The "empty lattice" model

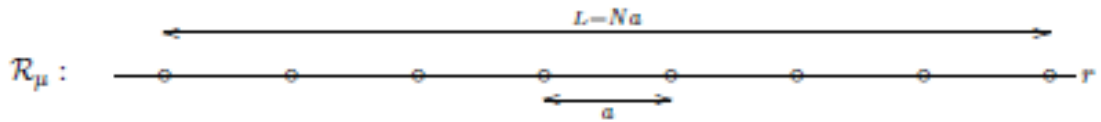
Outline

The 1D empty lattice model

The 1D crystal

Microscopic and Macroscopic Lattices

- Monodimensional crystal based on a microscopic Bravais lattice $\mathcal{R}_\mu$ with primitive cell length a
- Macroscopic solid sample: supercell of length $L = Na$ containing $N \sim N_A$ primitive cells
- Periodic boundary conditions introduce a macroscopic Bravais lattice $\mathcal{R}_M$ whose primitive cell has length L
  - $\Longrightarrow \mathcal{R}_M^*$ has spacing $2\pi/L$

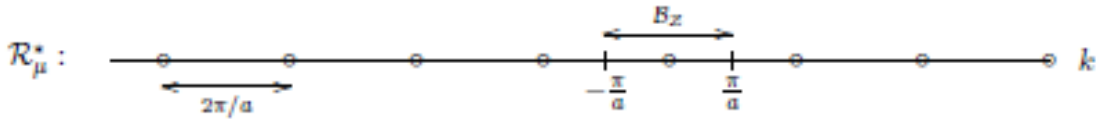


The 1D empty lattice model

The 1D Crystal: Reciprocal Lattice

Microscopic Reciprocal Lattice, $\mathcal{R}^*_\mu$

- Grid with spacing $g = 2\pi/a$
- Points: $G = jg = j\,\dfrac{2\pi}{a}, \quad j \in \mathbb{Z}$
- First Brillouin zone: interval $[-\pi/a,\, \pi/a] = [-g/2,\, g/2]$



Allowed wave vectors

- Only $\boldsymbol{k} \in \mathcal{R}^*_M$ are allowed
- Total of N allowed $\boldsymbol{k}$ points in the first BZ of $\mathcal{R}_\mu$

The 1D empty lattice model

The central equations in 1D

The central equation

$$\left(\frac{\hbar^2 k^2}{2m} - \epsilon\right) C_k + \sum_G U_G \, C_{k-G} = 0 \qquad k \in \mathcal{R}^*_M$$

- $G = jg \in \mathcal{R}^*_\mu$: microscopic reciprocal lattice vectors ($j \in \mathbb{Z}$)
- $\forall$ k's inside the first BZ of $\mathcal{R}^*_\mu$ there is a subsystem:

$$\left(\frac{\hbar^2 (k - jg)^2}{2m} - \epsilon\right) C_{k-jg} + \sum_i U_{ig} \, C_{k-jg-ig} = 0 \qquad j \in \mathbb{Z}$$

The 1D empty lattice model

The "Empty Lattice" assumption

The null periodic potential

- A constant function is trivially periodic for any period T:

$$f(x) = \text{const} \implies f(x+T) = f(x) \quad \forall x, T \in \mathbb{R}$$

- Assume $U(r) = 0 \; \forall r \in \mathbb{R}$
  - $\implies$ free electron periodic model

Distinction from the Fermi gas model

- In both models $U = 0$, but:
  - Fermi gas: no periodicity imposed
  - Empty lattice: $U = 0$ treated as a periodic potential
- $\implies$ Limit a crystalline solid approaches as $U(\boldsymbol{r}) \to 0$

The 1D empty lattice model

The central equation

Solution of the central equation

- Since $U(r) = 0$, all its Fourier coefficients vanish:

$$U_{jg} = \frac{1}{a} \int_0^a U(r)\, e^{-i(jg)r}\, dr = 0 \qquad \forall j$$

- The subsystem reduces to a set of independent equations:

$$\left(\frac{\hbar^2 (k - jg)^2}{2m} - \epsilon \right) C_{k-jg} = 0 \qquad j \in \mathbb{Z}$$

  - Each equation involves only one coefficient C_{k-jg}
  - No coupling between different j values

The 1D empty lattice model

The central equation

Solutions of the central equation

- If $\forall\ j\ \epsilon \neq \dfrac{\hbar^2(k-jg)^2}{2m}\ C_{k-jg} = 0 \Longrightarrow$ trivial solution
- Possible eigenvalues:

$$\epsilon = \frac{\hbar^2(k-jg)^2}{2m} \qquad j \in \mathbb{Z}$$

- for each $j \in \mathbb{Z}$: $C_{k-j'g} = 0$ for $j' \neq j$, $C_{k-jg} \neq 0$
- given a $k \in$ 1st BZ of $\mathcal{R}^*_\mu$ there are infinitely many eigenvalues, one per reciprocal lattice vector $G = j'g\ j' \in \mathbb{Z}$

The 1D empty lattice model

The central equation

Solutions of the central equation

- Eigenfunctions and eigenvalues:

$$\psi_{kn}(r) = \frac{1}{\sqrt{L}} e^{i(k-jg)r} \qquad \epsilon_{kn} = \frac{\hbar^2(k-jg)^2}{2m}$$

  - $k \in$ 1st BZ of $\mathcal{R}^*_\mu$, $j \in \mathbb{Z}$
- n is the band index : ordered by increasing energy for fixed k
  - n is uniquely determined by j
  - lowest eigenvalue always corresponds to $j = 0$: $\varepsilon_{k1} = \dfrac{\hbar^2 k^2}{2m}$
- Normalisation

$$\int_0^L |\psi_{kn}|^2 \, dr = C^2_{k-j'g} \, L = 1 \implies C_{k-j'g} = \frac{1}{\sqrt{L}}$$

The 1D empty lattice model

Solutions of the central equation

Comparison: Fermi Gas vs. Empty Lattice

	Fermi gas	**Empty lattice**
Eigenvalue	$\varepsilon_k = \dfrac{\hbar^2 k^2}{2m}$	$\varepsilon_{kn} = \dfrac{\hbar^2 (k - jg)^2}{2m}$
Eigenfunction	$\psi_k = \dfrac{1}{\sqrt{L}} e^{ikr}$	$\psi_{kn} = \dfrac{1}{\sqrt{L}} e^{i(k-jg)r}$

- Fermi gas: one eigenvalue per allowed k
- Empty lattice: infinitely many eigenvalues per k, indexed by band index n (determined by j)
- Microscopic reciprocal lattice $\mathcal{R}^*_\mu$ is completely absent in the Fermi gas model

The 1D empty lattice model

Solutions of the central equation

Verification of Bloch's Theorem

- Second form of Bloch's theorem:

$$\psi_{kn}(r+R) = e^{i(k-jg)(r+R)}/\sqrt{L} = e^{ikR}\underbrace{e^{-ijgR}}_{=1}\psi_{kn}(r) = e^{ikR}\psi_{kn}(r)$$

  - since $R = pa$, $j \in \mathbb{Z}$: $e^{-ij(2\pi/a)pa} = e^{-ijp2\pi} = 1$

- First form of Bloch's theorem

$$\psi_{kn}(r) = e^{ikr}\underbrace{\frac{1}{\sqrt{L}}e^{-ijgr}}_{u_{kn}(r)}$$

  - $u_{kn}(r)$ is periodic on $\mathcal{R}_\mu$: $u_{kn}(r+la) = e^{-ijl2\pi}\,u_{kn}(r) = u_{kn}(r)$

The dispersion relation

The 1D empty lattice model

General properties

- Link the allowed energies to the allowed k's:

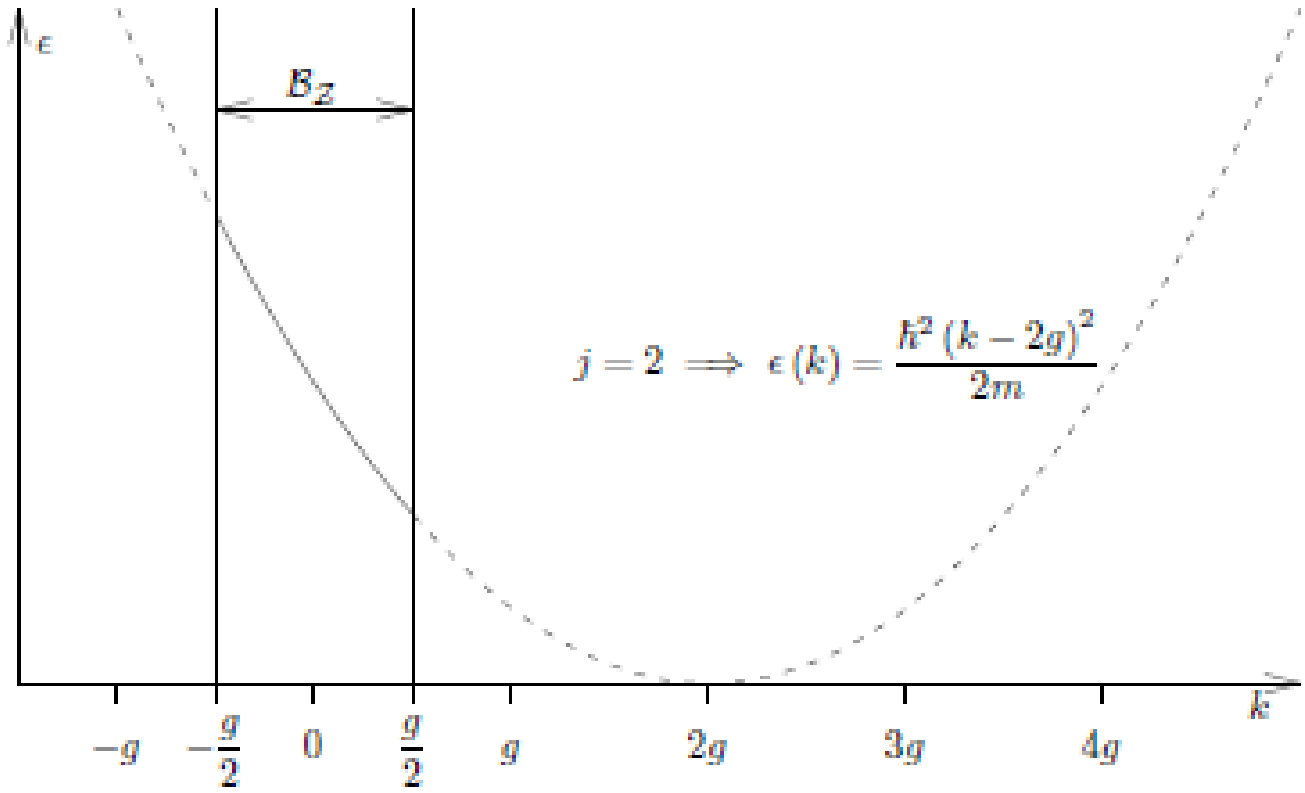
$$\varepsilon(k) = \frac{\hbar^2(k - jg)^2}{2m}$$

  - $k \in$ 1st BZ of $\mathcal{R}^*_\mu$, $\quad j \in \mathbb{Z}$
- For fixed j (which fixes n): a parabola translated by $G = jg \in \mathcal{R}^*_\mu$
  - to the right ($j > 0$) or to the left ($j < 0$)
  - graph in the 1st BZ: portion of the parabola clipped inside $[-\pi/a, \pi/a]$
- For a given k: infinitely many ε values, one per $j \in \mathbb{Z}$
- For fixed j: true function of k in the 1st BZ

The dispersion relation

The 1D empty lattice model

General properties

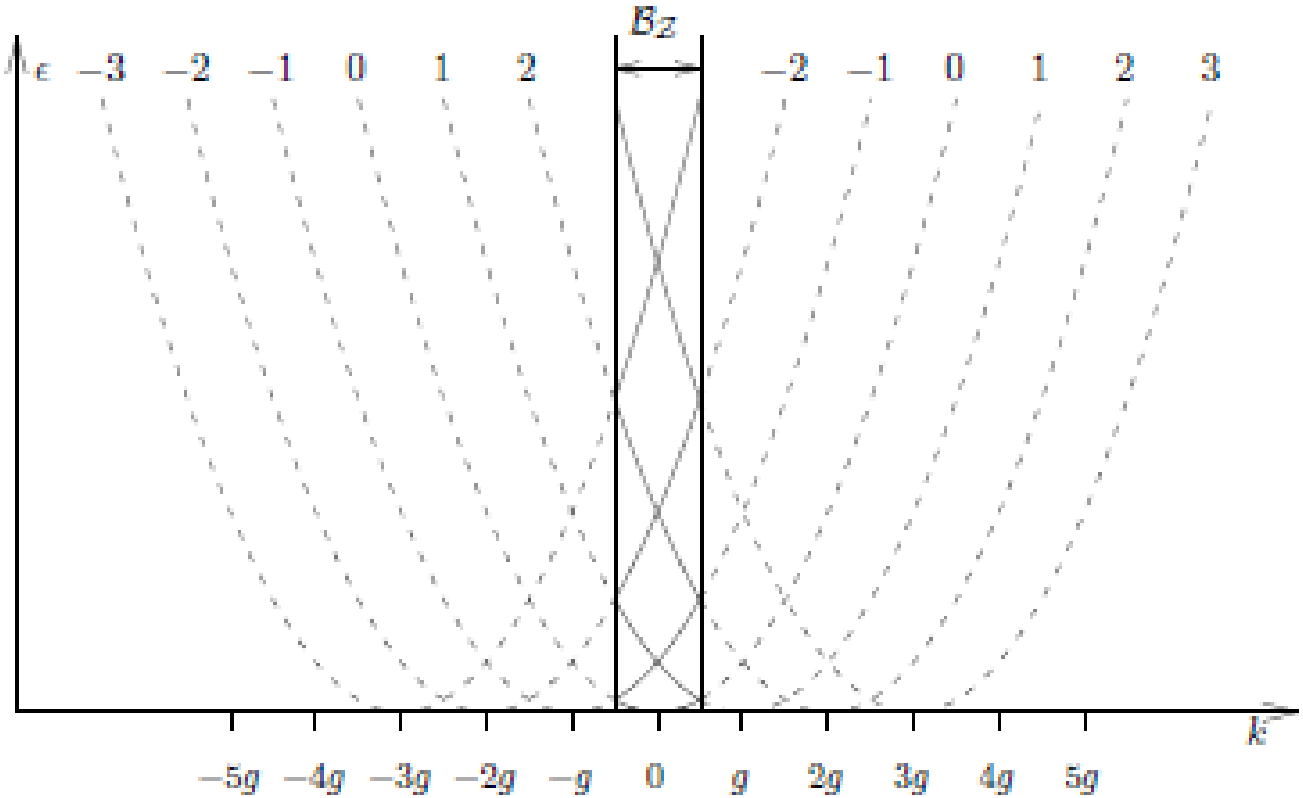


dispersion relation in the 1st BZ for $j = 2$

The dispersion relation

The 1D empty lattice model

General properties



dispersion relation in the 1st BZ for $j = 0, \pm 1, \pm 2, \pm 3$

The dispersion relation

Band Index and G vectors

Map between n and j

- For fixed $k \in$ 1st BZ of $\mathcal{R}^*_\mu$, the eigenvalues are ordered:

$$\epsilon_{1k} \leq \epsilon_{2k} \leq \epsilon_{3k} \leq \cdots \leq \epsilon_{nk} \leq \cdots$$

  - move vertically from k: each intersection is an eigenvalue
  - Band index $n \geq 1$ (positive integer)

	n:	1	2	3	4	5	6	7	$\cdots$
$k \leq 0$:	j:	0	-1	1	-2	2	-3	3	$\cdots$
$k \geq 0$:	j:	0	1	-1	2	-2	3	-3	$\cdots$

The dispersion relation

Band Index and G vectors

Map between n and j

- The relation between n and j reads:

$$n(j) = \begin{cases} 1 \quad \text{if j} = 0 \\ 2|j| + \frac{\frac{j}{|j|}+1}{2} \text{when k} = 0 \text{ j} \neq 0 \\ 2|j| + \frac{\frac{k}{|k|}\frac{j}{|j|}-1}{-2} \text{when k} \neq 0 \text{ j} \neq 0 \end{cases}$$

- For any $j \Longrightarrow$ one and only one $G = jq \in \mathcal{R}^*_\mu \Longrightarrow$ one and only one portion of the Fermi gas parabola in the 1st BZ
- $\epsilon_{1k} = \frac{\hbar^2 k^2}{2m}$ always corresponds to $j = 0 \Longrightarrow G = 0$
- greater $|j| \rightarrow$ higher eigenvalues

The dispersion relation

Band Index and G vectors

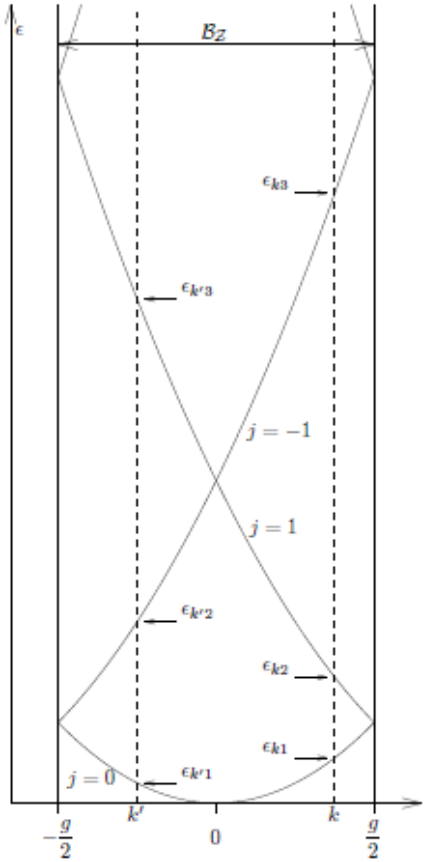
Degeneracy at zone boundaries

- At $k = 0$ and $k = \pm g/2 = \pm\pi/a$: two parabola portions share a common point $\Longrightarrow$ degenerate states
  - $k = g/2$: j_1 and $j_2 = 1 - j_1$
  - $k = -g/2$: j_1 and $j_2 = -j_1 - 1$
  - $k = 0$: j_1 and $j_2 = -j_1$
- Double degeneracy at the BZ boundaries and at $k = 0$
- Points where a non-zero $U(r)$ would open band gaps: the empty lattice is the zero-gap limit
- Gap size in nearly free electorn theory: $E_{\text{gap}} = 2|U_G|$

The dispersion relation

Band Index and G vectors

Degeneracy at zone boundaries



dispersion relation in the 1st BZ

The dispersion relation

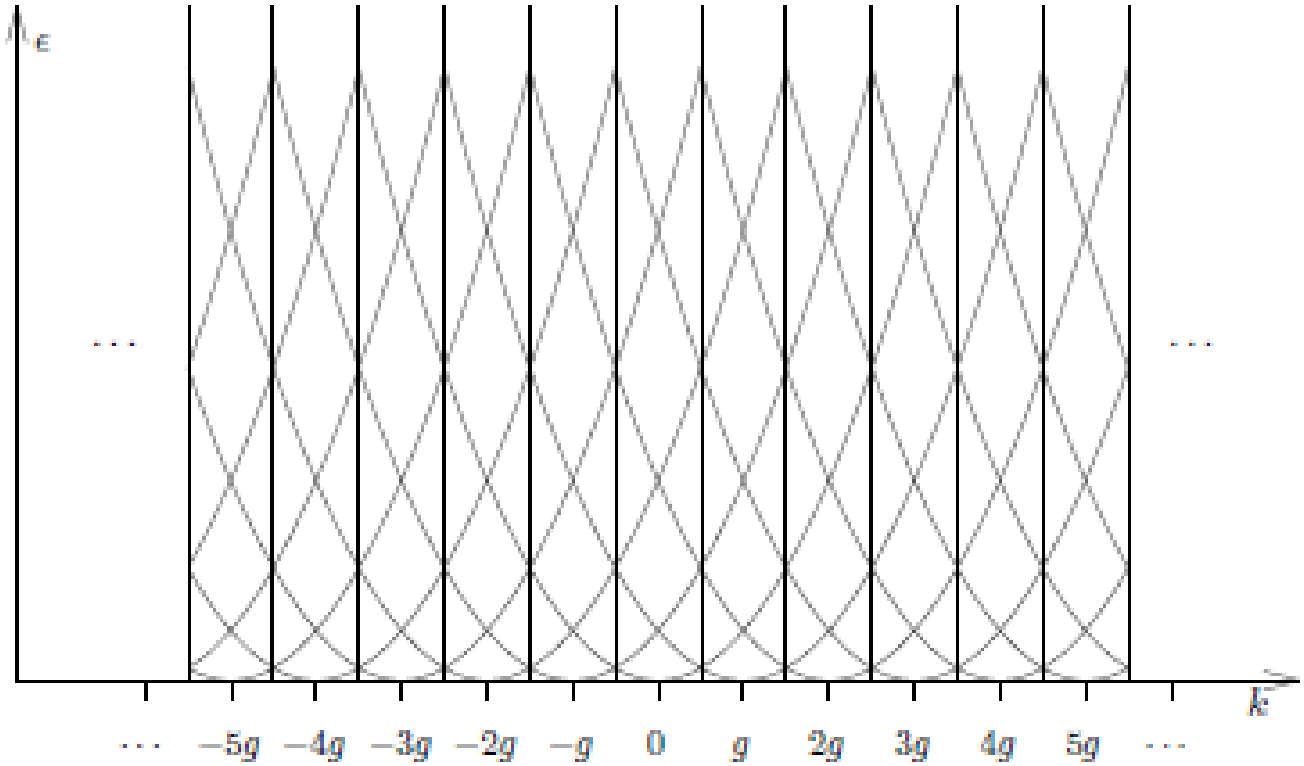
Periodicity of the dispersion relation in k-Space

Observations

- $\psi_{n\boldsymbol{k}}$ and $\varepsilon_{n\boldsymbol{k}}$ are periodic functions of k with the periodicity of $\mathcal{R}^*_\mu$
- The dispersion relation on the whole k axis is obtained by indefinitely replicating the first BZ
- The full dispersion relation is the collection of infinite Fermi gas parabolas, each centred on a reciprocal lattice point $G = jg$
- The parabola giving the $j = 0$ portion in one cell gives the $j = -1$ portion in the adjacent cell to the right, etc.
- The dispersion relation on the whole k axis is not a single parabola, but the infinite set of translated parabolas taken as a whole

The dispersion relation

Periodicity of the dispersion relation in k-Space



dispersion relation on the whole k axis

Different representations of the band structure

Lowest bands for the 1D "empty lattice" model

Examples: branches of the first three bands

- First band:

$$\epsilon_1(k) = \frac{\hbar^2}{2m}k^2 \qquad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$$

  - lowest portion of the Fermi gas parabola centered at the origin

- Second band:

$$\epsilon_2(k) = \begin{cases} \dfrac{\hbar^2}{2m}\left(k + \dfrac{2\pi}{a}\right)^2 & k \in [-\pi/a,\, 0] \\ \dfrac{\hbar^2}{2m}\left(k - \dfrac{2\pi}{a}\right)^2 & k \in [0,\, \pi/a] \end{cases}$$

Different representations of the band structure

Lowest bands for the 1D "empty lattice" model

Examples: branches of the first three bands

- Third band:

$$\epsilon_2(k) = \begin{cases} \dfrac{\hbar^2}{2m}\left(k - \dfrac{2\pi}{a}\right)^2 & k \in [-\pi/a,\, 0] \\ \dfrac{\hbar^2}{2m}\left(k + \dfrac{2\pi}{a}\right)^2 & k \in [0,\, \pi/a] \end{cases}$$

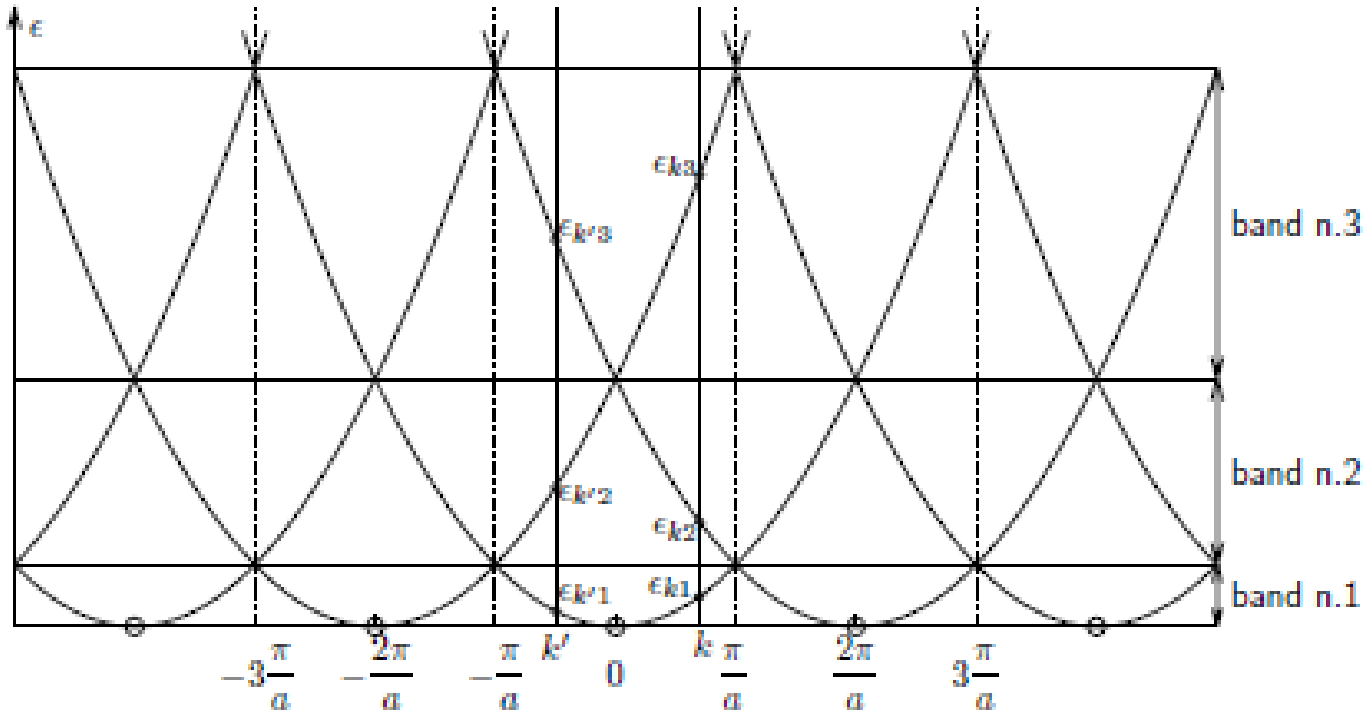
  - same two parabola portions as band 2, but with the left and right branches swapped

- Higher bands come from parabolas centred on reciprocal lattice points of progressively larger modulus

Different representations of the band structure

Lowest bands for the 1D "empty lattice" model

Examples: branches of the first three bands



Repeated zone representation for the first three bands of the 1D "empty lattice" model

Different representations of the band structure

Extension to the general case

Generalizations

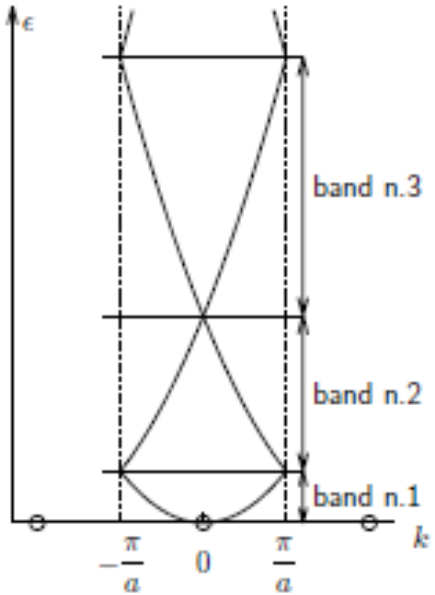
- All branches of all bands are obtained by evaluating $\epsilon(\boldsymbol{k} - \boldsymbol{G})$, $\boldsymbol{k} \in$ 1st BZ, $\forall \boldsymbol{G} \in \mathcal{R}^*_\mu$
- Valid for any dispersion relation
- $\forall$ branch there always $\exists!$ $\boldsymbol{G}$ such that the branch is obtained from $\epsilon(\boldsymbol{k} - \boldsymbol{G})$ inside the first BZ
- Branches are delimited on the k axis by:
  $\ldots, -\frac{3\pi}{a}, -\frac{2\pi}{a}, -\frac{\pi}{a}, 0, \frac{\pi}{a}, \frac{2\pi}{a}, \frac{3\pi}{a}, \ldots$
  - $\Longrightarrow$ boundaries of all Brillouin zones (and the point $k = 0$)
  - Holds in 2D/3D too (BZ boundaries become lines or planes)

Different representations of the band structure

Three Equivalent Representations

Reduced Zone Representation

- Plot $\epsilon(\boldsymbol{k} - \boldsymbol{G})$ for $\boldsymbol{k} \in$ 1st BZ, $\forall \boldsymbol{G} \in \mathcal{R}^*_\mu$
- All band branches shown inside the first BZ only
- No redundancy but the full dispersion relation picture is partially lost



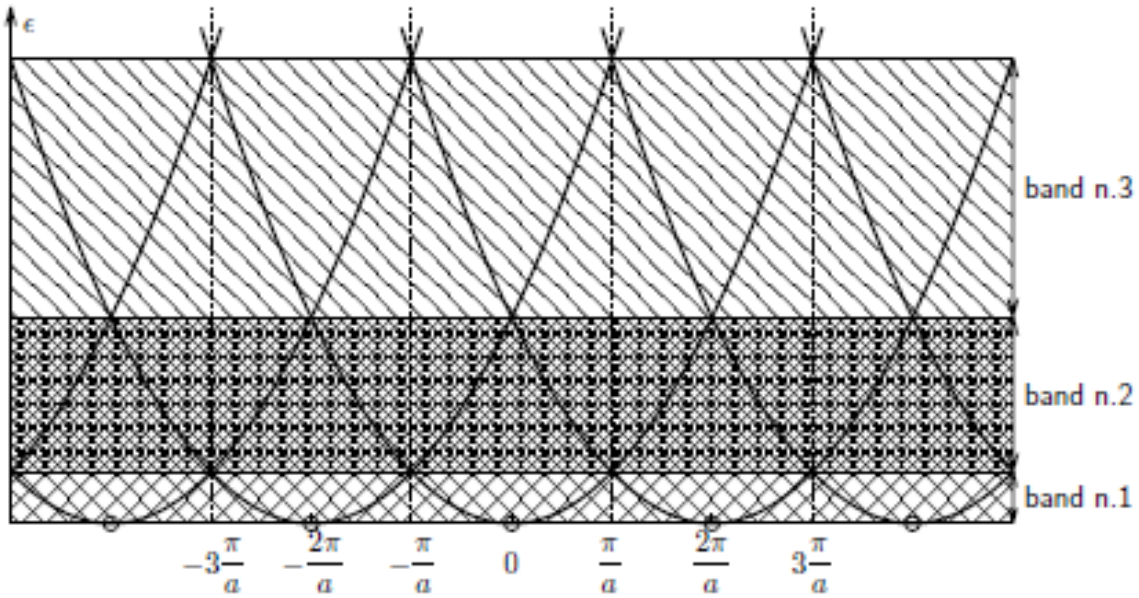
Reduced zone representation for the first three bands of the 1D "empty lattice" model

Different representations of the band structure

Three Equivalent Representations

Repeated Zone Representation

- Plot $\epsilon(\boldsymbol{k} - \boldsymbol{G})$ for $\boldsymbol{k}$ over the whole k-space, $\forall \boldsymbol{G} \in \mathcal{R}^*_\mu$
- Highly redundant; shows well the k-space periodicity of the dispersion relation



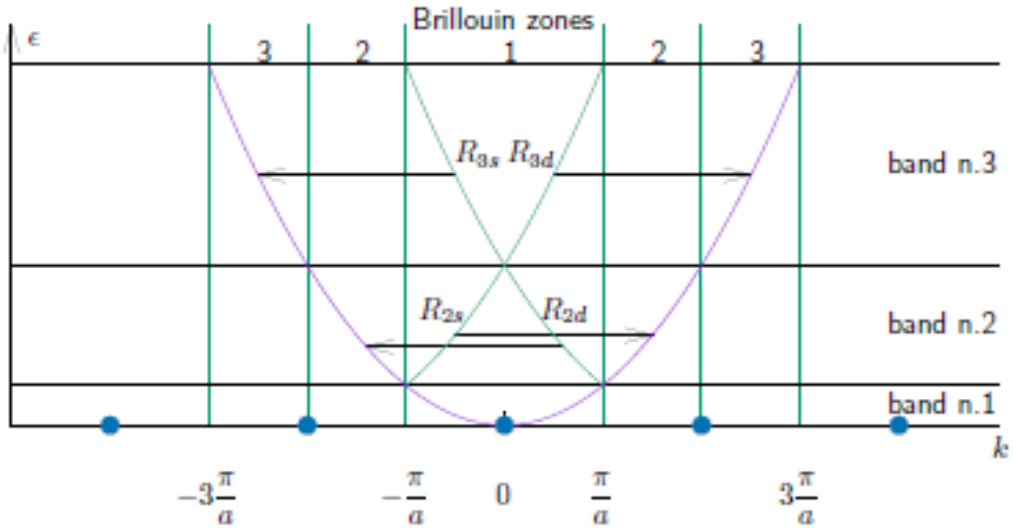
Repeated zone representation for the first three bands of the 1D "empty lattice" model

Different representations of the band structure

Three Equivalent Representations

Extended Zone Representation

- Plot the unshifted dispersion relation $\epsilon(\boldsymbol{k})$ for $\boldsymbol{k} \in \mathcal{R}^*_M$
- Each branch of the reduced zone is translated back by $-\boldsymbol{G}$
- Recovers the single Fermi gas parabola $\epsilon = \hbar^2 k^2 / 2m$



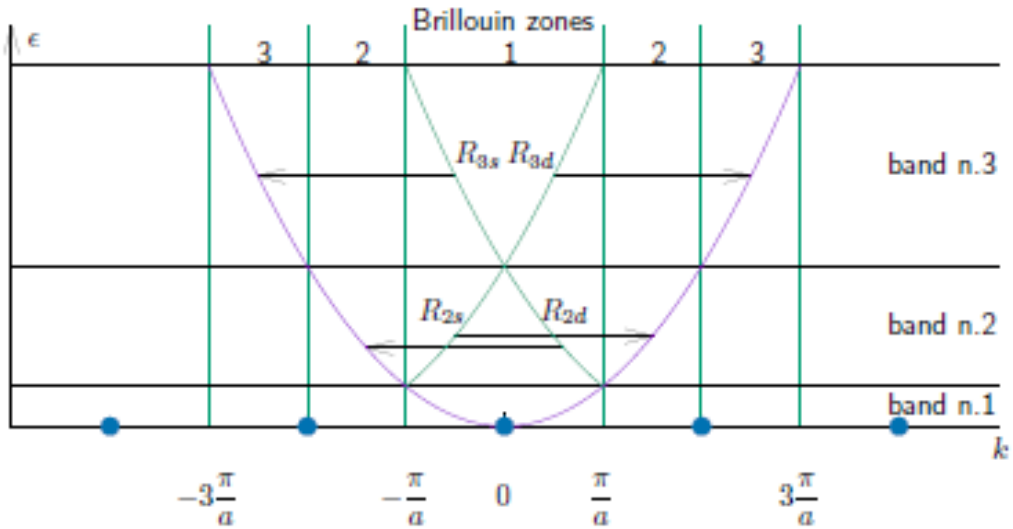
Extended zone representation for the first three bands of the 1D "empty lattice" model

Different representations of the band structure

Three Equivalent Representations

Extended Zone Representation

- band n is fully contained in the n-th Brillouin zone
- Band 1 $\leftrightarrow$ 1st BZ; bands 2,3 $\leftrightarrow$ 2nd, 3rd BZ; ...
- Alternatively: draw BZ boundaries on the unshifted dispersion relation



Extended zone representation for the first three bands of the 1D "empty lattice" model

Different representations of the band structure

Symmetry properties

Parity: $\epsilon_n(k) = \epsilon_n(-k)$

- Band 1: $\epsilon_1(k) = \frac{\hbar^2 k^2}{2m} \implies$ manifestly even
- Band 2: for $k \in [0, \pi/a]$, $\epsilon_2(k) = \frac{\hbar^2}{2m}(k - \frac{2\pi}{a})^2$; replacing $k \to -k$ $\implies \frac{\hbar^2}{2m}((-k) - \frac{2\pi}{a})^2 = \frac{\hbar^2}{2m}(k + \frac{2\pi}{a})^2 = \epsilon_2(-k)$ ✓
- Symmetry is a consequence of the quadratic dispersion relation:
  - the reduced zone band structure is always symmetric about the energy axis ($k = 0$)
  - all three representations inherit this symmetry

Extension to 2D and 3D

2D system with a square Bravais lattice

2D square lattice: dispersion relation

- Reciprocal lattice: square with spacing $2\pi/a$
  - $\boldsymbol{b}_1 = (2\pi/a, 0)$, $\boldsymbol{b}_2 = (0, 2\pi/a)$
- $\boldsymbol{G} \in \mathcal{R}_\mu = \frac{2\pi}{a}(n_x, n_y)$, $n_x, n_y \in \mathbb{Z}$
- Dispersion relation:

$$\varepsilon(\boldsymbol{k}) = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{2\pi n_x}{a}\right)^2 + \left(k_y - \frac{2\pi n_y}{a}\right)^2\right]$$

- We will consider the bands givem by the nine $\boldsymbol{G}$ vectors of smallest modulus ($n_x, n_y \in \{-1, 0, 1\}$)

Extension to 2D and 3D

2D system with a square Bravais lattice

2D square lattice: dispersion relation for the first 9 bands

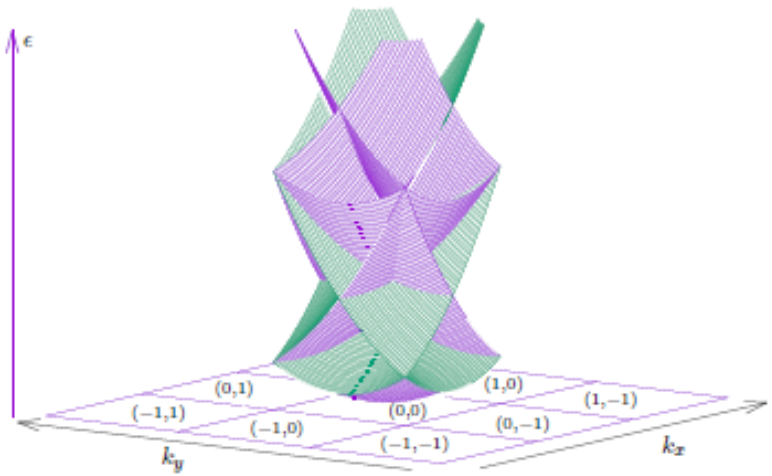
n_x	n_y	$\epsilon(\vec{k}) = \frac{\hbar^2}{2m}\left\vert\vec{k}-\vec{G}\right\vert^2$
-1	-1	$\frac{\hbar^2}{2m}\left(\left(k_x+\frac{2\pi}{a}\right)^2+\left(k_y+\frac{2\pi}{a}\right)^2\right)$
-1	0	$\frac{\hbar^2}{2m}\left(\left(k_x+\frac{2\pi}{a}\right)^2+k_y^2\right)$
-1	1	$\frac{\hbar^2}{2m}\left(\left(k_x+\frac{2\pi}{a}\right)^2+\left(k_y-\frac{2\pi}{a}\right)^2\right)$
0	-1	$\frac{\hbar^2}{2m}\left(k_x^2+\left(k_y+\frac{2\pi}{a}\right)^2\right)$
0	0	$\frac{\hbar^2}{2m}\left(k_x^2+k_y^2\right)$
0	1	$\frac{\hbar^2}{2m}\left(k_x^2+\left(k_y-\frac{2\pi}{a}\right)^2\right)$
1	-1	$\frac{\hbar^2}{2m}\left(\left(k_x-\frac{2\pi}{a}\right)^2+\left(k_y+\frac{2\pi}{a}\right)^2\right)$
1	0	$\frac{\hbar^2}{2m}\left(\left(k_x-\frac{2\pi}{a}\right)^2+k_y^2\right)$
1	1	$\frac{\hbar^2}{2m}\left(\left(k_x-\frac{2\pi}{a}\right)^2+\left(k_y-\frac{2\pi}{a}\right)^2\right)$

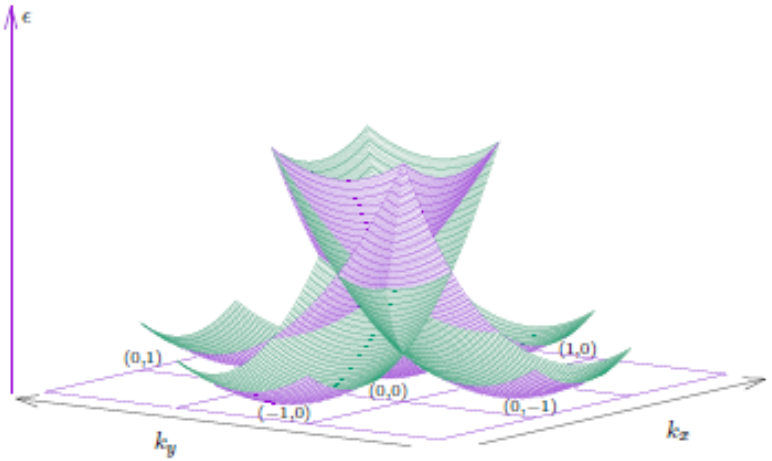
Extension to 2D and 3D

2D system with a square Bravais lattice

Reduced and repeated zone representation of the band structure

- Two ways of realizing the reduced zone representation:
  1. evaluate the branches of the nine parabolas (each centered on a lattice point of $\mathcal{R}^*_\mu$) on a grid of $\boldsymbol{k}$ points inside the 1st BZ (see previous slide)
  2. draw the set of infinite 2D Fermi gas parabolas centred on each reciprocal lattice point and clip inside the first BZ
- Replicate periodically $\Rightarrow$ repeated zone representation





Extension to 2D and 3D

2D system with a square Bravais lattice

Representation along fixed directions

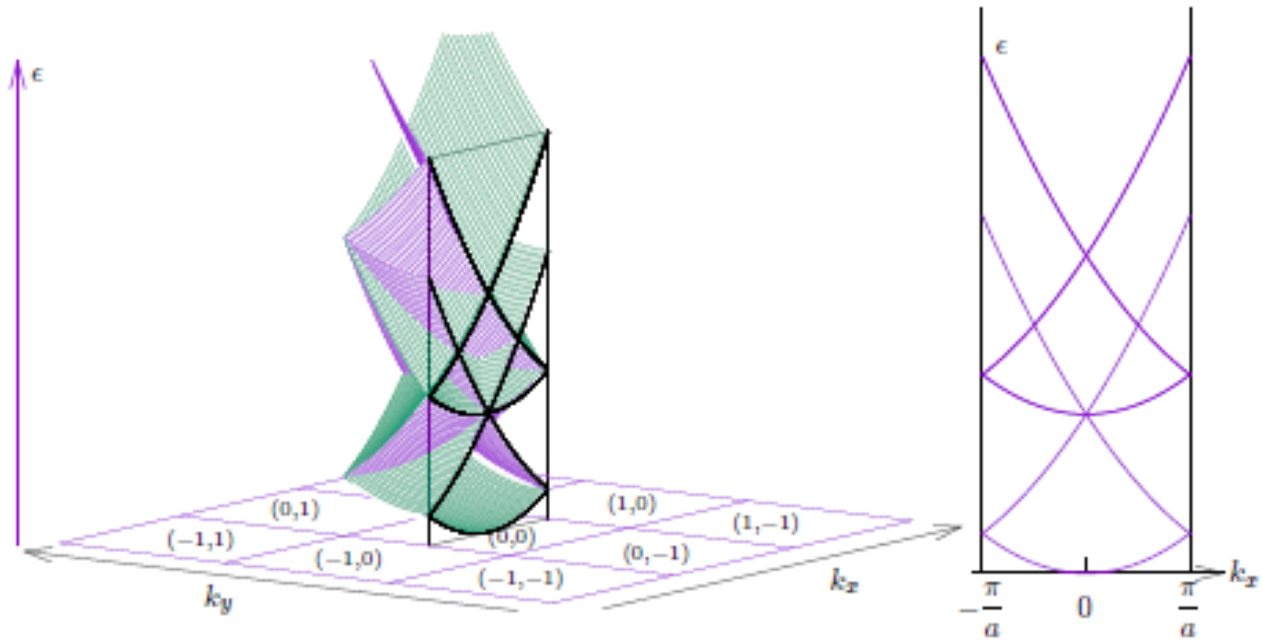
- For 3D systems the full representation is not possible: consider a section of the complete graph
  - along one or more line segments (trajectory in $\boldsymbol{k}$ space)
- Along $k_y = 0 \Longrightarrow$ the 2D dispersion is a function of k_x alone:

$$\epsilon(k_x) = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{2\pi n_x}{a}\right)^2 + \left(\frac{2\pi n_y}{a}\right)^2\right]$$

Extension to 2D and 3D

2D system with a square Bravais lattice

Representation along fixed directions



Extension to 2D and 3D

2D system with a square Bravais lattice

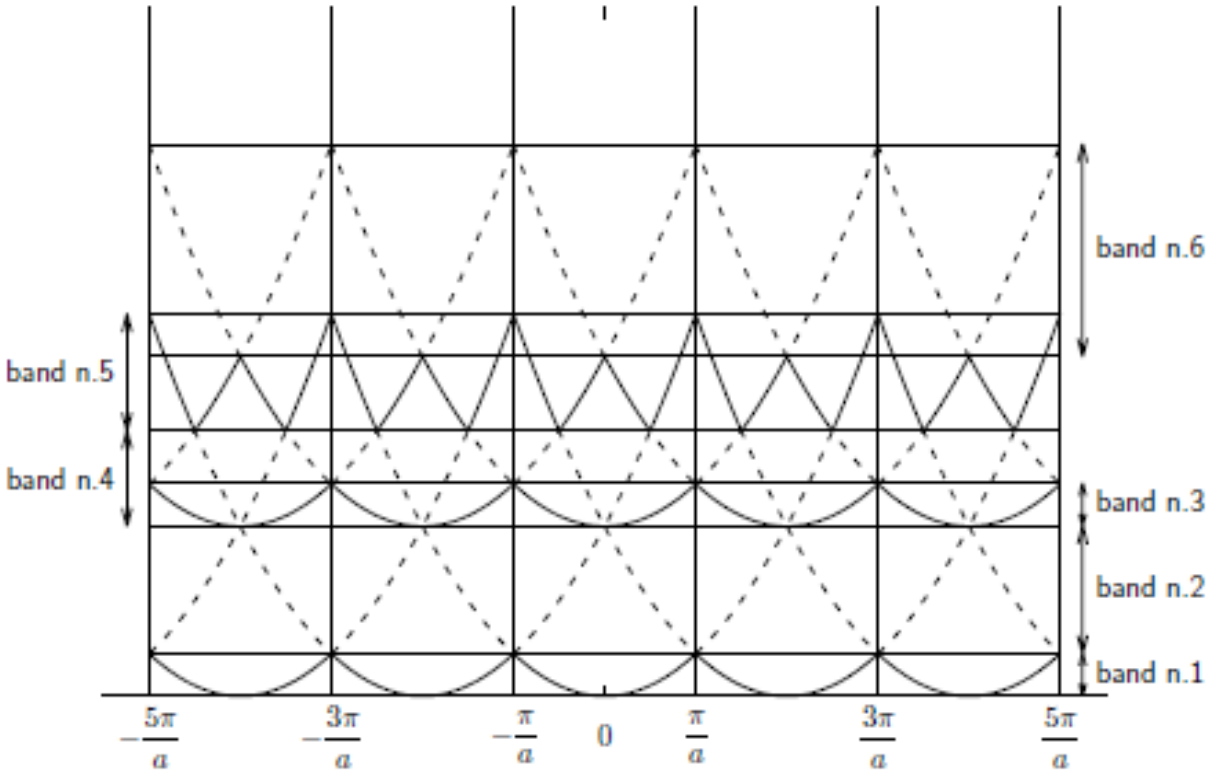
New feature # 1: bands can overlap

- In 1D bands are strictly ordered in energy $\Longrightarrow$ no overlap between bands
- In 2D/3D systems bands can overlap (either partially or completely)
- Along the $(k_x, 0)$ direction:
  - bands 1, 2: no overlap with any other band or with each other
  - band 3 completely overlaps band 4 (latter has a greater bandwidth
  - bands 5 and 6 partially overlap
  - for a fixed $\boldsymbol{k}$, $\epsilon_n(\boldsymbol{k}) \leq \epsilon_{n+1}(\boldsymbol{k})$ always
  - $\epsilon_{\boldsymbol{k}_1,n} > \epsilon_{\boldsymbol{k}_2,n+1}$ possible only for $\boldsymbol{k}_1 \neq \boldsymbol{k}_2$
- Band overlap is crucial for determining whether a material is a metal or an insulator

Extension to 2D and 3D

2D system with a square Bravais lattice

New feature # 1: bands can overlap



Band overlaps along the $k_y = 0$ direction

Extension to 2D and 3D

2D system with a square Bravais lattice

New feature # 2: higher degeneracies

- At $k_x = i\,2\pi/a$ ($i = 0, \pm 1, \ldots$): bands 2, 3, and 4 share a common point $\Rightarrow$ triple degeneracy
- Along $(k_x, 0)$ band nr. 3 is actually two perfectly degenerate bands from $(n_x, n_y) = (0, +1)$ and $(n_x, n_y) = (0, -1)$:

$$\epsilon(k_x) = \frac{\hbar^2}{2m}\left(k_x^2 + \left(\frac{2\pi}{a}\right)^2\right)$$

- Degeneracy becomes more and more frequent as the number of $\boldsymbol{G}$ vectors included increases
- In 3D, higher degeneracies are commonplace
- The quadratic dispersion also preserves mirror symmetry about the energy axis in 2D

Extension to 2D and 3D

2D system with a square Bravais lattice

New feature # 2: higher degeneracies

- Degeneracies for band nr. 4:

interval:	dispersion relation	$(n_x n_y)$
$-\frac{\pi}{a} \leq k_x \leq -\frac{1}{2}\frac{\pi}{a}$	$\frac{\hbar^2}{2m}\left(\left(k_x+\frac{2\pi}{a}\right)^2+\left(\frac{2\pi}{a}\right)^2\right)$	$(-1,\,1)\,,\;(-1,\,-1)$
$-\frac{1}{2}\frac{\pi}{a} \leq k_x \leq 0$	$\frac{\hbar^2}{2m}\left(k_x-\frac{2\pi}{a}\right)^2$	$(1,\,0)$
$0 \leq k_x \leq \frac{1}{2}\frac{\pi}{a}$	$\frac{\hbar^2}{2m}\left(k_x+\frac{2\pi}{a}\right)^2$	$(-1,\,0)$
$\frac{1}{2}\frac{\pi}{a} \leq k_x \leq \frac{\pi}{a}$	$\frac{\hbar^2}{2m}\left(\left(k_x-\frac{2\pi}{a}\right)^2+\left(\frac{2\pi}{a}\right)^2\right)$	$(1,\,1)\,,(1,\,-1)$

Extension to 2D and 3D

Partial representation along specific directions

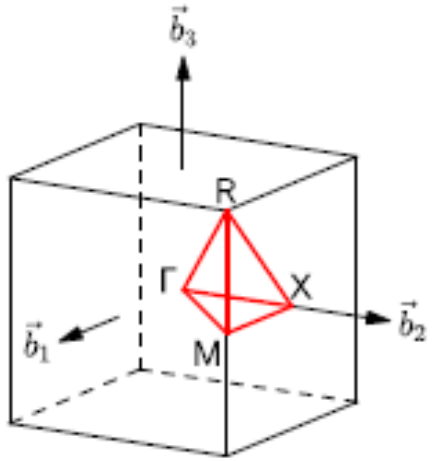
High-symmetry points of the 1st BZ

- Complete representation is not possible for a 3D system $\Longrightarrow$ partial representations along trajectories inside the 1st BZ
- For each of the 14 Bravais lattices, there is a special nomenclature of high-symmetry points in the 1st BZ
  - in its interior or on its faces
  - see `https://en.wikipedia.org/wiki/Brillouin_zone`

Extension to 2D and 3D

3D system with a simple cubic Bravais lattice

High-symmetry points of the SC BZ



Label	coordinates	description
Γ	$(0,0,0)$	Zone center
X	$(\pi/a)\,(1,0,0)$	direction $(0,1,0)$: face center
M	$(\pi/a)\,(1,1,0)$	direction $(1,1,0)$: edge midpoint
R	$(\pi/a)\,(1,1,1)$	direction $(1,1,1)$: corner

Extension to 2D and 3D

3D system with a simple cubic Bravais lattice

Dispersion along $\Gamma \to R$: the $k(1,1,1)$ segment

- Consider $\boldsymbol{k} = k(1,1,1)$ with $k \in [-\pi/a, \pi/a]$
- Include $\boldsymbol{G} = \frac{2\pi}{a}(n_x, n_y, n_z)$, $n_x, n_y, n_z \in \{0, \pm 1\} \implies 27$ vectors in total
- Band trajectories plotted along the body diagonal of the cubic BZ for $\boldsymbol{k} = k(1,1,1)$, $k \in [-\pi/a, \pi/a]$:

$$\epsilon(\boldsymbol{k} - \boldsymbol{G}) = \frac{\hbar^2}{2m} \sum_{i \in \{x,y,z\}} \left(k - \frac{2\pi n_i}{a} \right)^2$$

Extension to 2D and 3D

3D system with a simple cubic Bravais lattice

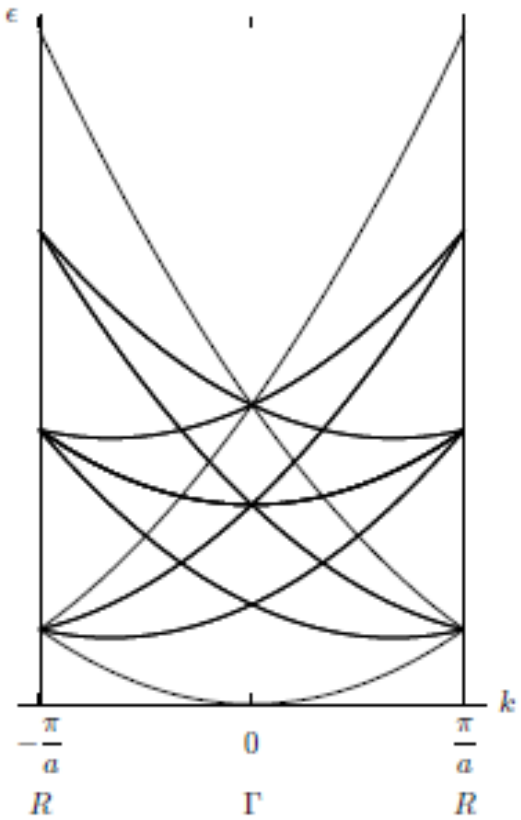
Dispersion along $\Gamma \to R$: the $k(1,1,1)$ segment

n_x	n_y	n_z	$\epsilon\left(\vec{k}-\vec{G}\right) = \frac{\hbar^2}{2m}\left(\left(k-\frac{2\pi}{a}n_x\right)^2+\left(k-\frac{2\pi}{a}n_y\right)^2+\left(k-\frac{2\pi}{a}n_z\right)^2\right)$
−1	−1	−1	$3\frac{\hbar^2}{2m}\left(\frac{2\pi}{a}+k\right)^2$
−1	−1	0	$\frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}+k\right)^2+k^2\right)$
−1	−1	1	$\frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2\right)$
−1	0	−1	$\frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}+k\right)^2+k^2\right)$
−1	0	0	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+2k^2\right)$
−1	0	1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
−1	1	−1	$\frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2\right)$
−1	1	0	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
−1	1	1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+2\left(k-\frac{2\pi}{a}\right)^2\right)$
0	−1	−1	$\frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}+k\right)^2+k^2\right)$
0	−1	0	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+2k^2\right)$
0	−1	1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
0	0	−1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+2k^2\right)$
0	0	0	$3\frac{\hbar^2}{2m}k^2$
0	0	1	$\frac{\hbar^2}{2m}\left(\left(k-\frac{2\pi}{a}\right)^2+2k^2\right)$
0	1	−1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
0	1	0	$\frac{\hbar^2}{2m}\left(\left(k-\frac{2\pi}{a}\right)^2+2k^2\right)$
0	1	1	$\frac{\hbar^2}{2m}\left(2\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
1	−1	−1	$\frac{\hbar^2}{2m}\left(2\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2\right)$
1	−1	0	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
1	−1	1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+2\left(k-\frac{2\pi}{a}\right)^2\right)$
1	0	−1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
1	0	0	$\frac{\hbar^2}{2m}\left(\left(k-\frac{2\pi}{a}\right)^2+2k^2\right)$
1	0	1	$\frac{\hbar^2}{2m}\left(2\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
1	1	−1	$\frac{\hbar^2}{2m}\left(\left(\frac{2\pi}{a}+k\right)^2+2\left(k-\frac{2\pi}{a}\right)^2\right)$
1	1	0	$\frac{\hbar^2}{2m}\left(2\left(k-\frac{2\pi}{a}\right)^2+k^2\right)$
1	1	1	$3\frac{\hbar^2}{2m}\left(k-\frac{2\pi}{a}\right)^2$

Extension to 2D and 3D

3D system with a simple cubic Bravais lattice

Dispersion along $\Gamma \to R$: the $k(1,1,1)$ segment



Extension to 2D and 3D

3D system with a simple cubic Bravais lattice

Dispersion along $\Gamma \to R$: the $k(1,1,1)$ segment

- Only 10 distinct bands visible out of 27 calculations $\Longrightarrow$ many degeneracies
- Example: $(n_x, n_y, n_z) = (1,0,0)$, $(0,1,0)$, $(0,0,1)$ all give the same expression $\frac{\hbar^2}{2m}\left[(k - \frac{2\pi}{a})^2 + 2k^2\right] \Rightarrow$ 3-fold degeneracy
- Mirror symmetry about the energy axis is preserved
- High degeneracies at Γ and R reflect the cubic symmetry of the lattice

The Fermi surface and its representations

The Fermi surface

Branches of the Fermi surface

- Three different scenarios concerning the position of a band with respect to ε_F:
  1. empty band: $\epsilon_F < \epsilon_n^{\min} \Rightarrow$ all states unoccupied
  2. full/completely occupied band: $\epsilon_n^{\max} < \epsilon_F \Rightarrow$ all states occupied
  3. partially occupied/filled band: $\epsilon_n^{\min} < \epsilon_F < \epsilon_n^{\max} \Rightarrow$ Fermi surface of band n defined by $\epsilon_n(\boldsymbol{k}) = \epsilon_F$
- Each partially occupied band contributes one branch of the Fermi surface
- Branch n encloses all $\boldsymbol{k}$ points corresponding to occupied states in band n
- The Fermi surface is periodic on $\mathcal{R}_\mu^* \Longrightarrow$ reduced, extended, or repeated zone representation

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

Reduced zone representation of the Fermi "surface"

- Can be represented in a single step. Solution of the equation:

$$\varepsilon_F = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{2\pi n_x}{a}\right)^2 + \left(k_y - \frac{2\pi n_y}{a}\right)^2\right]$$

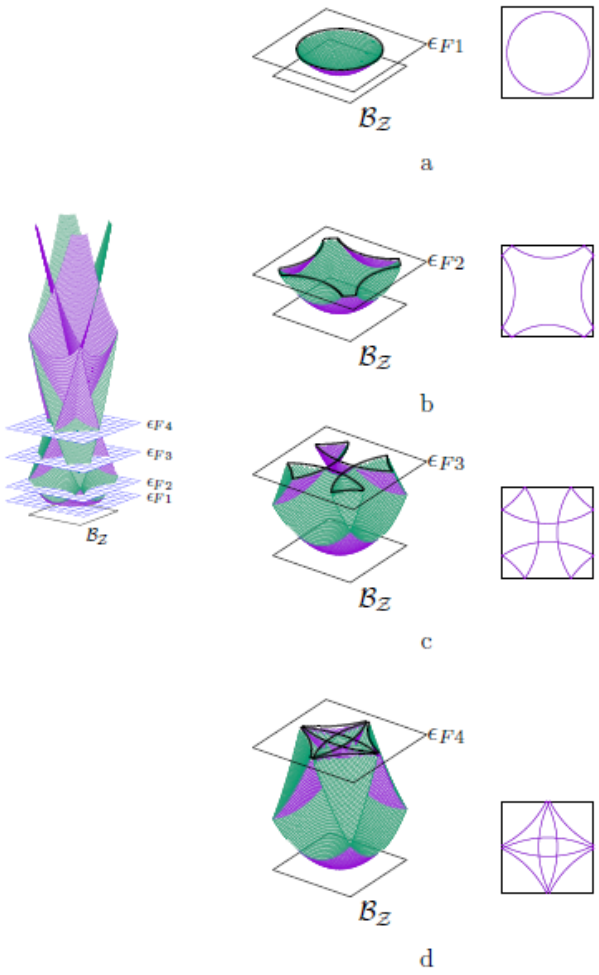
Intersection of the dispersion relation with the horizontal plane $\varepsilon = \varepsilon_F$:

- $\varepsilon = \varepsilon_{F_1}$: circle centered at the origin
- more complicated for greater values of ε_F

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

Reduced zone representation of the Fermi "surface"



The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

Repeated zone representation of the Fermi "surface"

- Dispersion relation given by the infinite set of 2D parabolas each centered on a lattice point of $\mathcal{R}^*_\mu$.
- For the single parabola centered at $\boldsymbol{G} = \frac{2\pi}{a}(n_x, n_y) \in \mathcal{R}^*_\mu$:

$$\left(k_x - \frac{2\pi n_x}{a}\right)^2 + \left(k_y - \frac{2\pi n_y}{a}\right)^2 = \frac{2m}{\hbar^2}\epsilon_F$$

  - circle of radius $\sqrt{(2m/\hbar^2)\epsilon_F}$ centered at $(n_x, n_y)\, 2\pi/a$
- Repeated zone representation $\Longrightarrow$ set of infinite circles.

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

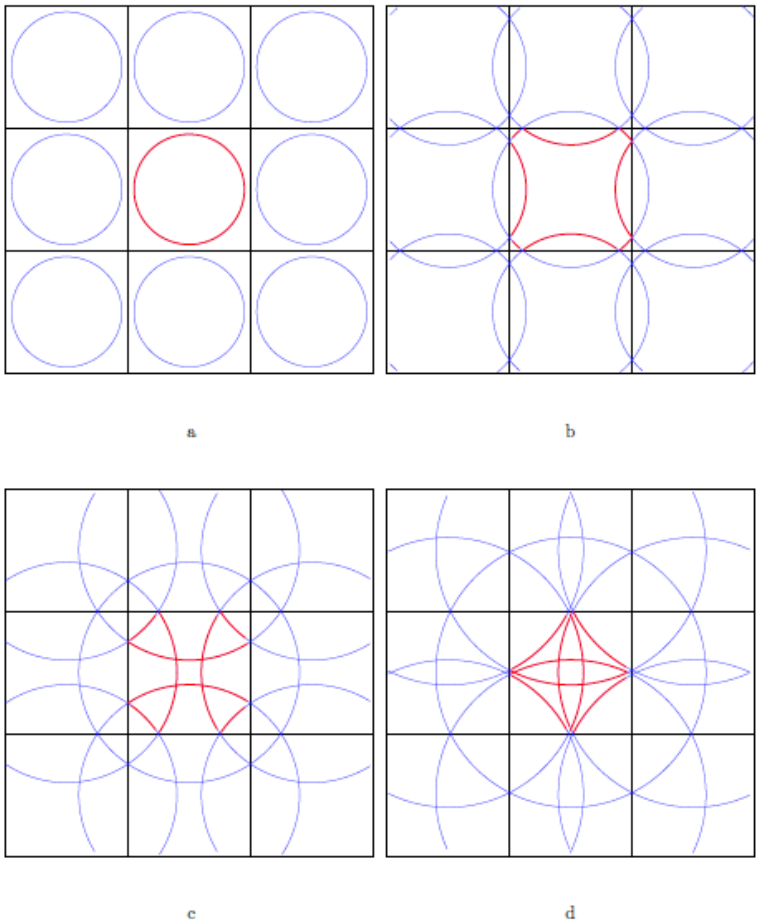
Repeated zone representation of the Fermi "surface"

- Small ϵ_F: each circle fully confined in its primitive cell; simple non-intersecting circles
- Larger ϵ_F (radius $> \pi/a$): circles overflow the cell and intersect; Fermi surface becomes complex
- Reduced zone representation: clip all circles inside the first BZ

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

Repeated zone representation of the Fermi "surface"



Repeated zone representation for four values of ε_F

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

Extended zone representation of the Fermi "surface"

- Reduced zone Fermi surface $\Longrightarrow$ intersection of the plane $\epsilon = \epsilon_F$ with the 2D dispersion relation surface $\epsilon(k_x, k_y)$
- Small ϵ_F: circle entirely inside the first BZ $\Longrightarrow$ only band 1 is partially occupied
- Larger ϵ_F: circle crosses BZ boundaries $\Longrightarrow$ multiple bands partially occupied $\Longrightarrow$ Fermi surface has multiple branches

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

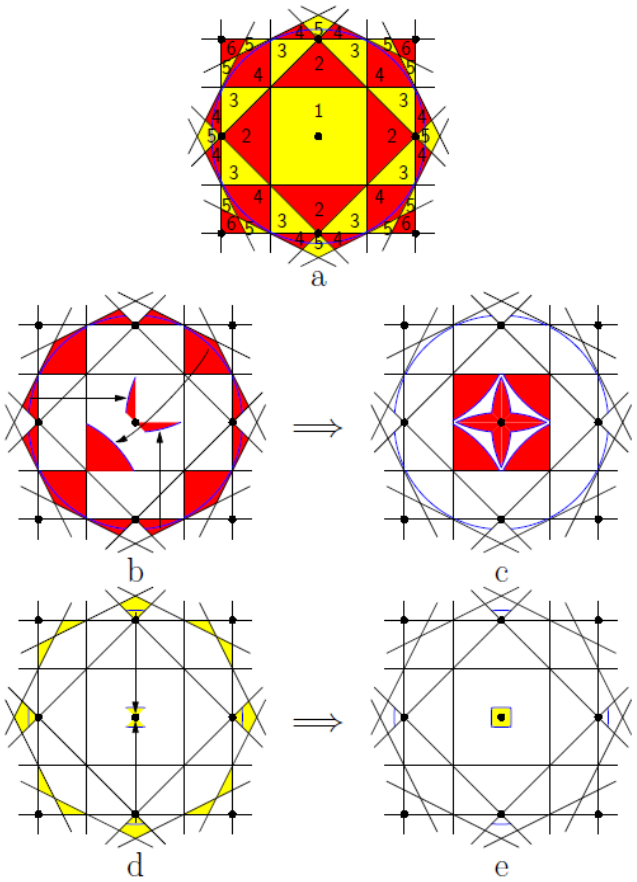
Extended zone representation of the Fermi "surface"

- How to identify the different branches:
  - Plot the single circle centered at the origin
  - Superimpose the grid of Brillouin zones
  - The portion of the circle in the i-th BZ is the branch of the Fermi surface from band i
- Example for $\varepsilon_F = \varepsilon_{F_4}$
  - Zones 1, 2, 3 fully inside the circle $\Rightarrow$ bands 1, 2, 3 are fully occupied
  - Circle crosses zones 4 and 5 $\Rightarrow$ bands 4 and 5 are partially occupied (Fermi surface has two branches)
  - To recover branches in the reduced zone: fold the portions of the circle in zones 4 and 5 back into the first BZ using $\mathcal{R}_\mu^*$ translations
  - Folded result coincides with the reduced zone representation
  - See `http://lampx.tugraz.at/~hadley/ss2/fermisurface/2d_fermisurface/2dsquare.php`

The Fermi surface and its representations

The Fermi surface for a 2D square Bravais lattice

Repeated zone representation of the Fermi "surface"



Branches of the Fermi surface for $\varepsilon_F = \varepsilon_{F_4}$

The Fermi surface and its representations

The Fermi surface for 3D systems

Generalization to 3D systems

- The 3D dispersion relation is a function of three independent variables (k_x, k_y, k_z): not directly representable
- The Fermi surface is defined implicitly by $\epsilon(\boldsymbol{k}) = \epsilon_F$: a surface in 3D k-space, still representable
- Each hyperparabola centred on a reciprocal lattice point $\boldsymbol{G}$ gives a *sphere* of radius $\sqrt{(2m/\hbar^2)\epsilon_F}$ centred on $\boldsymbol{G}$
  - Small ϵ_F: spheres confined within primitive cells; simple Fermi surface
  - Larger ϵ_F: spheres overflow their cells, intersect, and produce complex multi-sheet Fermi surfaces
  - Analysis proceeds exactly as in 2D: extended zone + BZ grid $\Rightarrow$ branch identification