

Quiz: Last time we established  $c_n = A e^{i k n a}$  are the coefficients for a traveling wave LCAO solution. Write out the full wave fn  $\Psi(x, t)$ .

Act out the wave fn. Each person is a coefficient multiplying an atomic orbital.

When talking about phonons we saw similar traveling waves.

What are the similarities / differences?

- In both cases we are looking for a sequence of numbers  
 $\chi_1, \chi_2 \dots \chi_n$   
 $c_1, c_2 \dots c_n$
- Bands of allowed freqs / energies

(2)

The quantity  
that changes  
from lattice site  
to lattice site

Governing  
eqn

Phonon

$x_n$

displacement of the  
 $n^{\text{th}}$  atom.

Has to be real #.

$$-m\omega^2 x_n = Kx_{n-1} - 2Kx_n + Kx_{n+1}$$

Electron  
LCAO state

$c_n$

coefficient multiplying  
the  $n^{\text{th}}$  atomic orbital.

Can be complex #.

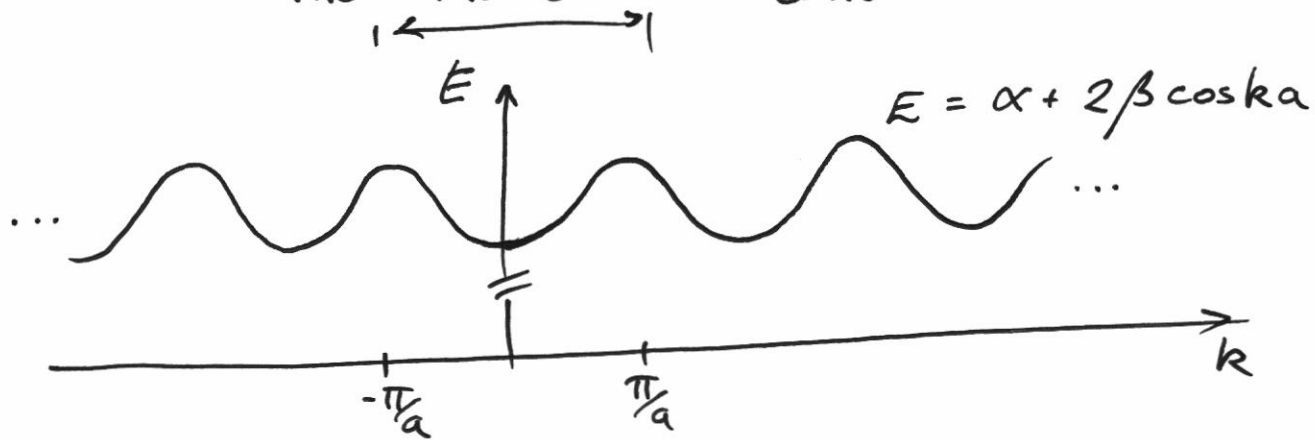
$$Ec_n = \beta c_{n-1} + \alpha c_n + \beta c_{n+1}$$

Question to consider:

The governing eqns are essentially the same,  
so why do the dispersion relations have different  
shapes?

# THE FIRST BRILLOUIN ZONE

(3)



The dispersion relation is well-defined for all  $k$ , but all the eigenstates are described with  $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$ .

What happens when  $k$  is outside this range?

Consider a value of  $k$  that is inside the 1<sup>st</sup> B.Z.

$$c_{n,k} = A e^{ikna}$$

Consider another value, ~~at~~  $k' = k + \frac{2\pi}{a}$   
(outside the 1<sup>st</sup> B.Z.)

$$\begin{aligned} c_{n,k'} &= A e^{ik'na} = A e^{i(k + \frac{2\pi}{a})na} \\ &= A e^{ikna} e^{i2\pi n} \\ &= A e^{ikna} \end{aligned}$$

The  $k$  eigenstate has the same coefficients as the  $k'$  eigenstate.

They are the same state!

(4)

A strange prediction:

I apply a force to an electron in a periodic potential.

The force leads to a change in momentum.

$$F = \frac{dp}{dt} \quad \text{where } p = \hbar k.$$

The electron moves into states with larger  $k$ , but eventually it returns to exactly the same state!

Do you subscribe to the philosophy of Paul Dirac?

"Have faith in the logic of mathematics as a means to physical reasoning."

\* Bloch Oscillations do occur in nature,  
see paper by Dahan et al. Phys. Rev. Lett. 76 4508 (1996)