In the Dirac comb, in between the delta functions the potential is V(x)=0, and the solutions are simple:

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

Because we know the solution in the range 0<x<a, then we know it everywhere, according to Bloch's theorem:

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

This gives the wave function in the "right" cell, if I have the wave function in the "left" cell. Sometimes I have the wave function in the "right" cell, and I want the wave function in the "left cell": $\psi(x) = e^{-iKa}\psi(x+a)$.

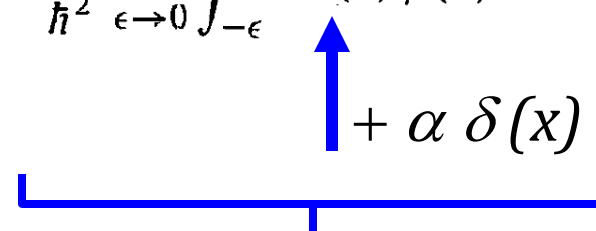$$\psi(x) = e^{-iKa}[A \sin k(x + a) + B \cos k(x + a)], \quad (-a < x < 0)$$

$$\psi(x + a)$$

To fix A and B, as with the delta function potential in QM411, we will use:

(1) the wave function has to be continuous at x=0.
(2) the first derivative cannot be continuous for a delta function, but its discontinuity we know how to calculate.

Reminder: see page 84 of the book:

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

$$\Delta\left(\frac{d\psi}{dx}\right) \equiv \lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}\bigg|_{+\epsilon} - \frac{d\psi}{dx}\bigg|_{-\epsilon}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)\,dx$$

$$+\,\alpha\,\delta(x)$$

$$=\frac{2m\alpha}{\hbar^2}\psi(0)$$

(1) Continuity at x=0 requires that wave function

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

at x=0, i.e. $\psi(x=0) = B$, be equal to

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

at x=0, which is $\psi(x=0) = e^{-iKa}[A\sin(ka) + B\cos(ka)]$

Thus, the first equation is:

$$B = e^{-iKa}[A\sin(ka) + B\cos(ka)]$$

3

(2) The derivative of each of the two wave functions can be easily calculated and then specialized for x=0.

$$kA - e^{-iKa}k[A\cos(ka) - B\sin(ka)] = \frac{2m\alpha}{\hbar^2}B$$

$$\lim_{\epsilon \to 0}\left(\frac{d\psi}{dx}\bigg|_{+\epsilon} - \frac{d\psi}{dx}\bigg|_{-\epsilon}\right) = \frac{2m\alpha}{\hbar^2}\psi(0)$$

So we have the two equations for A and B, easy to solve. There is no "independent" term i.e. each term has either A or B in front. Then a condition must be satisfied:

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

Introducing: $z \equiv ka,$ and $\beta \equiv \dfrac{m\alpha a}{\hbar^2}$
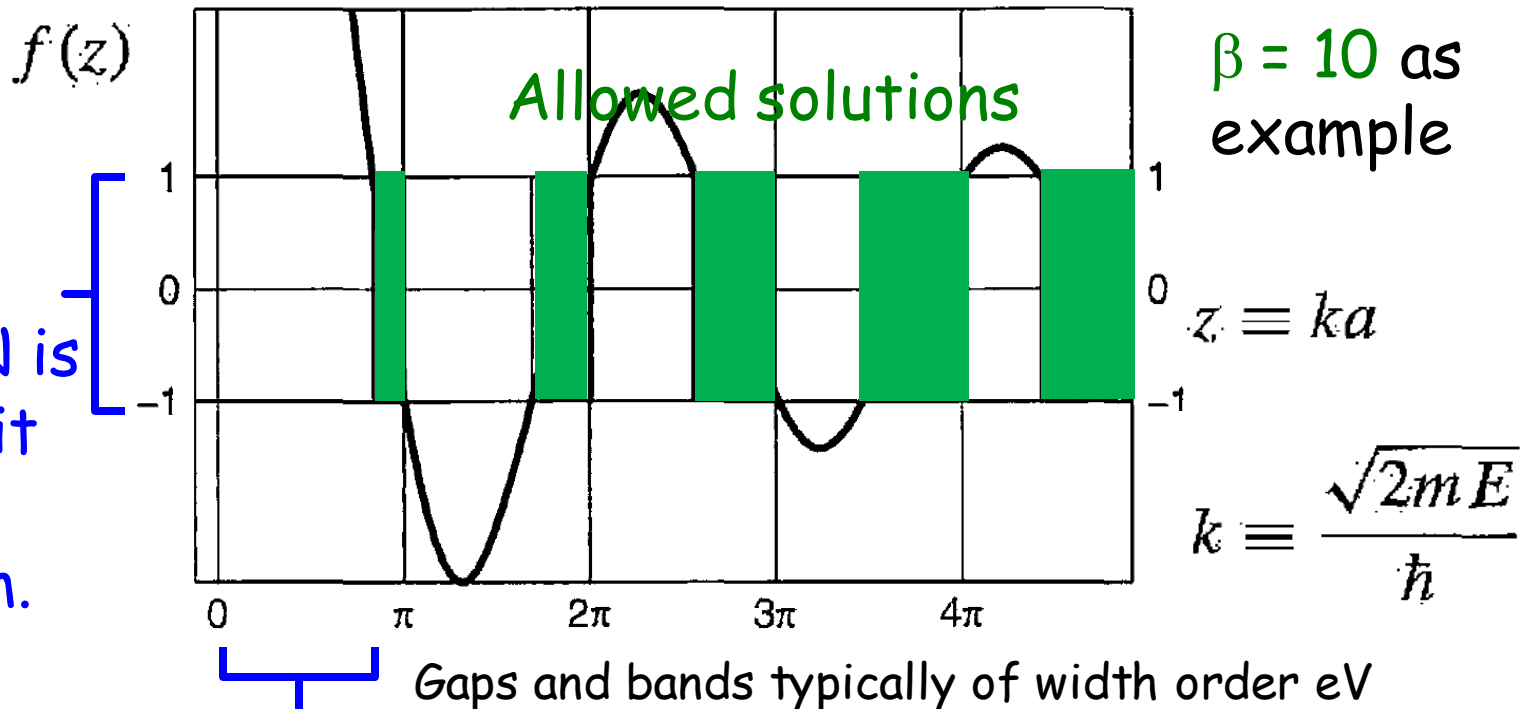
then we arrive to:

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

Bounded between -1 and 1   Unbounded

Allowed solutions β = 10 as example

Range of cos(Ka). Ka=2πn/N is so dense it forms a continuum.

$z \equiv ka$

$k \equiv \dfrac{\sqrt{2mE}}{\hbar}$

Gaps and bands typically of width order eV

5

Repeating: $Ka = 2\pi n/N$ is so dense it forms almost a continuum.

E

N states

N states

N states
(degenerate by pairs see HW18 problem, so N/2 actual lines at large N)

band

gap

band

gap
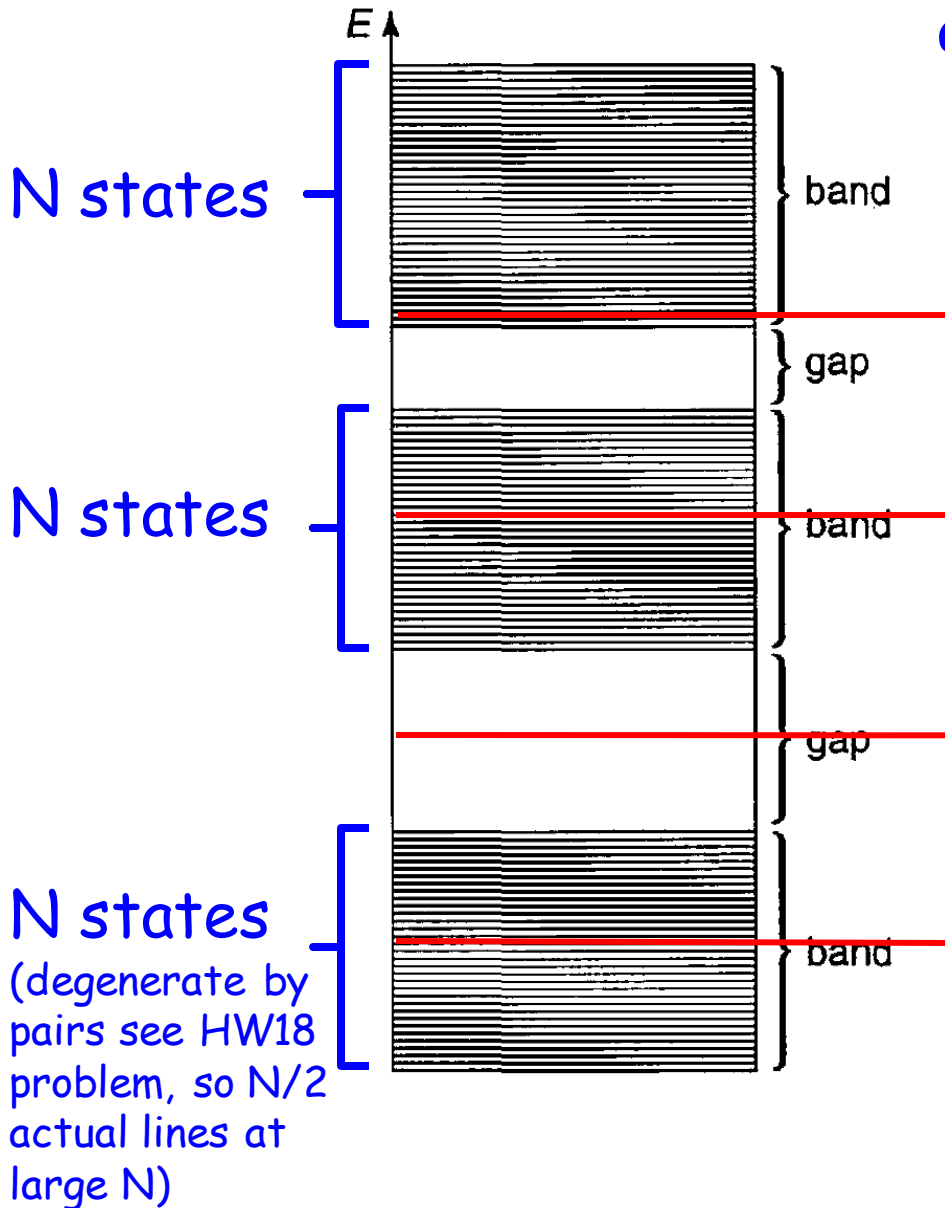
band

q=4+ε (semiconductor)-> second band fully occupied + a few more electrons (2e/state)

q=3 (metal)-> second band half occupied (2e/state)

q=2 (insulator)-> first band fully occupied (2e/state)

q=1 (metal) -> half-band occupied (2e/state)

6

5.4 Quantum Statistical Mechanics

In this section, for the first time, we will introduce the concept of temperature T in QM.

At T=0, the system is in the state that minimizes the energy. At nonzero T, excited states start participating. If the system is immersed in a large "heat bath" its energy is raised, thus excited states are populated because there is thermal energy to excite the system.
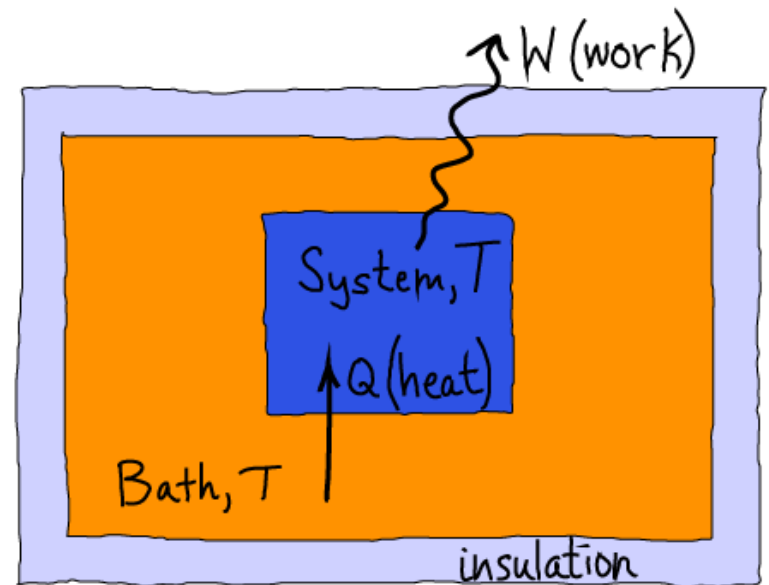
Thermodynamics is a probabilistic theory, even classically. We have N (large) number of particles and it is impossible to keep track of their individual movement.

In thermodynamics we need to address questions such as: *what is the probability that one particle has a particular energy Ej?*

With enough T, which translates into enough energy, I can populate excited states.

Again, this is a probabilistic theory even in a perfect classical gas. It is probabilistic because N is huge.

Ground state of q=3 is all occupied below, all empty above.

E

band

gap

$k_B T$

band

gap

band
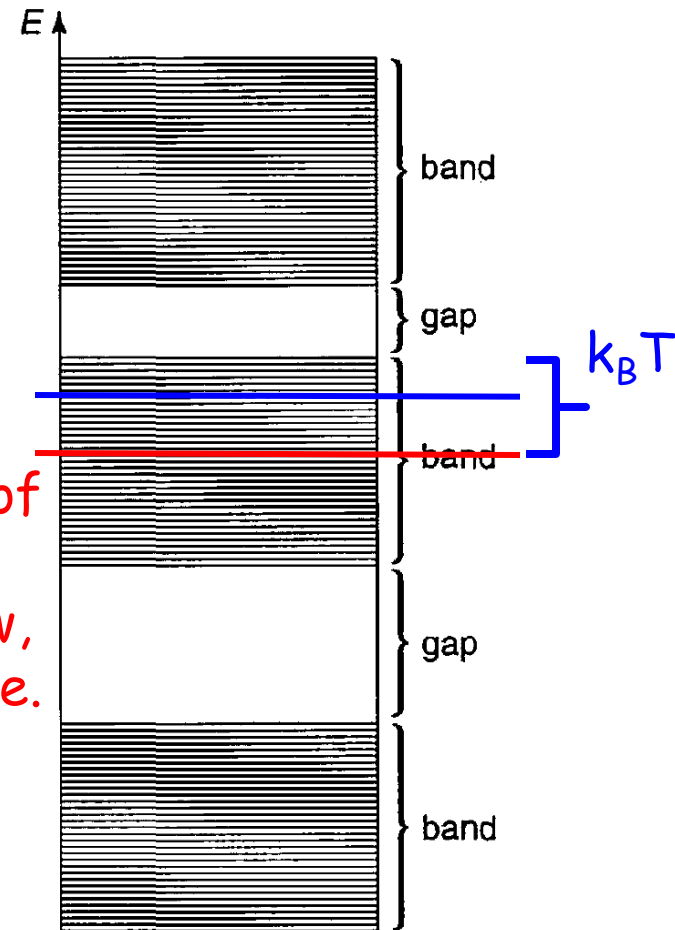
Intuitively, because of the contact with the large "heat bath? at constant T, the energy of the system is now larger than the ground state and it is also constant.

But this "excited" state is not frozen: particles constantly move. When on particle moves up in energy, another moves down; when a molecule starts rotating, another stops; etc. At the microscopic level there is plenty of activity.

The **fundamental assumption of statistical mechanics** is that in **thermal equilibrium** every combination of energy (i.e. every state) of the N particles that produces the same total energy has the **same probability**.

QM here will only affect the results by the way in which we count distinct states. For instance classical particles vs fermions will lead to a different number of excited states with energy say E_j.