# Bloch Wavefunctions

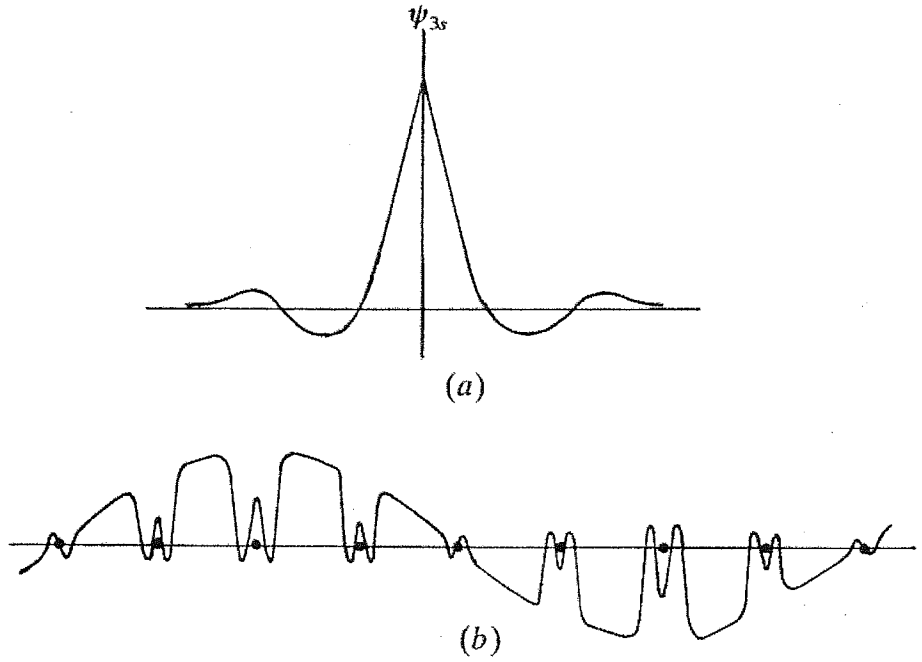
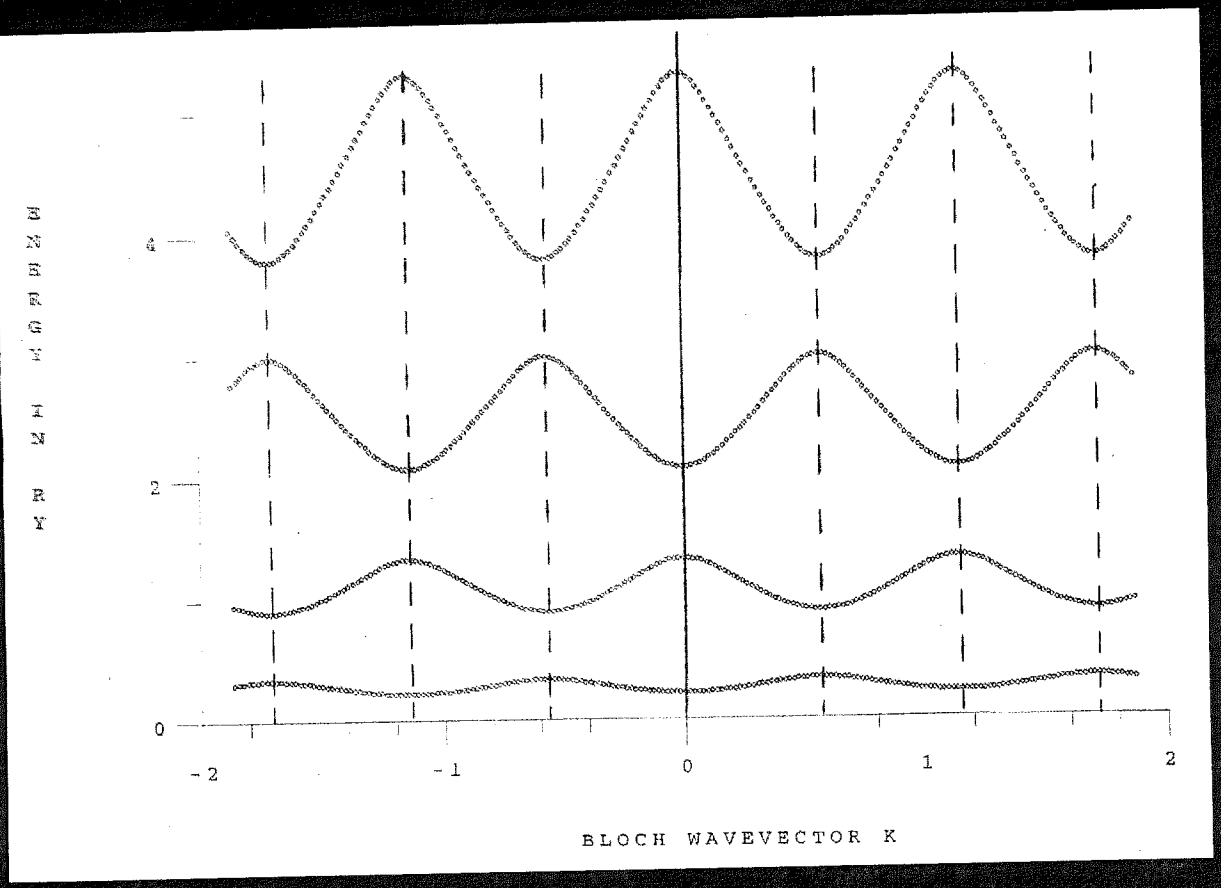



**Figure 7.18** The wave function for a 3s electron in sodium is shown in schematic fashion, (a). In sodium metal the ion core is very small compared to the atomic diameter, the Bloch functions for the 3s electrons have a marked plane wave component except for the immediate vicinity of the core region, (b).

This result gives evidence to support the nearly-free electron approximation, in which the periodic potential is assumed to have a very small effect on the plane-wave character of a free electron wavefunction. It also explains why the free-electron gas model is so successful for the simple metals!

handout chapter 7

# Numerical Results of the Krönig-Penney Model




The 1st BZ has a maximum k value given by:

$$k_{\max} = \frac{\pi}{a+b} = \frac{\pi}{5.5a_0} = 0.57\frac{rad}{a_0}$$

You can see the same qualitative 1-D band structure we deduced from the approximate band gap calculation earlier!

$K' = Q$ and $\kappa = k$

# Graphical Approach

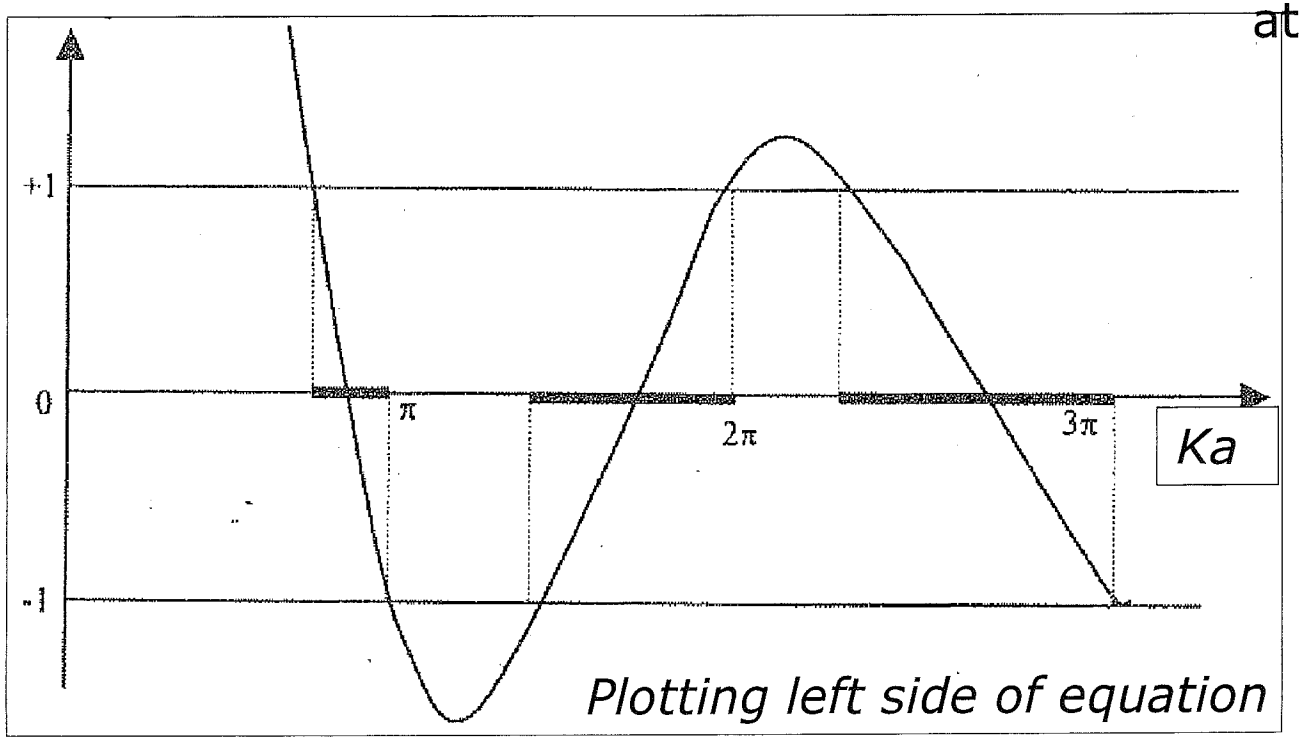
$$\left(\frac{\kappa^2 - K^2}{2K\kappa}\right)\sin(Ka)\sinh(\kappa b) + \cos(Ka)\cosh(\kappa b) = \cos[k(a+b)]$$

small *b*

$$\left(\frac{b\kappa^2}{2K}\right)\sin(Ka) + \cos(Ka) = \cos(ka)$$

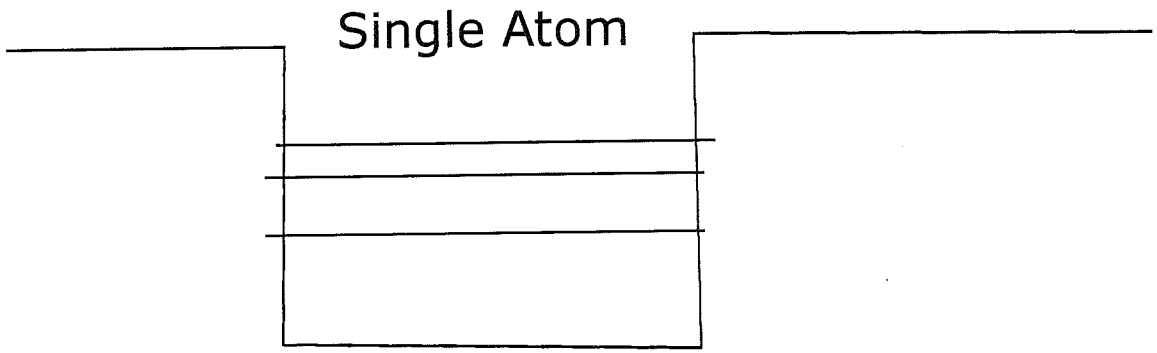
Right hand side cannot exceed ±1, so values exceeding will mean that there is no wavelike solutions of the Schrodinger eq. (forbidden band gap)

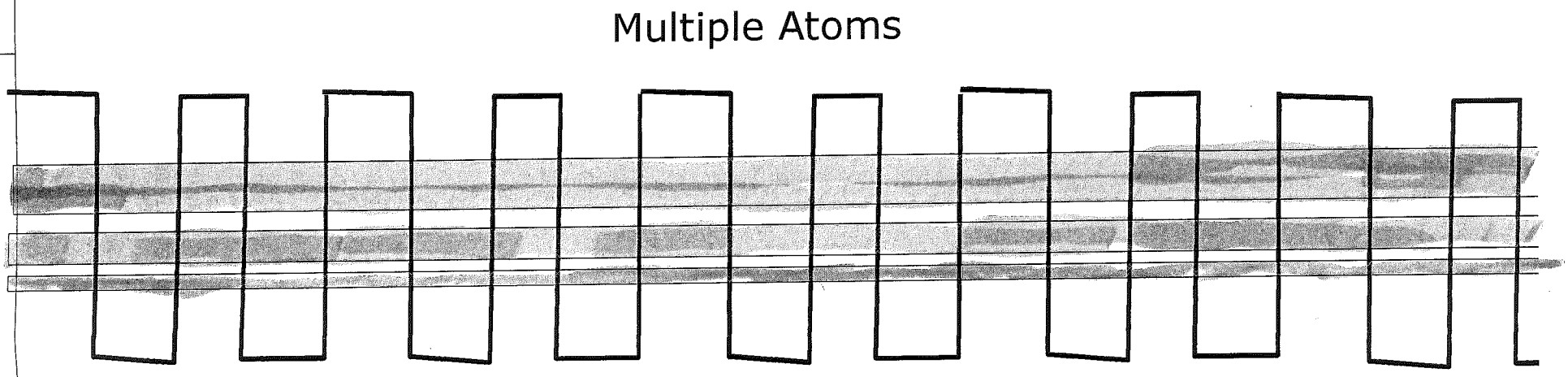
Gap occurs at Ka=Nπ or K=Nπ/a




$$E = \frac{\hbar^2 K^2}{2m}$$

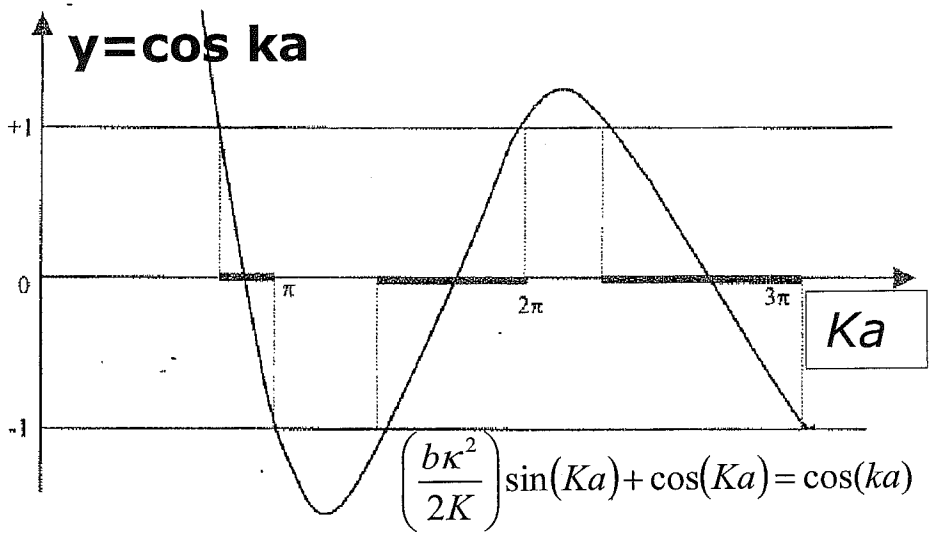
# Not really much different



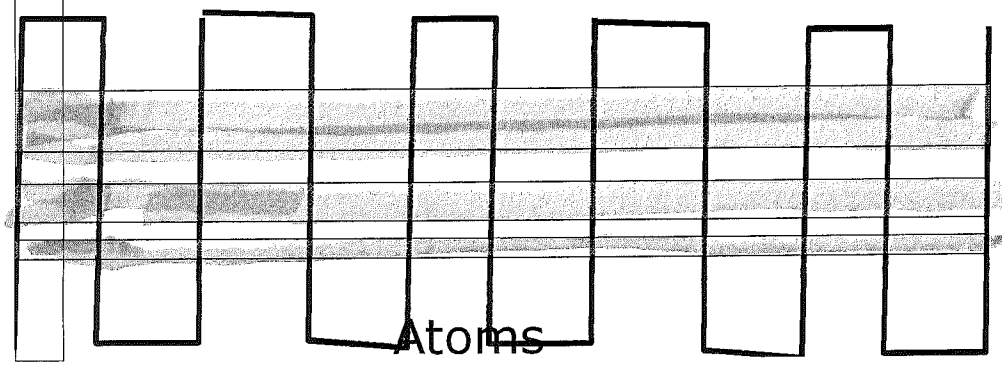



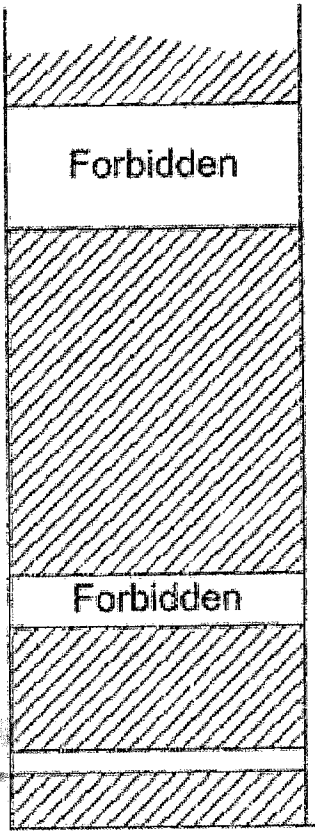
# Different Ways to Plot It
# Extended Zone Scheme

**Note that the larger the energy, the larger the band/gap is (until some limit).**



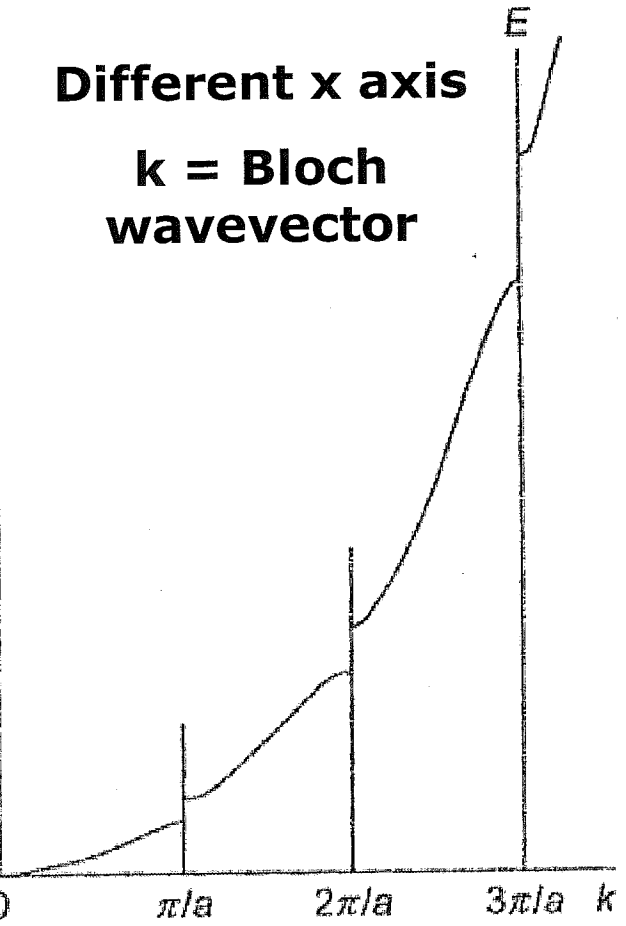

The range $-\pi<ka<\pi$ is called the first ***Brillouin zone***.



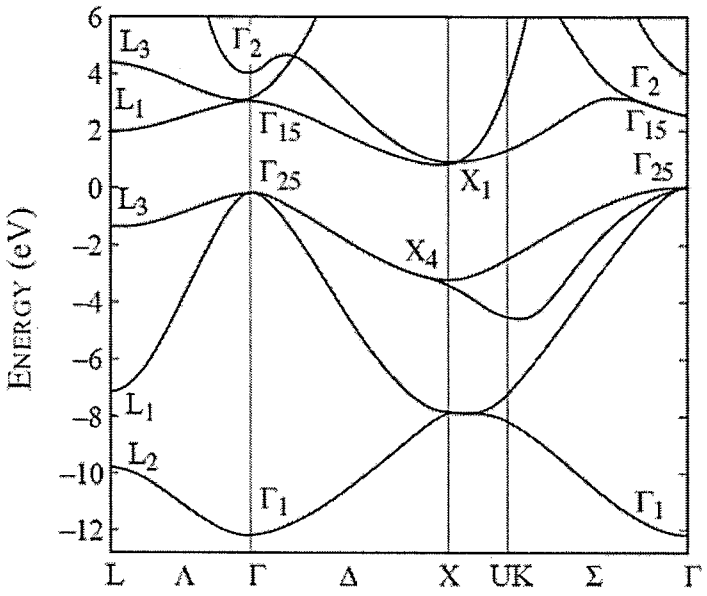

**Different x axis**

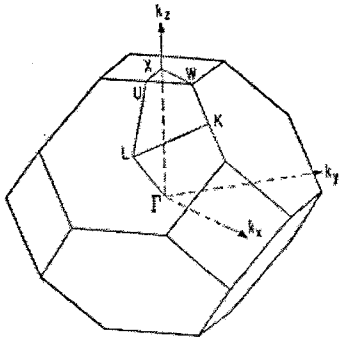
**k = Bloch wavevector**



# Band Theory, Kittel chapter 7

Calculate the dispersion relation for electrons in a crystal




silicon