Palestinian Advanced Physics School

Condensed Matter Physics

Professor David Tong

BIRZEIT UNIVERSITY

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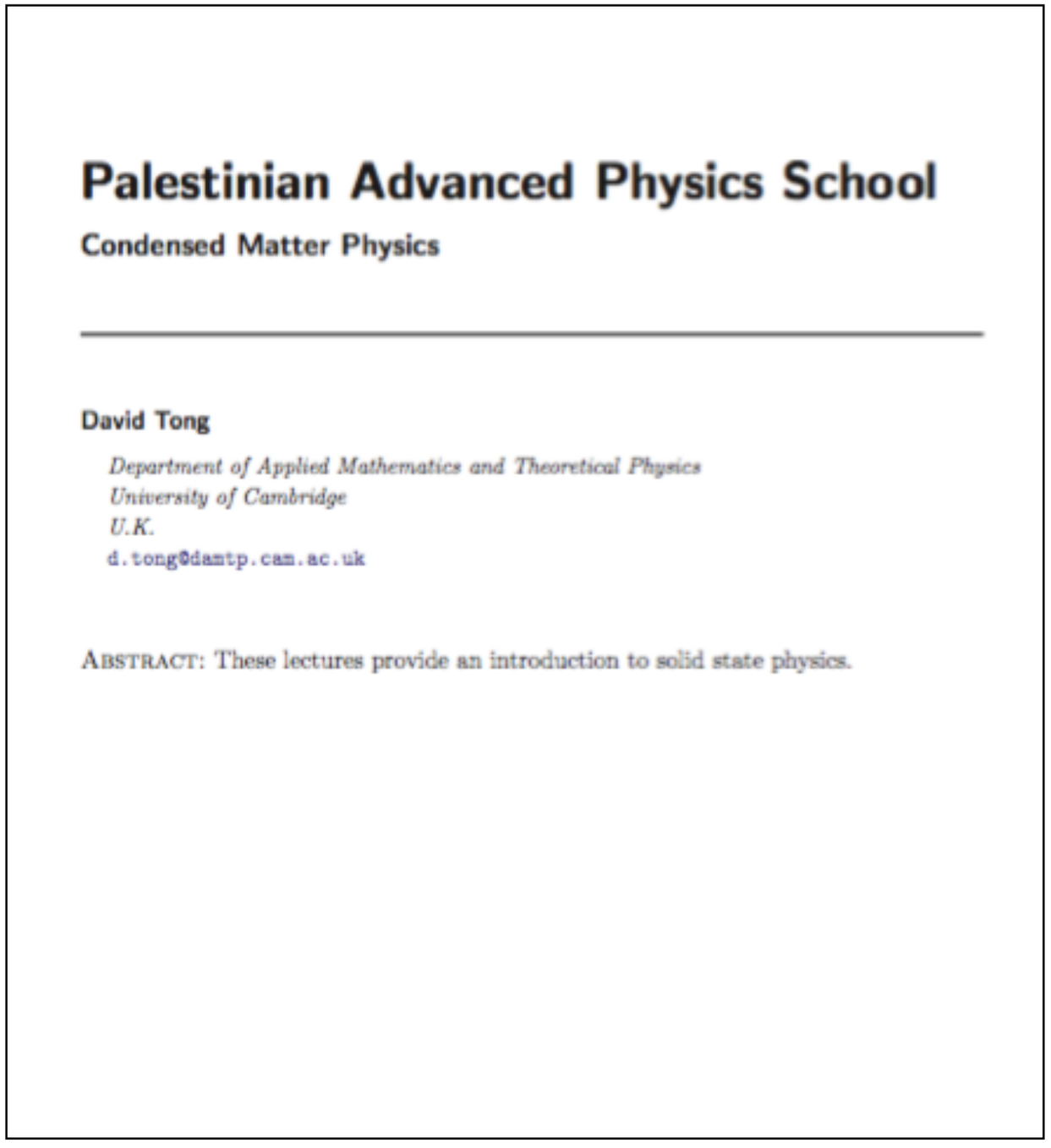
Lecture Notes on School Website



Palestinian Advanced Physics School

Condensed Matter Physics

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ABSTRACT: These lectures provide an introduction to solid state physics.

Condensed Matter Physics

Just solve this!

$$H = \sum_{j=1}^{N_e} \frac{\mathbf{p}_j^2}{2m} + \sum_{\alpha=1}^{N_i} \frac{\mathbf{P}_\alpha^2}{2M_\alpha} + \frac{e^2}{4\pi\epsilon_0}\left[\sum_{j\neq k} \frac{1}{|\mathbf{r}_j - \mathbf{r}_j|} - \sum_{j,\alpha} \frac{Z_\alpha}{|\mathbf{r}_j - \mathbf{R}_\alpha|} + \sum_{\alpha\neq\beta} \frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}\right]$$

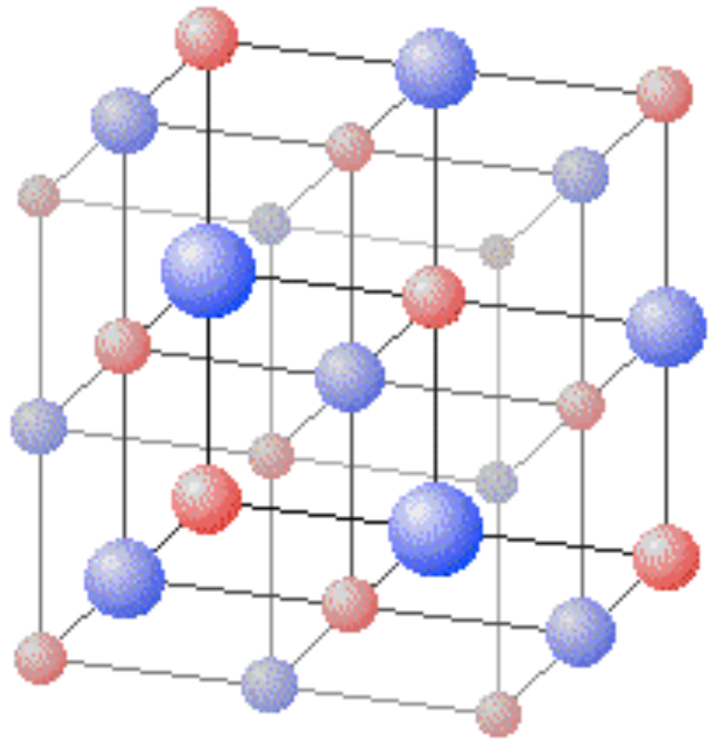
Electrons: mass m, charge –e, position r_j, momentum p_j

Ions: mass M_α, charge $+Z_\alpha e$, position R_α, momentum P_α

Lecture 1: Band Structure

Band Structure

Inside a solid, the ions are arranged on a lattice

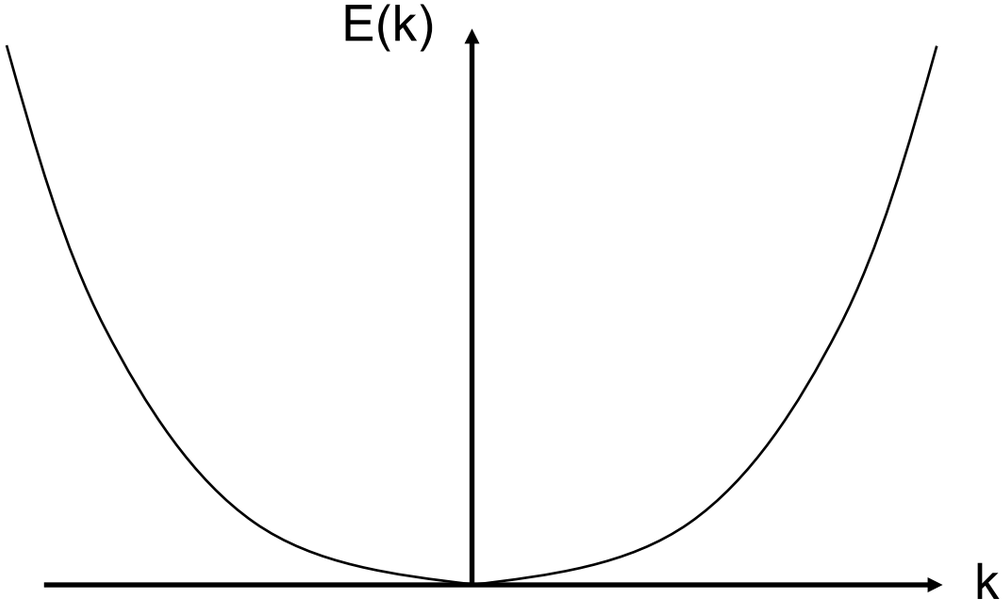


How does the electron move through this? How does its energy change?

Band Structure

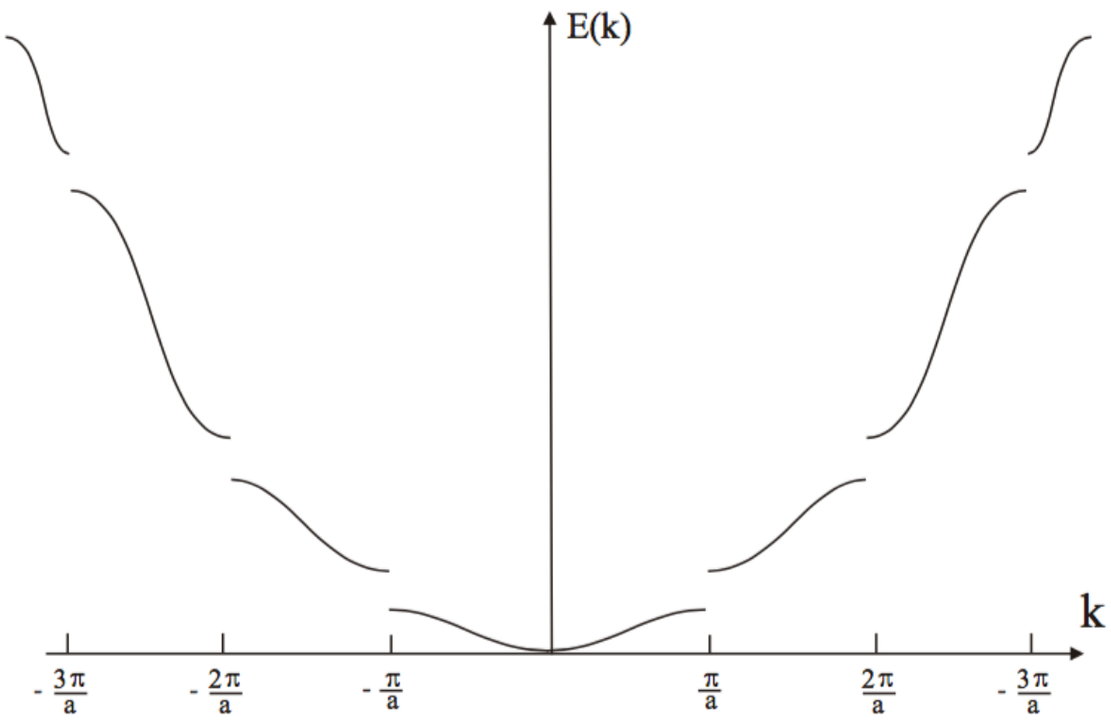
A particle moving in empty space has energy

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \qquad p = mv = \hbar k$$



Band Structure

A particle moving through a lattice has energy which is similar to empty space, but with gaps

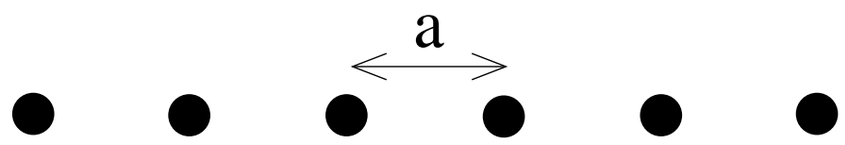


Plan for the Lecture

- Tight binding model
- Nearly free electron model

Tight Binding Model

Consider a one-dimensional lattice. Each atom is separated by distance *a*



One electron moves on this lattice. It can sit at any lattice site. When the electron sits on the n^{th} lattice site, we will denote its quantum state as:

$$|n\rangle$$

We take n=1,…,N and set $\langle n|m\rangle = \delta_{nm}$

We also make the chain of ions into a circle by imposing periodic boundary conditions

$$|N+1\rangle \equiv |1\rangle$$

Tight-Binding Model

We describe the electron by the tight-binding Hamiltonian

$$H = E_0 \sum_n |n\rangle\langle n| - t \sum_n \Big(|n\rangle\langle n+1| + |n+1\rangle\langle n| \Big)$$

t is called the “hopping parameter”

To get some intuition for this Hamiltonian, in a small time interval

$$|\psi\rangle \mapsto |\psi\rangle - \frac{i\Delta t}{\hbar} H|\psi\rangle + \mathcal{O}(\Delta t^2)$$

- The term proportional to E_0 leaves the electron alone
- The hopping term makes the electron move one place to the left or to the right

Tight-Binding Model

$$H = E_0 \sum_n |n\rangle\langle n| - t \sum_n \Big(|n\rangle\langle n+1| + |n+1\rangle\langle n| \Big)$$

We want to solve this. We want to find energy eigenstates that solve

$$H|\psi\rangle = E|\psi\rangle$$

A general state can be written as $|\psi\rangle = \sum_m \psi_m |m\rangle$. This gives us the equation

$$E_0 \sum_m \psi_m |m\rangle - t\Big(\sum_m \psi_{m+1}|m\rangle + \psi_m |m+1\rangle \Big) = E \sum_n \psi_m |m\rangle$$

If we take the overlap with a state $\langle n|$ we get a bunch of linear equations

$$\langle n|H|\psi\rangle = E\langle n|\psi\rangle \quad \Rightarrow \quad E_0\psi_n - t(\psi_{n+1} + \psi_{n-1}) = E\psi_n$$

Tight-Binding Model

Recap: a state $|\psi\rangle = \sum_m \psi_m |m\rangle$ is an energy eigenstate if

$$E_0\psi_n - t(\psi_{n+1} + \psi_{n-1}) = E\psi_n$$

This is solved by

$$\psi_n = e^{ikna}$$

This looks like a plane wave state $\psi(x) = e^{ikx}$ which has momentum $p = \hbar k$

But on the lattice, our state is the same if we shift $k \to k + 2\pi/a$

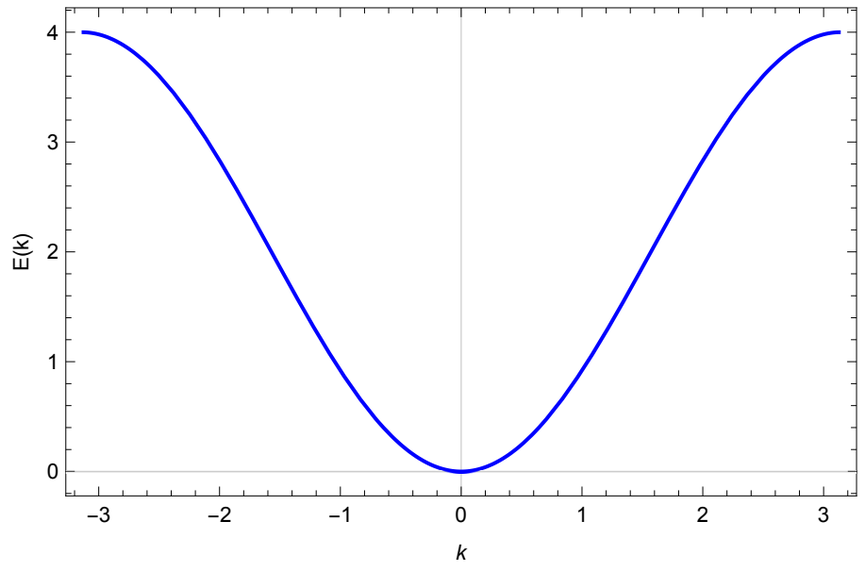
<u>Important lesson</u>: On a lattice, the momentum can only sit in the range $-\frac{\pi}{a} \leq k < \frac{\pi}{a}$

This range of momentum is called the *Brillouin zone*

Tight-Binding Model

The state with momentum *k* has energy

$$E(k) = E_0 - 2t\cos(ka)$$



Some comments:

- The electrons want to move! The eigenstates look like plane waves
- The energies lie in a *band*: $E_0 - 2t \leq E(k) \leq E_0 + 2t$
- For small momentum, $k \ll \pi/a$, we can Taylor expand

$$E(k) \approx (E_0 - 2t) + ta^2k^2$$

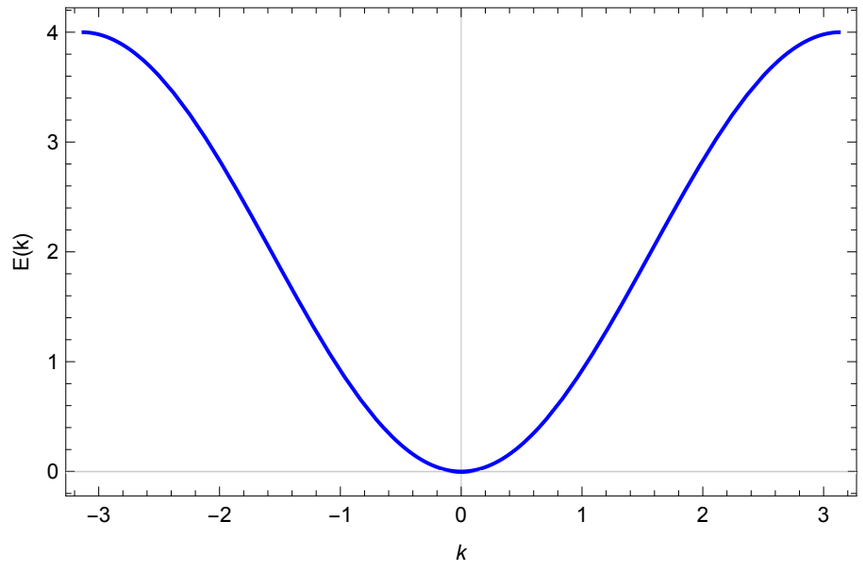
Up to the constant, this looks like a free particle $E_{\text{free}} = \dfrac{\hbar^2 k^2}{2m^\star}$ with effective mass

$$m^\star = \hbar^2/2ta^2$$

Tight-Binding Model

The state with momentum *k* has energy

$$E(k) = E_0 - 2t\cos(ka)$$



One more comment:

- How many quantum states do we have? To see this, we need to remember that the lattice is periodic, which means that

$$\psi_{N+1} = \psi_1 \qquad \Longrightarrow \qquad e^{ikNa} = 1$$

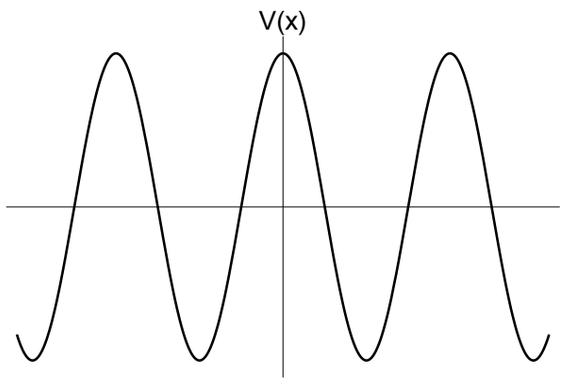
- For this to work, *k* must be quantised in units of $2\pi/aN$
- In the Brillouin zone $-\frac{\pi}{a} \leq k < \frac{\pi}{a}$ we have *N* different quantum states
- This is the same number that we started with!

Nearly Free Electron Model

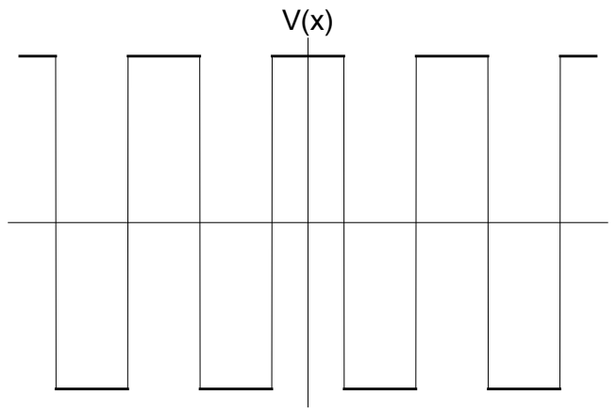
Here's a completely different way to think about electrons moving in a lattice. The electron can move anywhere along a line, but feels a periodic potential *V(x)*

$$H = \frac{p^2}{2m} + V(x) \qquad \text{with} \qquad p = -i\hbar\frac{d}{dx} \qquad \text{and} \qquad V(x+a) = V(x)$$

The potential can have any shape. e.g



or



We again put the particle on a circle of length *L* such that $\frac{L}{a} = N \in \mathbf{Z}$

Nearly Free Electron Model

$$H = \frac{p^2}{2m} + V(x)$$

When the potential vanishes, the energy eigenstates $\left|k\right\rangle$ are plane waves

$$\psi_k(x) = \langle x|k\rangle = \frac{1}{\sqrt{L}} e^{ikx} \qquad \text{with energy} \qquad E_0(k) = \frac{\hbar^2 k^2}{2m}$$

These are orthonormal: $$\langle k|k'\rangle = \frac{1}{L}\int dx\ e^{i(k'-k)x} = \delta_{k,k'}$$

We will treat the potential *V(x)* using perturbation theory. Except the two states $\left|k\right\rangle$ and $\left|-k\right\rangle$ have the same energy. We must use *degenerate* perturbation theory!

Nearly Free Electron Model

Claim: When the momentum is $k = \dfrac{\pi n}{a}$, with *n* an integer, the potential will scatter the state +*k* state to the –*k* state. Note that this first happens at the edge of the Brillouin zone, $k = \pi/a$

Proof: Consider the two states $|k\rangle$ and $|k'\rangle = |-k\rangle$. To do perturbation theory, we should compute

$$\langle k|V|k'\rangle$$

Because the potential is periodic, we can Fourier transform

$$V(x) = \sum_{n\in\mathbf{Z}} V_n\, e^{2\pi i n x/a} \quad \Longleftrightarrow \quad V_n = \frac{1}{a}\int_0^a dx\; V(x)\, e^{-2\pi i n x/a}$$

Using this, the matrix elements are given by

$$\langle k|V|k'\rangle = \frac{1}{L}\int dx\; \sum_{n\in\mathbf{Z}} V_n\, e^{i(k'-k+2\pi n/a)x} = \sum_{n\in\mathbf{Z}} V_n\, \delta_{k-k',2\pi n/a}$$

This is non-zero only when $k = k' + \dfrac{2\pi n}{a} \quad \Longrightarrow \quad k = \dfrac{\pi n}{a}$

Nearly Free Electron Model

The potential can scatter the particle only when it has momentum $k = \dfrac{\pi n}{a}$.

The energy eigenstates will be some linear combination $\alpha|k\rangle + \beta|k'\rangle$. To figure this out, we diagonalise the matrix

$$\begin{pmatrix} \langle k|H|k\rangle & \langle k|H|k'\rangle \\ \langle k'|H|k\rangle & \langle k'|H|k'\rangle \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \Longrightarrow \quad \begin{pmatrix} E_0(k) + V_0 & V_n \\ V_n^\star & E_0(k') + V_0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Eigenvalues are given by

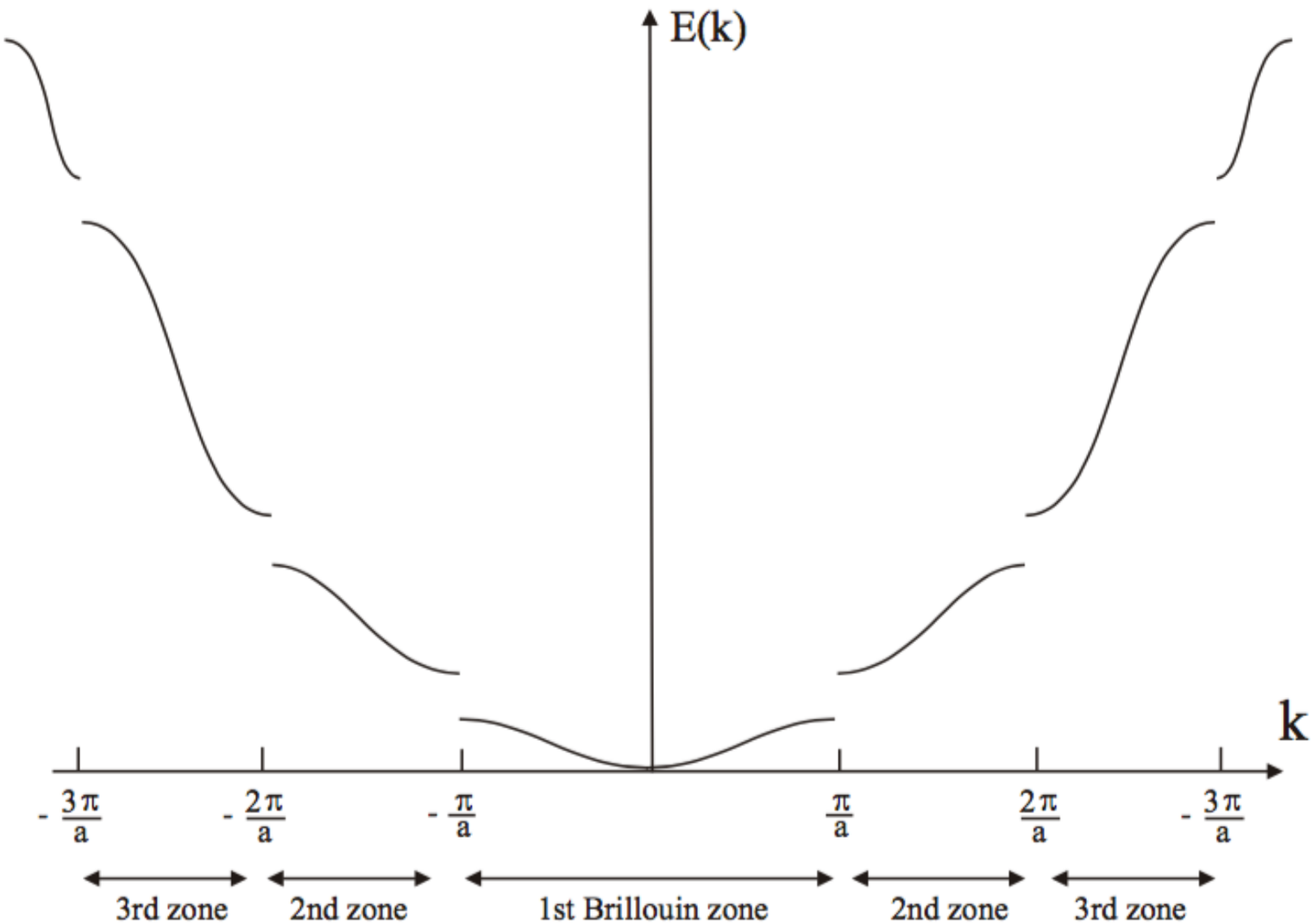
$$(E_0(k) + V_0 - E)^2 - |V_n|^2 = 0 \quad \Longrightarrow \quad E = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2} + V_0 \pm |V_n|$$

$$k = \frac{\pi n}{a}$$

A gap opens up at these values of the momenta

Nearly Free Electron Model

The energy shows a *band structure*

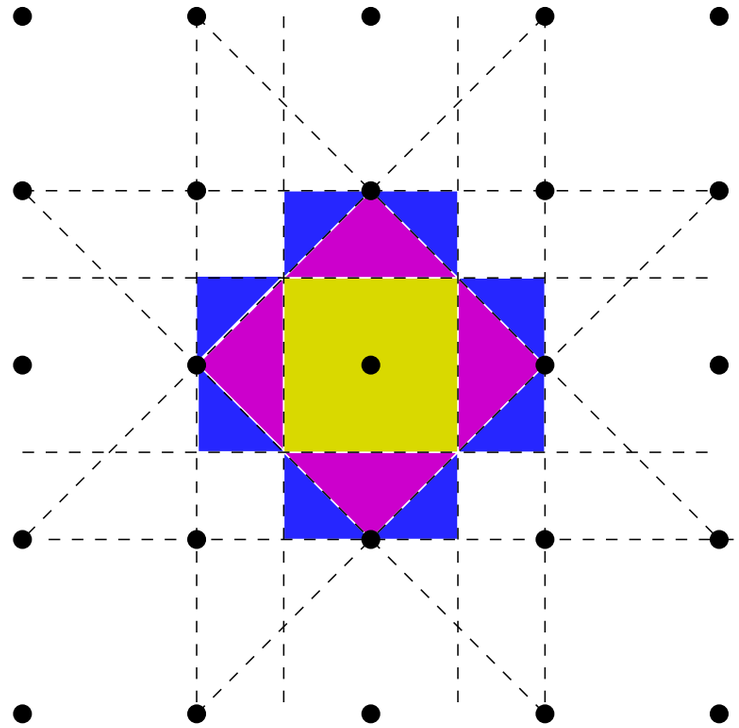


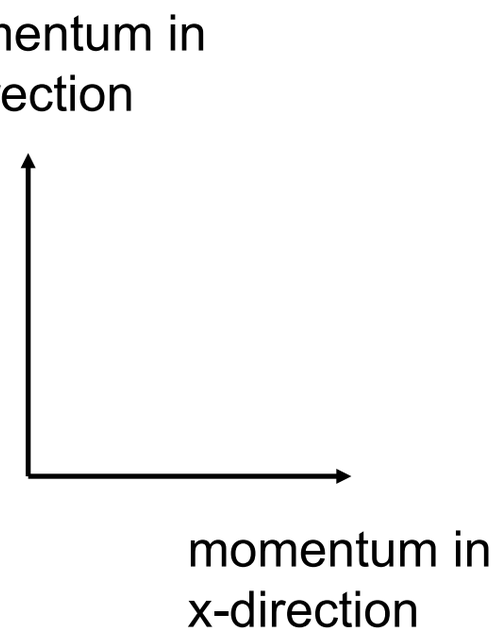
There are gaps in the energy as you go from one Brillouin zone to the next.

Other Lattices

In 2d and 3d there are many different possible lattices. Each lattice has an associated *Brillouin zone,* which is a region of momentum space

e.g. 2d square lattice:

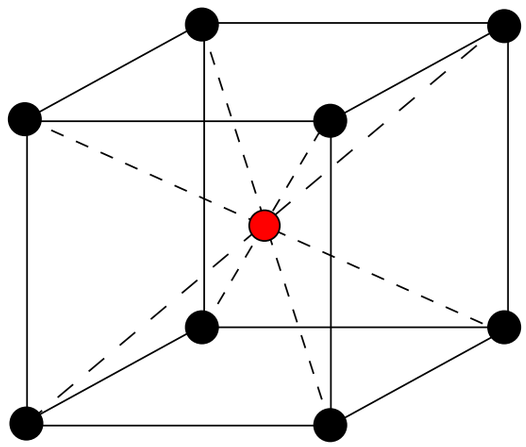




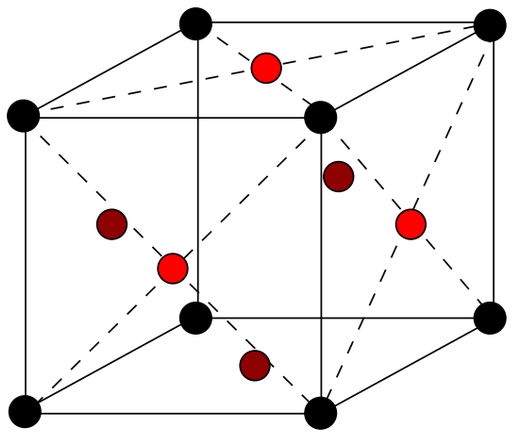
The energy of an electron is fixed by the momentum **k**, but with gaps in the spectrum when you cross the boundary of a Brillouin zone.

Other Lattices

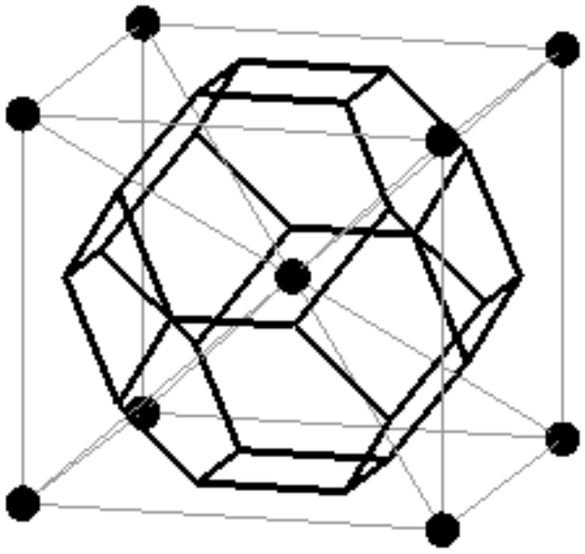
BCC



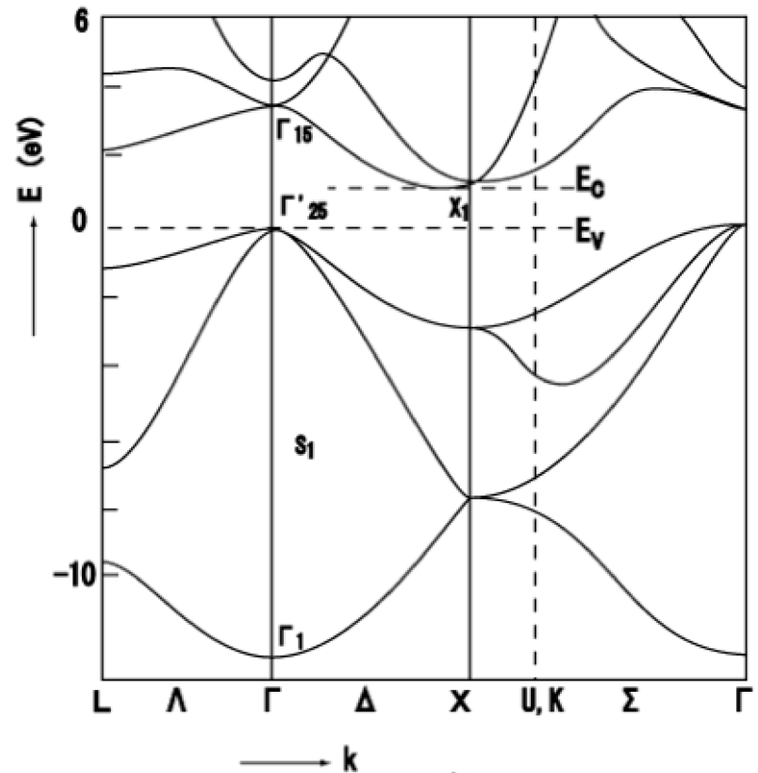
FCC



The Brillouin zone for BCC



What an energy spectrum really looks like!



Silicon