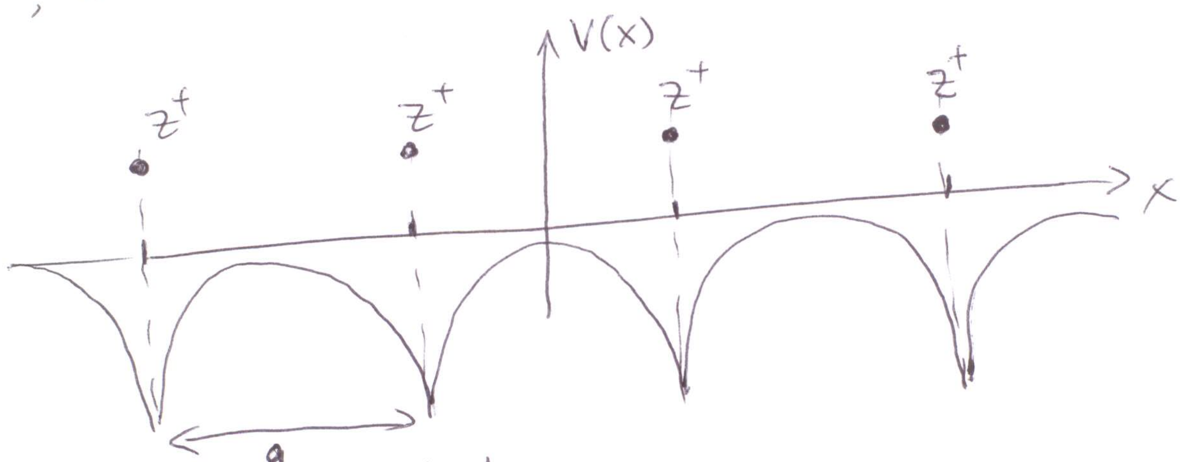
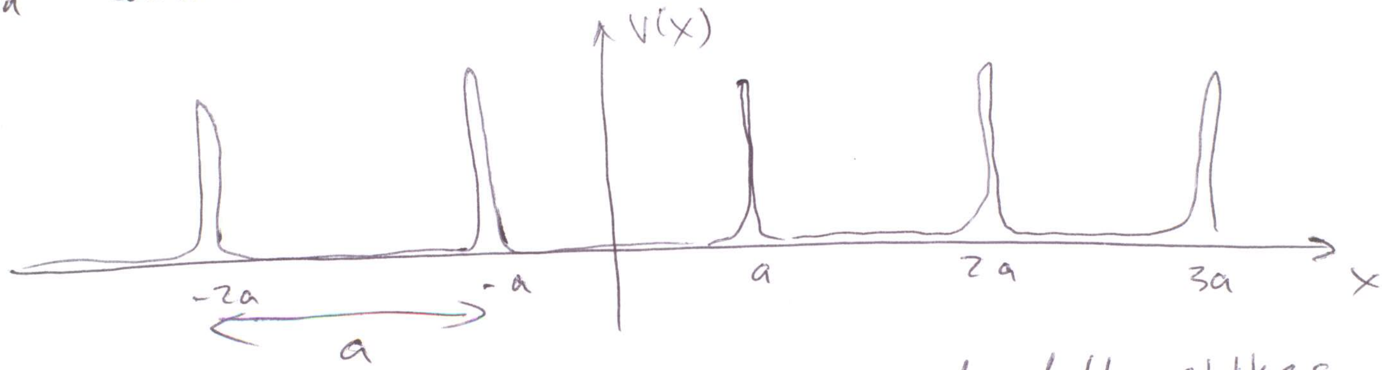
Periodic potentials and band structure

So far we studied cases when the potential is localized within a certain region of space. An electron moving in the field of a nucleus fits into this picture. However in physics we often encounter another importan class of problems — when a particle moves in a periodic (in space) potential, such as a crystal lattice. It is very instructive to see what a periodic potential does with energy levels.

For simplicity (we are only interested in the qualitative picture here) we will consider a 1D system. Say, a lattice of positive ions looks as follows:



In fact, we can simplify the potential even more and consider a one-dimensional Dirac comb,



which is a sum of evenly spaced delta spikes.

$$V(x) = \alpha \sum_j \delta(x - ja)$$

The spikes are made positive to avoid dealing with positive and negative energy solutions. The sign of the spikes actually does not make any qualitative difference.

The above potential is periodic, i.e.

$$V(x+a) = V(x)$$

It can be shown that for such a periodic potential the solutions to the Schrödinger equation satisfy the condition

$$\psi(x+a) = e^{iKa}\psi(x)$$

where K is some constant (independent of x) called crystal wave vector. This constitutes the so called Bloch theorem and $e^{ika}\psi(x)$ is called the Bloch wave.

Let $\hat{T}$ be the translation operator:

$$\hat{T}_a f(x) = f(x+a)$$

For a periodic potential $\hat{T}$ commutes with the Hamiltonian:

$$[\hat{T}_a, \hat{H}] = 0$$

(this is obvious because T_a does not change $\hat{H}$ when it acts on it)

Hence we can choose eigenfunctions of $\hat{H}$ in such a way that they are simultaneously eigenfunctions of $\hat{T}_a$:

$$T_a\psi = \lambda\psi, \text{ or } \psi(x+a) = \lambda\psi(x)$$

where λ is not zero (that would result in $\psi(x)=0$ for all x, which is physically meaningless) and can be represented as $\lambda = e^{iKa}$

We will see in a moment that K is actually real.

As we deal with $N \approx 10^{23}$ lattice sites we just might impose the condition

$$\psi(x+Na) = \psi(x)$$

which hardly changes anything, yet makes things more straightforward. Then

$$e^{iNka}\psi(x) = \psi(x) \quad \Rightarrow \quad e^{iNka} = 1 \quad \Rightarrow \quad Nka = 2\pi n$$

and $\quad k = \dfrac{2\pi n}{Na} \qquad n = 0, \pm 1, \pm 2, \dots$

Here k comes out real. We actually need to solve the Schrödinger equation within a single lattice period $(0 \leq x \leq a)$ only. Recursive application of

$$\psi(x+a) = e^{ika}\psi(x)$$

generates the solution everywhere else.

In the region $0 < x < a$ our potential is zero, so the Schrödinge equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad \text{or} \qquad \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

the general solution is

$$\psi(x) = A\sin kx + B\cos kx \qquad (0 < x < a)$$

According to the Bloch theorem

$$\psi(x) = e^{-ika}\psi(x+a) = e^{-ika}\left[A\sin k(x+a) + B\cos k(x+a)\right] \quad -a < x < 0$$

At $x = 0$ ψ must be continuous, so

$$B = e^{-ika}\left[A\sin ka + B\cos ka\right]$$

The derivative of ψ has discontinuity proportional to the strength of the delta function, which, if we recall it, follows from integrating the SE from $-\epsilon$ to $+\epsilon$:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}\,dx+\int_{-\epsilon}V(x)\,\psi(x)\,dx=E\int_{-\epsilon}\psi(x)\,dx \qquad \epsilon\to 0$$

$$\left.\frac{d\psi}{dx}\right|_{+\epsilon}-\left.\frac{d\psi}{dx}\right|_{-\epsilon}=\frac{2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon}V(x)\,\psi(x)\,dx$$

$$\psi'(+\epsilon)-\psi'(-\epsilon)=\frac{2m\alpha}{\hbar^2}\psi(0)$$

In our case

$$kA-e^{-ika}k\left[A\cos ka-B\sin ka\right]=\frac{2m\alpha}{\hbar^2}B$$

Now, substituting $A\sin ka=\left[e^{ika}-\cos ka\right]B$ into the last equation and cancelling kB yields

$$\left[e^{ika}-\cos ka\right]\left[1-e^{-ika}\cos ka\right]+e^{-ika}\sin^2 ka=\frac{2m\alpha}{\hbar^2 k}\sin ka$$

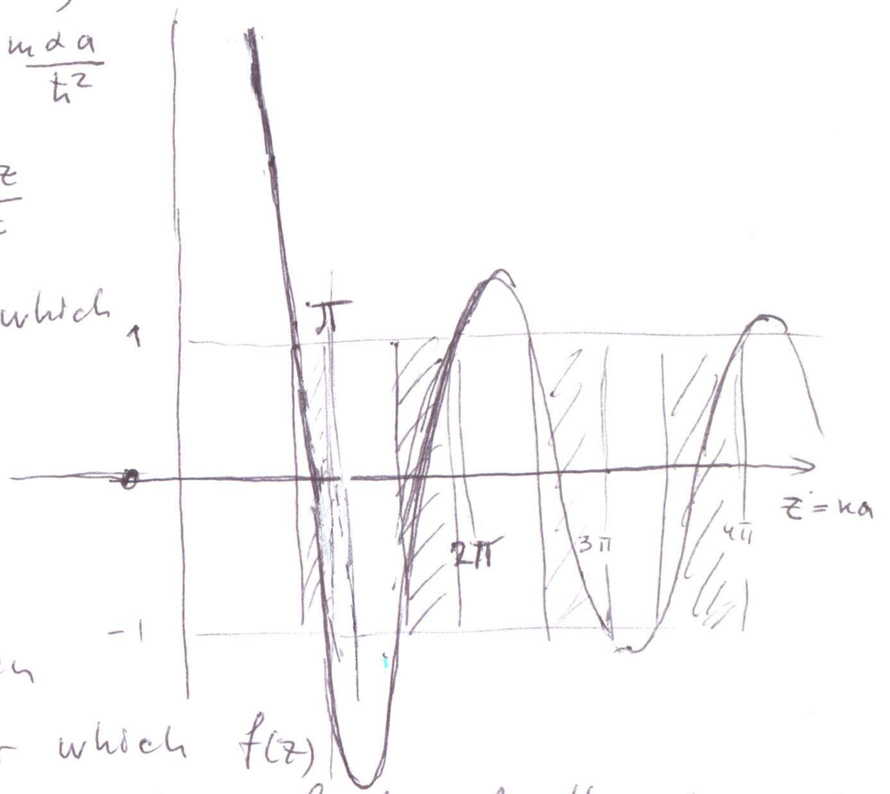
or

$$\cos Ka=\cos ka+\frac{m\alpha}{\hbar^2 k}\sin ka$$

The above formula determines possible values of k (and, thus energy). To simplify notations let us assume that

$$z\equiv ka \qquad \beta\equiv\frac{m\alpha a}{\hbar^2}$$

$$f(z)\equiv\cos(z)+\beta\frac{\sin z}{z}$$

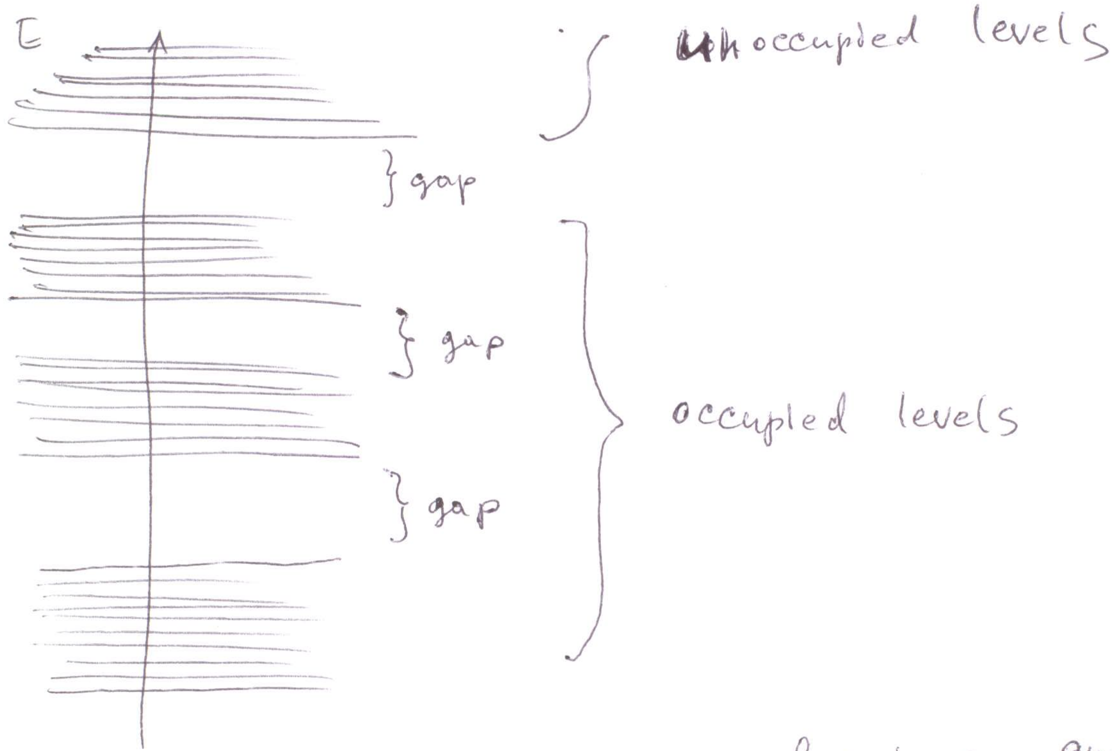


for those z values for which $f(z)$ stays outside of range $[-1,+1]$ the solutions do not exist. Thus the corresponding $z=ka$ range is forbidden.

The intervals of z for which $f(z)$ is within $[-1,+1]$ range we have bands of allowed energies

Within a given band pretty much any energy value is possible since $Ka = \frac{2\pi n}{N}$ $N \approx 10^{23}$ and $\cos Ka$ runs essentially over a continuous range

If we now imagine that we have $N \approx 10^{23}$ electrons (noninteracting) in this lattice they will fill those closely spaced energy levels till a certain point between the valence and conduction bands:



This is because electrons are fermions and cannot be placed into the same states.