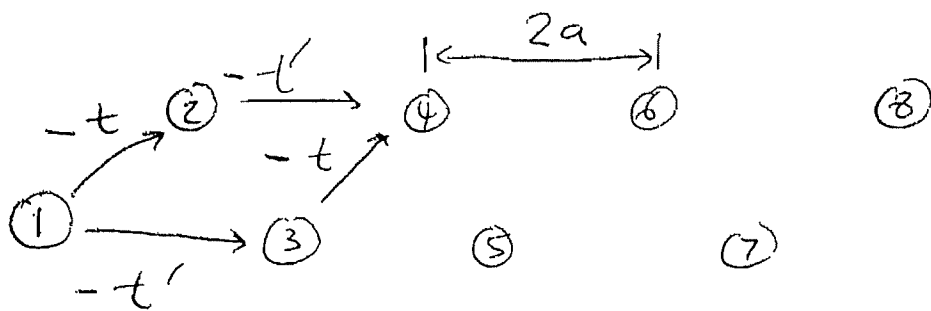


Solutions

1) Energy Bands IV : An Example  
 with two atoms per unit cell.

Consider the following one-dimensional crystal, described in the tight-binding model :



The crystal has two identical atoms per unit cell, with coupling  $-t$  along the diagonal to the

nearest-neighbor, and coupling  $\underline{2}$   
 $-t'$  to the nearest neighbor along  
the axis of the molecule.

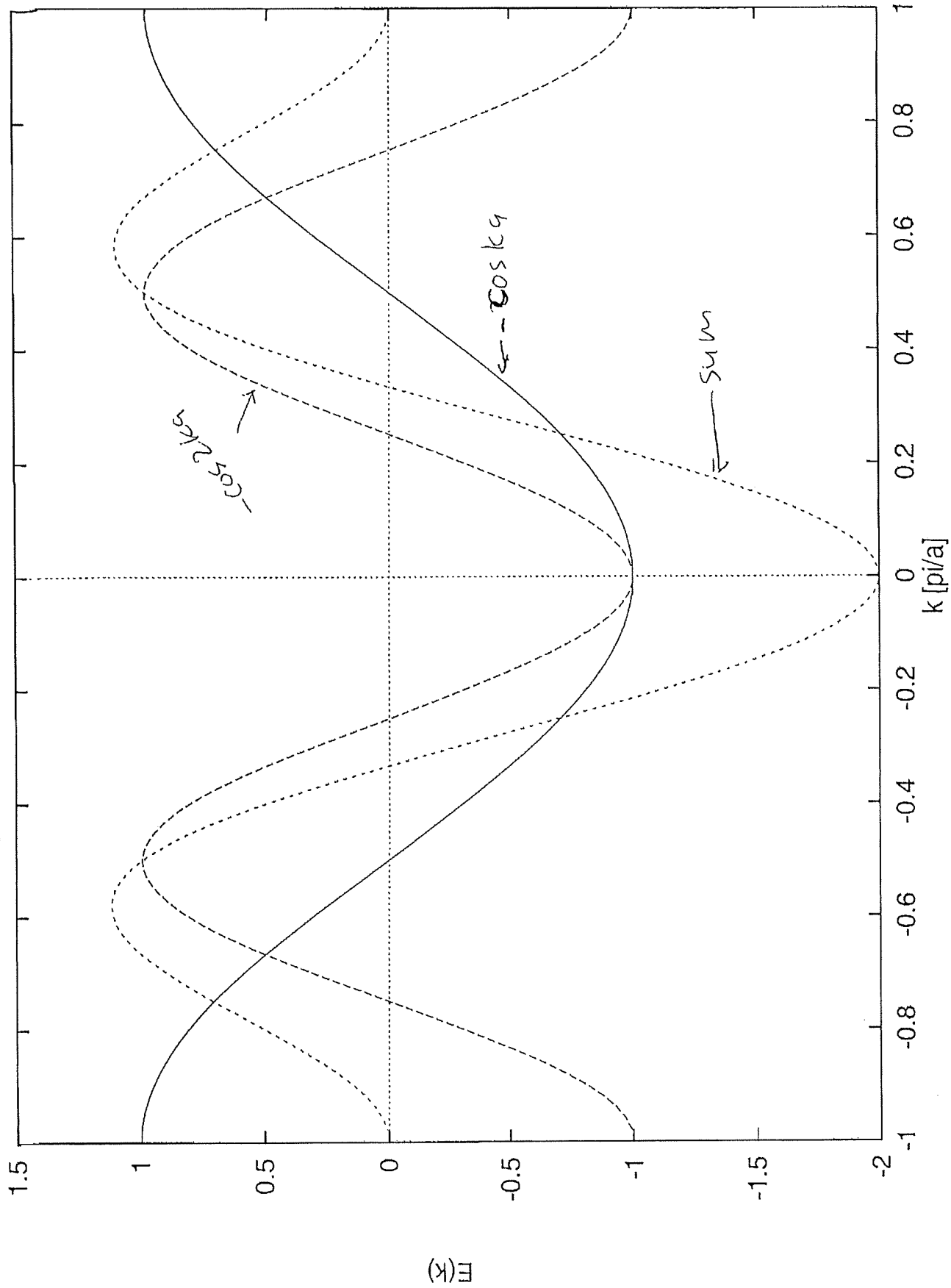
The dispersion relation is

$$\varepsilon(k) = -2t \cos ka - 2t' \cos 2ka.$$

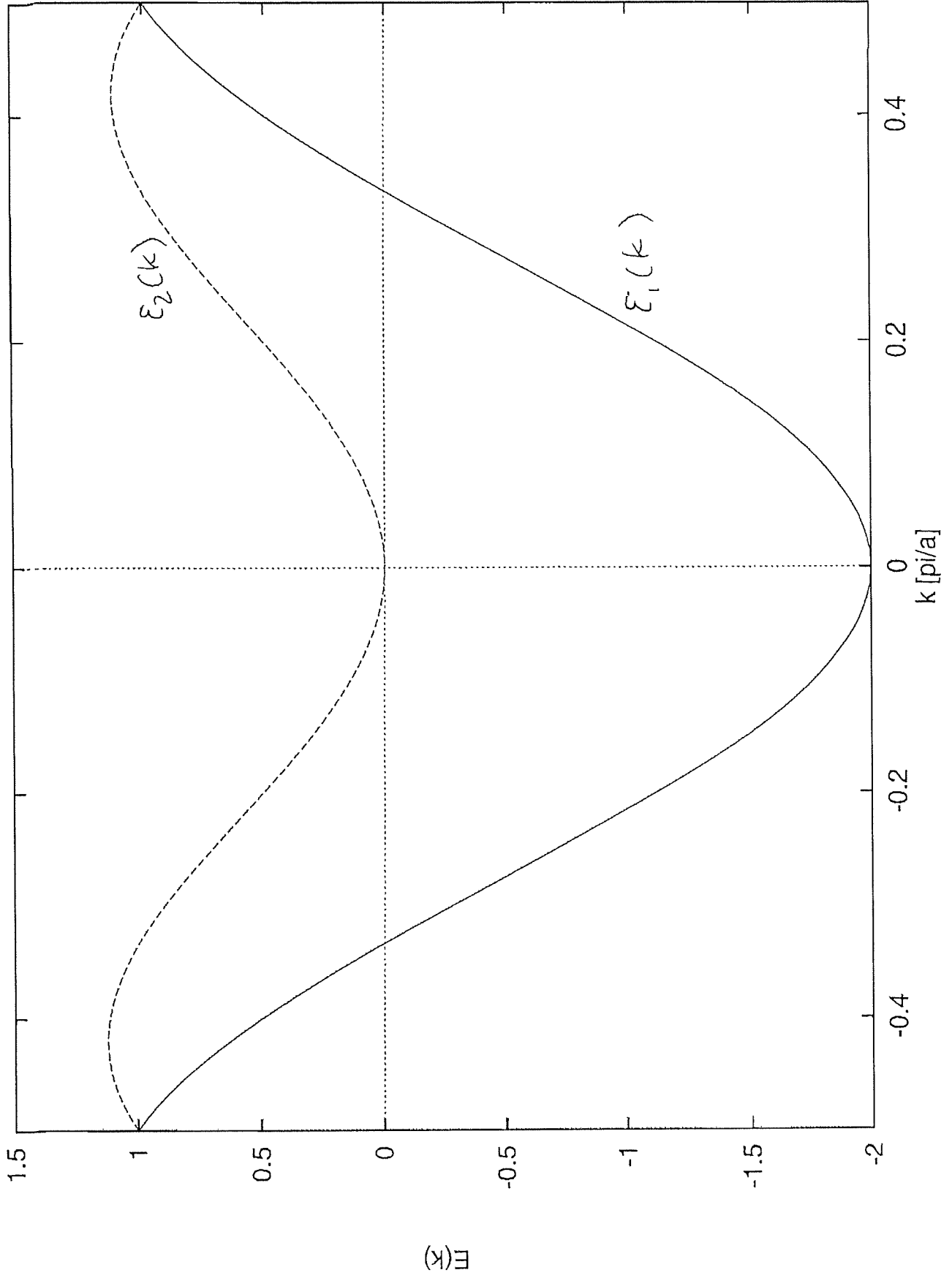
The lattice spacing is  $2a$ ,  
so the 1st Brillouin zone is

$$k \in \left( -\frac{\pi}{2a}, \frac{\pi}{2a} \right].$$

$t' = 1/2$ : Extended Zone Scheme



$t = i' = 1/2$  Reduced Zone Scheme



bands overlap

11

8

Two things to note:

i) In a 1D system, we can always choose  $t > 0$  by an appropriate choice of the relative phases of the basis orbitals on nearest-neighbor atoms. However, the ratio  $t'/t$  is independent of gauge choice, and is determined by the symmetry of the orbitals. The choice above  $t'/t > 0$  is appropriate for e.g. s-orbitals.

ii) The degeneracy of  $\epsilon_1$  &  $\epsilon_2$

at  $k = \pm \frac{\pi}{2a}$  will  
generically be lifted by  
higher order terms.

9

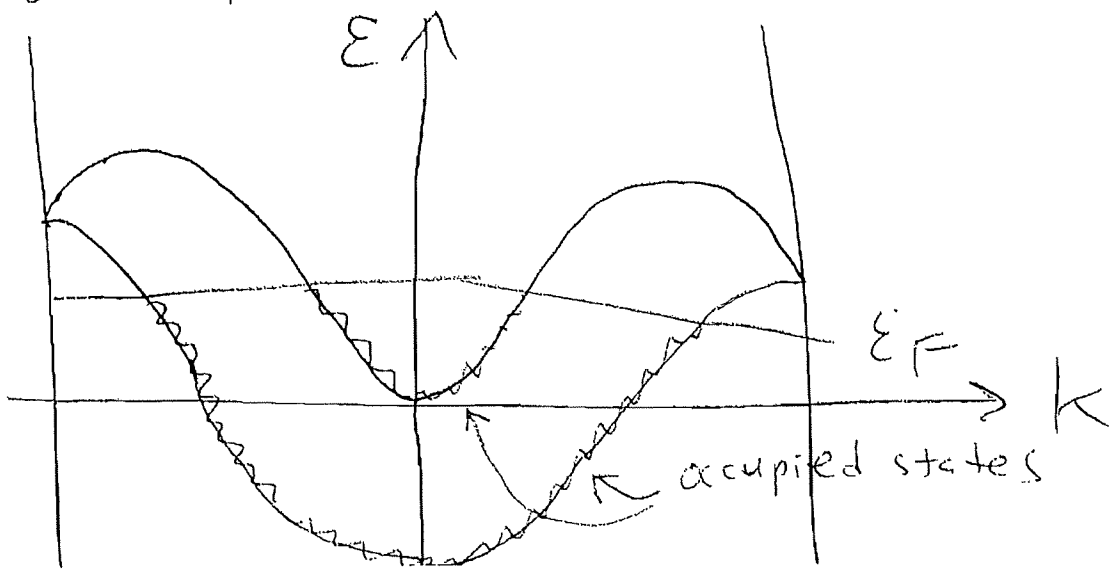
Metal or insulator?

If our 1D chain consists  
of atoms with a single  
valence electron, then  
we have two valence  
electrons per unit cell.

Including spin, the total #  
of orbitals per energy band is  
two per unit cell of the crystal

Thus, the chain of atoms has just enough valence electrons to fill a single band, and could a priori be an insulator.

However, the energy bands overlap, so instead of one filled and one empty band, it has two partially filled bands, and is a metal:



# Physics 460

## Problem Set # 7 Solutions

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2) Let  $g = e/\sqrt{E}$ . The Schrödinger equation becomes

$$\left[ -\frac{\hbar^2}{2m^*} \nabla^2 + \frac{g^2}{|\vec{r}|} \right] \psi(\vec{r}) = E \psi(\vec{r}).$$

This has the same form as the Sch. eq. for a hydrogen atom with  $m \rightarrow m^*$  and

$$e \rightarrow g.$$

a) For the H atom,  $a = \frac{\hbar^2}{m e^2}$

$$\Rightarrow a_d = \frac{\hbar^2}{m^* g^2} = \frac{e \hbar^2}{m^* e^2}$$



$$a_d = \epsilon \frac{m}{m^*} a = \frac{11.7}{0.2} 0.53 \text{ \AA}$$

$$= 58.5 a = 31 \text{ \AA}$$

b) For the H atom, the

ionization energy is  $\frac{me^4}{2\hbar^2}$ .

$$\Rightarrow E_d = \frac{m^* \hbar^4}{2\hbar^2} = \frac{m^* e^4}{2\epsilon^2 \hbar^2}$$

$$E_d = 13.6 \text{ eV} \frac{m^*}{m} \frac{1}{\epsilon^2} = 20 \text{ meV}$$

c) An impurity band will form when there is appreciable overlap of the wavefunctions of electrons bound on neighboring impurities. If the # of impurities per unit volume is  $n_d$ , the mean distance between them is  $n_d^{-1/3}$ .

The wavefunctions will overlap appreciably if

$$a_d n_d^{1/3} > 1$$

$$n_d > a_d^{-3}$$

$$n_d > (3.1 \times 10^{-9} \text{ m})^{-3}$$

$$n_d > 3.4 \times 10^{25} \text{ m}^{-3}$$

B

CC