

Comments about TEST1: From Chapter 4 + HW 14 problem 4.35:

$\uparrow\uparrow$

$\uparrow\downarrow$

$\downarrow\uparrow$

$\downarrow\downarrow$

$2^2=4$ states

$\uparrow\uparrow$

$$\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$$

$\downarrow\downarrow$

$$\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

The 4 states are grouped as $S=1$ (3 states) and $S=0$ (1 state)

$\uparrow\uparrow\uparrow$

$\uparrow\uparrow\downarrow, \uparrow\downarrow\uparrow, \downarrow\uparrow\uparrow$

$\uparrow\downarrow\downarrow, \downarrow\uparrow\downarrow, \downarrow\downarrow\uparrow$

$\downarrow\downarrow\downarrow$

$2^3=8$
states

The first and second electrons are grouped into triplet and singlet: $S=1$ and 0 .

The third electron remains $1/2$.

Then you group 1 and $1/2$ giving $3/2$ (4 states) and $1/2$ (2 states).

And then 0 and $1/2$ gives $1/2$ (2 states).

Problem 5, Test 1: 4 electrons

$2^4 = 16$
states

↑↑↑↑

↓↑↑↑, ↑↓↑↑, ↑↑↓↑, ↑↑↑↓

↓↑↓↑, ↑↑↓↓, ↑↓↓↑,

↓↓↑↑, ↑↓↑↓, ↓↑↑↓

↑↓↓↓, ↓↑↓↓, ↓↓↑↓, ↓↓↓↑

↓↓↓↓

If this was your answer you received ~2/8 points depending on whether it was the complete 16 or not. Check!

The **first and second** electrons are grouped into triplet and singlet: $S=1$ and 0 .
The **third and fourth** electrons are grouped into triplet and singlet: $S=1$ and 0 .

Then, you must combine
 1 with $1 \rightarrow$ Total = $2, 1, 0$
 1 with $0 \rightarrow$ Total = 1
 0 with $1 \rightarrow$ Total = 1
 0 with $0 \rightarrow$ Total = 0

$S=2 \rightarrow 5$ states

$S=1 \rightarrow 3$ states

$S=1 \rightarrow 3$ states

$S=1 \rightarrow 3$ states

$S=0 \rightarrow 1$ state

$S=0 \rightarrow 1$ state

} $2^4 = 16$
states

How do we find the TOTAL energy of the system? We have to integrate in k . For this purpose use spherical symmetry and infinitesimal shells.

Vol. of a shell (octant; $4\pi/8=\pi/2$)

$$\frac{2[(1/2)\pi k^2 dk]}{(\pi^3/V)} = \frac{V}{\pi^2} k^2 dk$$

2 electrons per point

Vol. of one elementary block

$$dE = \frac{\hbar^2 k^2}{2m} \frac{V}{\pi^2} k^2 dk$$

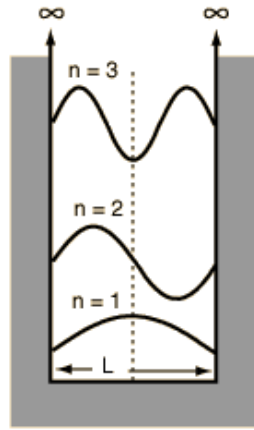
Energy at the shell

Number of states per shell

$$E_{\text{tot}} = \frac{\hbar^2 V}{2\pi^2 m} \int_0^{k_F} k^4 dk = \frac{\hbar^2 k_F^5 V}{10\pi^2 m} = \frac{\hbar^2 (3\pi^2 Nq)^{5/3}}{10\pi^2 m} V^{-2/3}$$

$$k_F = (3\rho\pi^2)^{1/3}$$

1D illustration for simplicity



x = 0 at left wall of box.

As we move up in the well, the energy and momentum grows and the electron hits harder and harder the wall.

Similar to molecules hitting the walls in a perfect gas, but this happens in QM even at zero temperature!

Thus, the electrons exert a pressure on the walls.

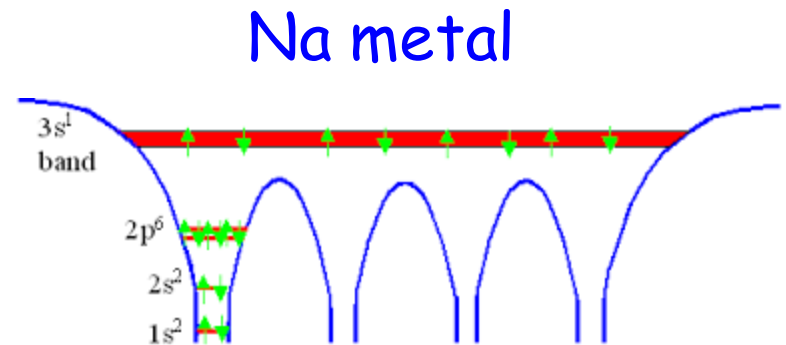
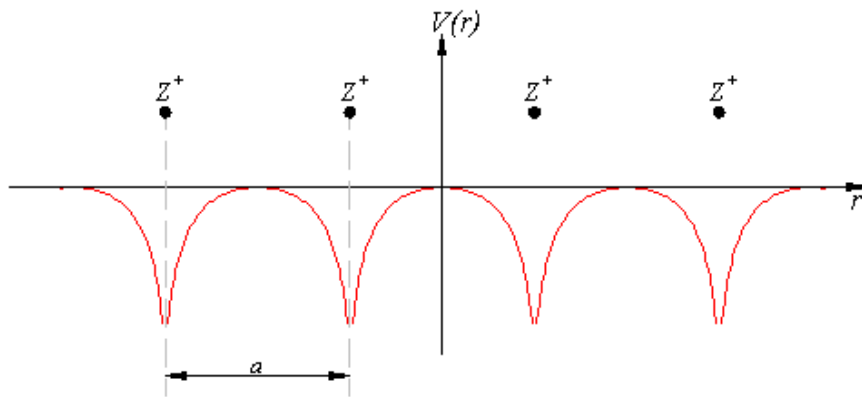
$$dE_{\text{tot}} = -\frac{2}{3} \frac{\hbar^2 (3\pi^2 Nq)^{5/3}}{10\pi^2 m} V^{-5/3} dV = -\frac{2}{3} E_{\text{tot}} \frac{dV}{V}$$

$$P = \frac{2}{3} \frac{E_{\text{tot}}}{V} = \frac{2}{3} \frac{\hbar^2 k_F^5}{10\pi^2 m} = \frac{(3\pi^2)^{2/3} \hbar^2}{5m} \rho^{5/3}$$

5.3.2 Band Structure

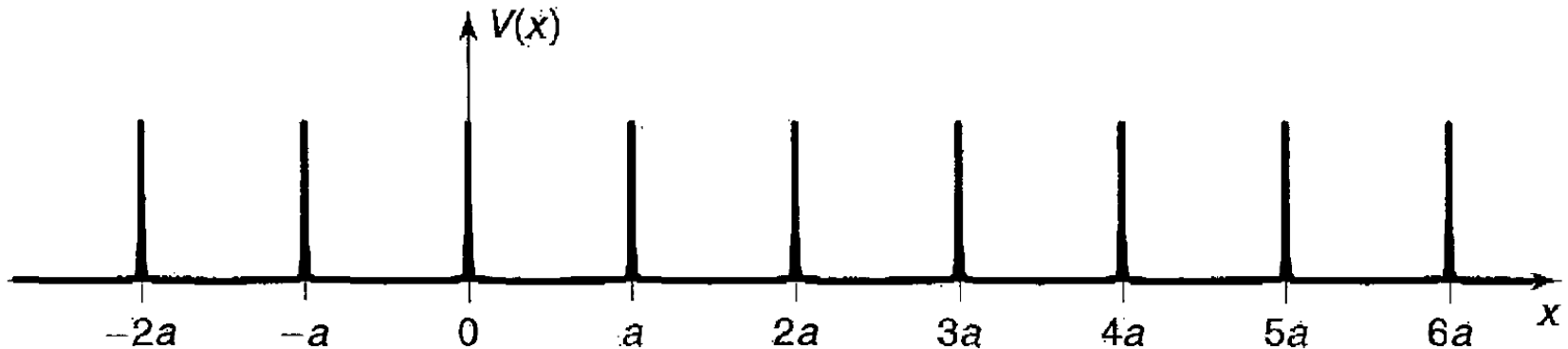
This is an improvement on the free electron gas.

We will consider the same set of Nq electrons but now in a **periodically arranged positive charge potential**, assumed rigid, that mimics the nuclei.



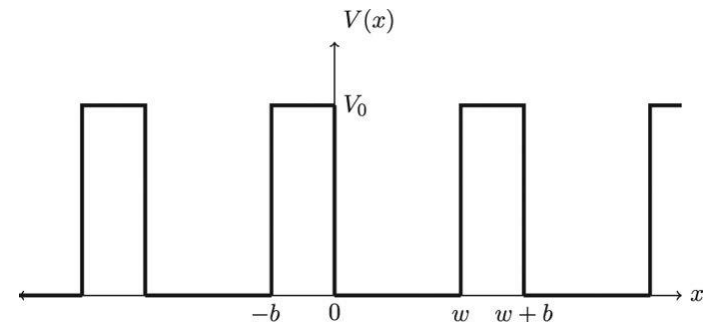
Qualitatively, the new key property is the **periodicity**, not the details of the potential used.

Because the periodicity is the key aspect, the book uses a 1D "Dirac comb" as example.



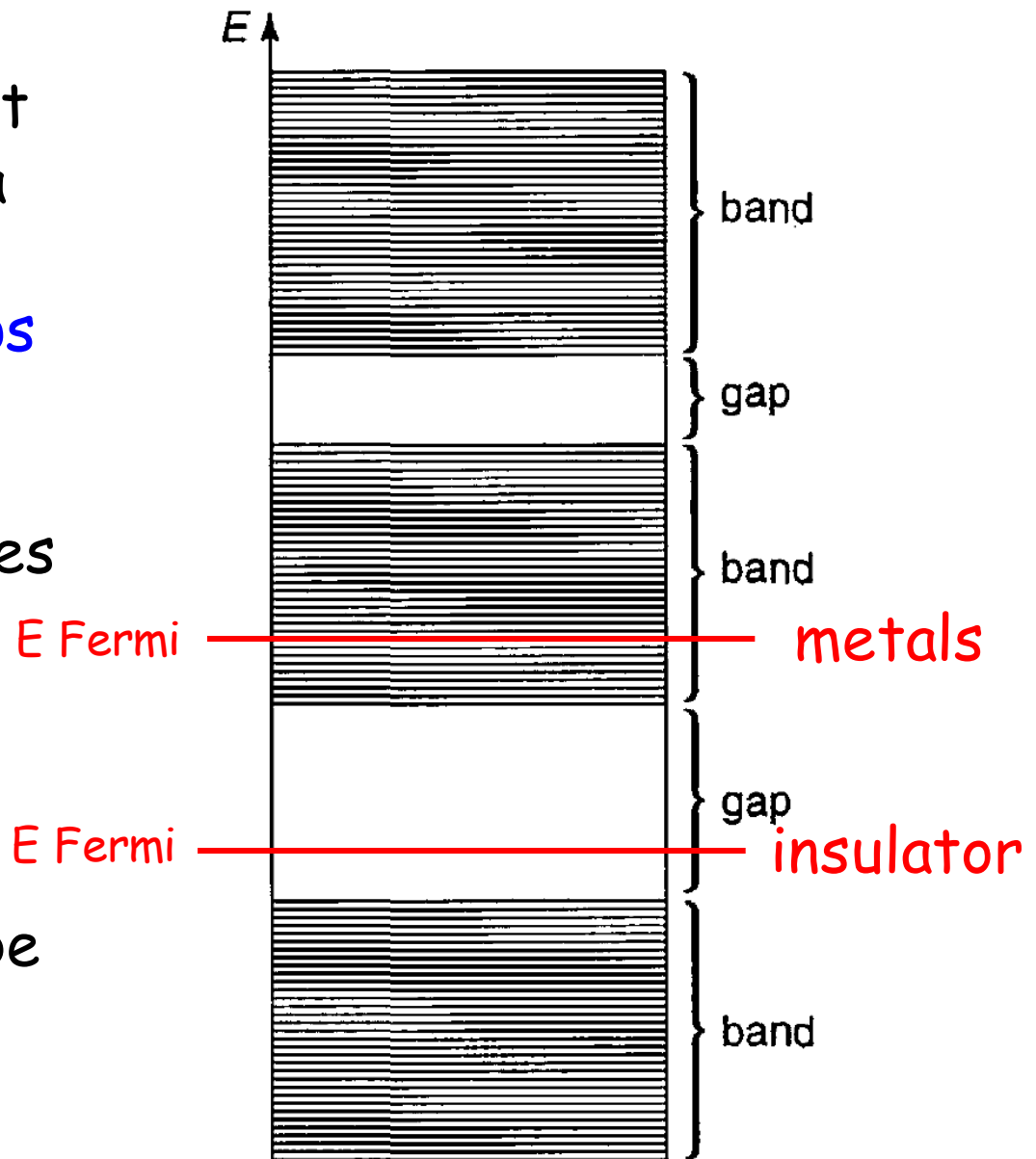
It is a periodic **positive** potential for **simplicity** to avoid the bound states that make more difficult the math.

Alternatively, think of the space in between the deltas as the "nuclei" potential



The remarkable result we will find by using a periodic potential is that there will be **gaps** (no solutions in some energy ranges) in between allowed states bands.

This physics cannot be found with just the free electron gap approximation.



The key aspect to emphasize is the periodicity:

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

Sch Eq same as usual:
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

For a periodic potential, we will prove the **Bloch's theorem**:

Consider the displacement operator D . It takes any function or operator and changes x to $x+a$:

$$Df(x) = f(x + a)$$

$$D \frac{d}{dx} = \frac{d}{d(x+a)} = \frac{d x}{d(x+a)} \frac{d}{dx} = \frac{d}{dx}$$

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

if periodic

Then $[D, H] = 0$ and the eigenfunctions can also be eigenfunctions of D : $D\psi = \lambda\psi$ i.e. $\psi(x+a) = \lambda\psi(x)$

So far this seems "trivial": naively for a periodic potential, the solutions of the Sch Eq should be periodic. However, "physics" tells us that actually it is the probability that should be periodic, not the wave functions:

$$|\psi(x+a)|^2 = |\psi(x)|^2$$

The statement $\psi(x+a) = \lambda\psi(x)$ considering the only constraint $|\psi(x+a)|^2 = |\psi(x)|^2$ becomes less trivial and gives:

$$\lambda = e^{iKa}$$

Thus, the Bloch's theorem says:

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

So the wave functions are more complicated than the probabilities ...

What is the value of K ? For this purpose I have to use another common trick: **periodic boundary conditions**.

Instead of a very long line of length $\sim Na$ with $N \sim 10^{23}$ we will use a **circle** with the same perimeter. The physics cannot depend on this boundary effect.

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

This trick fixes the value of K because

$$\psi(x + a) = e^{iKa} \psi(x) \quad \longrightarrow \quad \psi(x + \underbrace{a}_{\substack{\uparrow \\ N}}) = e^{iKa} \psi(x) = \psi(x).$$

$$e^{iNKa} \psi(x) = \psi(x)$$

If $e^{iNKa}\psi(x) = \psi(x)$, then $e^{iNKa} = 1$ i.e. $NKa = 2\pi n$.

$$K = \frac{2\pi n}{Na}, \quad (n = 0, \pm 1, \pm 2, \dots).$$

This theorem is independent of the "Dirac comb" we will use. **It is valid for any periodic potential.** The value is that you solve in the range $0 < x < a$, and then simply repeat the solution with different values of K .