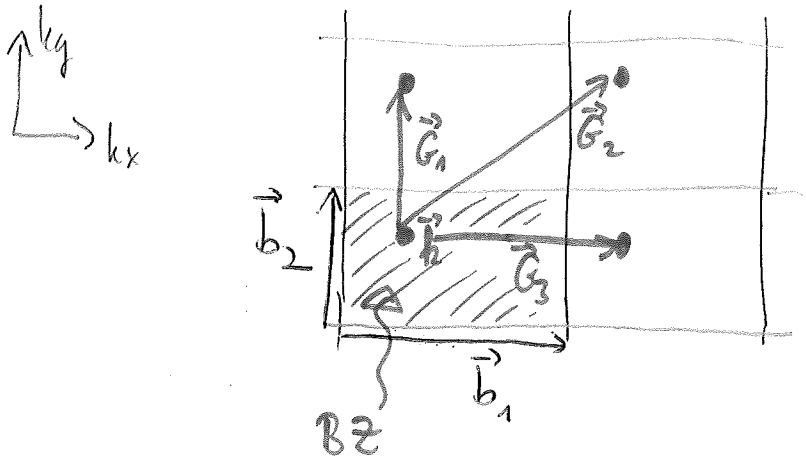
Momentum Conservation on the lattice

Scattering in a periodic lattice $\vec{k} \longrightarrow \vec{k}'$ with

$$\vec{k}' - \vec{k} = \vec{G} \in \{\vec{G}\}$$

$\Rightarrow$ momentum conservation up to reciprocal lattice vector

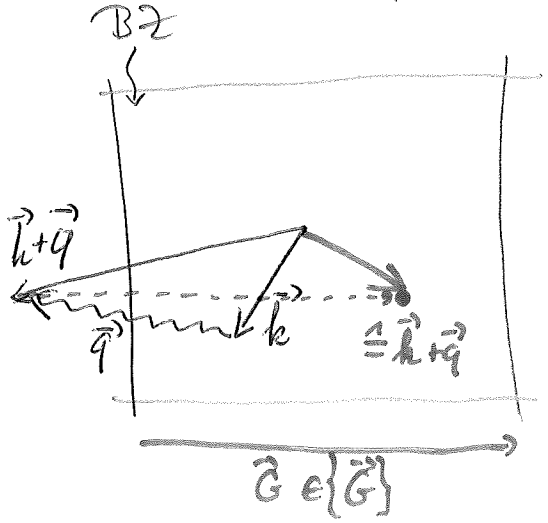
> State $|\psi\rangle$ has "good quasi-momentum $\vec{k}$"
>
> $\Leftrightarrow$ $|\psi\rangle$ superposition of states with momentum $\vec{k}+\vec{G}$, $\vec{G} \in \{\vec{G}\}$



without loss of generality, $\vec{k}$ can be taken from 1st Brillouin zone (BZ)

$\equiv$ Wigner-Seitz unit cell of reciprocal lattice

Illustration: Umklapp scattering



scattering of electron with $\vec{k}$ off something else (phonon, another electron) with quasimomentum $\vec{q}$

Momentum conservation: algebraic formulation

In a periodic crystal, $\hat{H}$ (Hamiltonian) commutes with all translation operators:

$$\boxed{\left[\hat{H}, \hat{T}_R\right] = 0 \quad \forall \ \vec{R} \in \{\vec{R}\}}$$

$$\left(\hat{T}_R \Psi\right)(\vec{r}) = \Psi(\vec{r} - \vec{R})$$

$\Rightarrow$ eigenfunctions of $\hat{H}$ and $\hat{T}_R$ are the same

$$\hat{T}_R |\Psi\rangle = c(\vec{R}) |\Psi\rangle \quad \forall \vec{R}$$

$$\vec{R} = \sum_i n_i \vec{a}_i \Rightarrow T_{\vec{R}} = \left(T_{\vec{a}_1}\right)^{n_1} \left(T_{\vec{a}_2}\right)^{n_2} \left(T_{\vec{a}_3}\right)^{n_3}$$

(because translation operators commute)

$$\Rightarrow T_R |\Psi\rangle = c(\vec{a}_1)^{n_1} c(\vec{a}_2)^{n_2} c(\vec{a}_3)^{n_3} |\Psi\rangle \cdot \forall n_i \in \mathbb{Z}$$

because $\| |\Psi\rangle \| = \| T_R |\Psi\rangle \| \Rightarrow |c(\vec{R})| = 1$

$\Rightarrow$ implicitly define $\vec{k}$ such that $c(\vec{a}_i) = e^{i \vec{k} \cdot \vec{a}_i}$ $\quad i = 1,2,3$

$$\Rightarrow c(\vec{R}) = \exp\left(i \sum_j \vec{a}_j \cdot n_j\right) = e^{i \vec{k} \cdot \vec{R}}$$

$\vec{k}$: <u>quasimomentum</u>: Quantum number that characterizes how wave function behaves under <u>translation</u>: $|\Psi\rangle$ has quasimomentum $\vec{k}$

$$\Leftrightarrow T_R |\Psi\rangle = e^{i \vec{k} \cdot \vec{R}} |\Psi\rangle \ \forall \vec{R} \in \{\vec{R}\}$$

- Note: $\vec{k}$ and $\vec{k}+\vec{G}$ with $\vec{G} \in \{\vec{G}\}$ are the same q.-mom.
- compare: L^2, L_z: quantum numbers which characterize trafo under rotations, etc.

Electrons in a periodic crystal

Goal: Solve Schrödinger equation for electrons (e) in the solid

Approximations:
- nuclei fixed (Born-Oppenheimer appr.), valid for $m_e \ll m_{nuclei}$
- e-e interaction neglected (deep reason: Landau's Fermi-liquid theory)

$\Rightarrow$ goal: determine eigenvalue spectrum of

$$H = \frac{\vec{p}^2}{2m} + V(\vec{r}) \qquad V(\vec{r}) = V(\vec{r}+\vec{R})$$
$$\forall\, \vec{R} \in \{\vec{R}\} \equiv \text{Bravais lattice}$$

Bloch theorem

$\hat{H}$ commutes with all translations $T_{\vec{R}}$, $\vec{R} \in \{\vec{R}\}$

$\Rightarrow$ eigenstates of $\hat{H}$ have good quasimomentum

$$T_{\vec{R}} |\psi(\vec{r})\rangle = |\psi(\vec{r}+\vec{R})\rangle$$

$$e^{i\vec{k}\cdot\vec{R}} |\psi(\vec{r})\rangle$$

($\vec{k}$: quasimomentum)

$\Rightarrow e^{-i\vec{k}\cdot\vec{R}}\,\psi(\vec{r}) \equiv u_{\vec{k}}(\vec{r})$ is periodic,

$u_{\vec{k}}(\vec{r}+\vec{R}) = u_{\vec{k}}(\vec{r})$

Bloch theorem

$\Rightarrow$ (Bloch) eigenfunctions of $\hat{H}$ can be written as $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})$, where $\vec{k}$ can be restricted to the first Brillouin zone, and $u_{\vec{k}}(\vec{r}+\vec{R}) = u_{\vec{k}}(\vec{r})\ \forall\ \vec{R}$

Note: an analogous theorem is used for time-periodic systems (Floquet theorem, 1883)

Bloch theorem $\Longrightarrow$ Schrödinger eq. gives eq. for $u_{\vec{k}}$

$\hat{\vec{p}} \to -i\hbar\vec{\nabla} \Rightarrow \hat{\vec{p}}\, e^{i\vec{k}\vec{r}} f(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}(\vec{p}+\hbar\vec{k}) f(\vec{r})$

$\Longrightarrow \left[\frac{(\vec{p}+\hbar\vec{k})^2}{2m} + V(\vec{r})\right] u_{\vec{k}}(\vec{r}) = \varepsilon_{\vec{k}}\, u_{\vec{k}}(\vec{r})$,

to be solved on one unit cell (e.g., Wigner-Seitz) with periodic boundary conditions

This defines an eigenvalue problem on a finite volume

$\Longrightarrow$ discrete energy spectrum for each $\vec{k}$, each level only finitely degenerate

$\Longrightarrow$ Energy bands $E_n(\vec{k})$, $n = 1, 2, 3, \ldots$

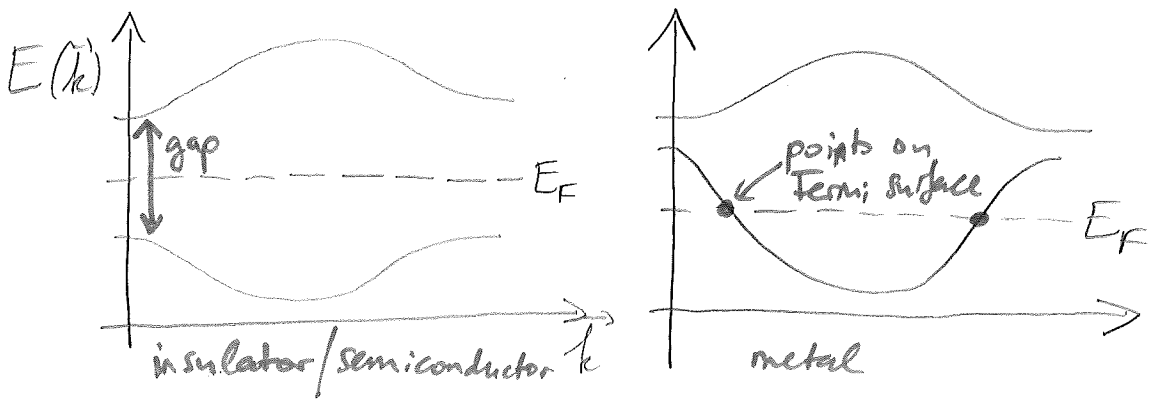
= end 1st lecture → start w/ exercise tomorrow

Wed: exercise only

- $E_n(\vec{k})$ is continuous as fct. of $\vec{k}$
- periodic over the BZ

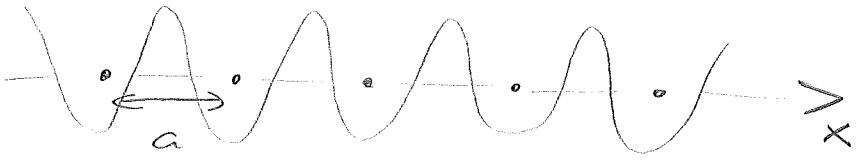
$$E_n(\vec{k}+\vec{G}) = E_n(\vec{k}) \quad , \vec{G} \in \{\vec{G}\}$$

- the level spectrum (band structure) is crucial for most properties of solids:
  - for independent electrons, levels filled up to E_F = Fermi energy; if E_F is in a band gap, electrons (actually: quasiparticles) can only be excited with minimum energy
    => <u>insulator</u> (semiconductor if gap smaller than $k_B T_{room}$)
  - in a <u>metal</u>, levels with $E_n(\vec{k}) = E_F$ form the <u>Fermi surface</u>, which can be multiply connected and in several bands. Its topology is important for many material properties: transport, ordered states, ...

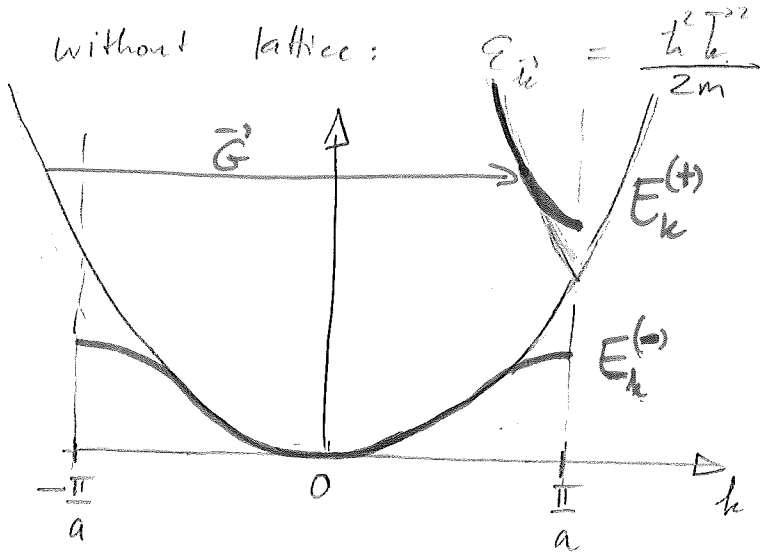


Example: band structure for 2D square lattice

- **1D case:**



$$\vec{G} = \frac{2\pi}{a}\hat{x}$$



weak potential: perturbative analysis close to degenerate point: $\vec{k} \approx \frac{\vec{G}}{2}$

$\Rightarrow$ take into account two plane waves

$$u_{k'}(\vec{r}) = \sum_{\vec{G}} C_{\vec{G}}^{(k)} e^{i\vec{G}\cdot\vec{r}}$$

only $C_0, C_G \neq 0$ $\Rightarrow$

Schrödinger equation becomes 2×2 eigenvalue problem

$$\begin{pmatrix} \varepsilon_k & V_G \\ V_G^* & \varepsilon_{k-G} \end{pmatrix} \begin{pmatrix} C_0 \\ C_G \end{pmatrix} = E_k \begin{pmatrix} C_0 \\ C_G \end{pmatrix}$$

$$E_k^{(\pm)} = \frac{1}{2}\left((\varepsilon_k + \varepsilon_{k-G}) \pm \sqrt{(\varepsilon_k - \varepsilon_{k-G})^2 + 4|V_G|^2} \right)$$

with $V(x) = 2V_0 \cos(kx)$ $\qquad G = \frac{2\pi}{a}$

at $k \simeq G/2$ $\qquad (\epsilon_k = \epsilon_{k-G} \equiv \epsilon_0)$

$$\begin{pmatrix} \epsilon_0 & V_0 \\ V_0 & \epsilon_0 \end{pmatrix} \begin{pmatrix} C_0 \\ C_G \end{pmatrix} = E \begin{pmatrix} C_0 \\ C_G \end{pmatrix}$$

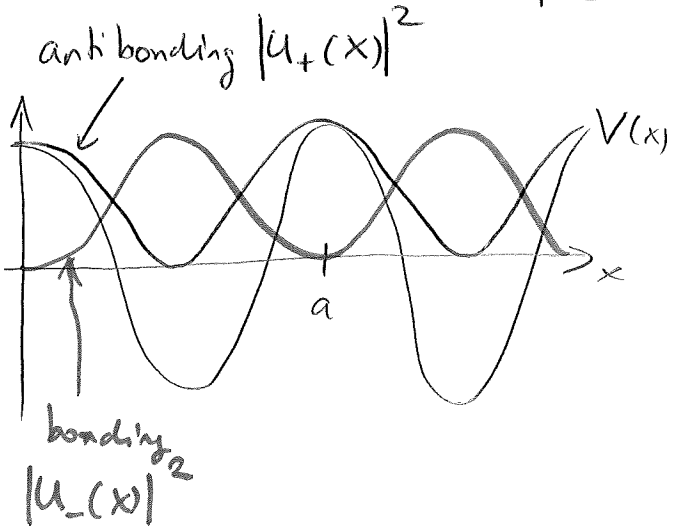
Solutions:

- $\begin{pmatrix} C_0 \\ C_G \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}/\sqrt{2} \quad \Rightarrow E^{(+)} = \epsilon_0 + V_0$

$$|u_+(x)|^2 \sim |1 + e^{iGx}|^2 \sim \cos\left(\frac{Gx}{2}\right)^2$$

- $\begin{pmatrix} C_0 \\ C_G \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}/\sqrt{2} \quad \Rightarrow E^{(-)} = \epsilon_0 - V_0$

$$|u_-(x)|^2 \sim |1 - e^{iGx}|^2 \sim \sin\left(\frac{Gx}{2}\right)^2$$



more examples

Summary: Bloch waves in a periodic potential

Setting $\frac{\hbar^2}{2m} \equiv 1$ and the lattice constant $a = 1$

Schrödinger equation: $\left(\hat{p}^2 + U(x)\right)\Psi(x) = \varepsilon\,\Psi(x)$ (*)

Bloch theorem suggests the ansatz with <u>good quantum number</u> k (crystal momentum):

$$\Psi_k(x) = e^{ikx}\,u_k(x)$$

Bloch wave $u_k(x) = \sum_{G \in \{G\}} \boxed{C_G(k)}\, e^{iGx}$

$C_G(k)$: expansion coefficient for plane waves with reciprocal lattice vector G

"Fourier-like decomposition"

$$C_G(k) = \int_0^1 dx\; e^{-iGx}\,u_k(x)$$

Plug ansatz into (*) using $\hat{p}^2 \to -\nabla_x^2$:

$$\Rightarrow \sum_G (k+G)^2 C_G(k)\, e^{iGx} + \sum_{GG'} U_{G'}\, e^{iG'x}\, C_G(k)\, e^{iGx} = \varepsilon_k \sum_G C_G(k)\, e^{iGx} \qquad (**)$$

where we have used $U(x) = \sum_{G'} e^{iG'x}\,U_{G'}$

$\equiv$ plane-wave expansion of potential

Why does this work? Because the potential can be expressed

with only few plane waves !

(e.g., $U(x) = V_0 \cos(2\pi x) \Rightarrow U_G = \begin{cases} \frac{V_0}{2} & \text{if } G = \pm 2\pi \\ 0 & \text{else} \end{cases}$

From (**) we obtain the Schrödinger equation for the Fourier coefficients $C_{\tilde{G}}(k)$ by:

- multiplying with $e^{-i\tilde{G}x}$
- integrating over the unit cell $\int_0^1 dx$

using $\int_0^1 dx\, e^{i(G-\tilde{G})x} = \delta_{G\tilde{G}}$!

$$\Rightarrow \boxed{\underbrace{(k+\tilde{G})^2 C_{\tilde{G}}(k)}_{\text{kinetic energy}} + \underbrace{\sum_{G'} U_{\tilde{G}-G'} C_{G'}(k)}_{\text{potential energy}} = \varepsilon_k C_{\tilde{G}}(k)}$$

$\Rightarrow$ write in matrix form for $\tilde{G} \in \{G\}$

$\Rightarrow$ diagonalize the matrix

$\Rightarrow$ eigenvalues = energy bands

Exercise: Band structure of 2D potential

Use $U_{(\pm 2\pi, 0)} = U_{(0, \pm 2\pi)} = V_0$

$U_{(\pm 2\pi, \pm 2\pi)} = V_1$

$U_{\vec{G}} = 0$ else

$\sum_{\vec{G}}$: cut off with N_{wave}

finite # of plane waves

=> check convergence for different values of V_0, V_1 !

(please try)