Week 7 - Energy Bands
Comprehension Check

Total points = 25 (scaled by a factor of 1/10 in the system)

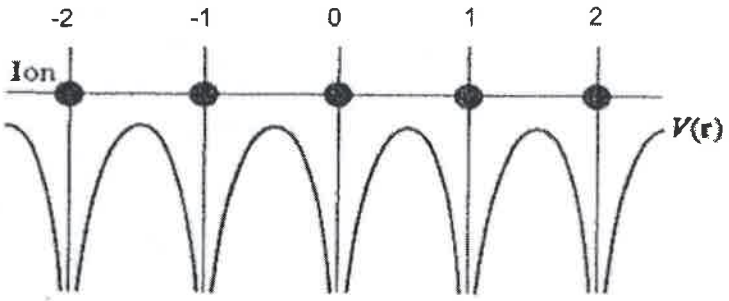
Question 1 (8 points)

Discuss the scenario(s) under which a material conducts electricity. Be brief.

① odd integer of valence electrons per primitive cell results in half filled band

② even integer of valence electrons per primitive cell + overlapping bands

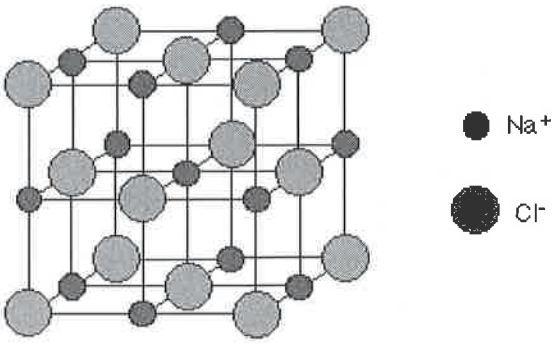
Question 2 (8 points)



For the periodic structure shown above, the distance between neighboring ions is 0.3 nm. The numbers above the ions are indices of the ionic sites. Use Bloch's theorem to relate the electron wavefunction at site #1 to the wavefunction at site #0.

$\psi(1) = \psi(0)\, e^{iKT}$ where $T = 0.3\,nm$, K in units of nm^{-1}

Question 3 (9 points)



How many valence electrons per primitive cell are there in crystalline salt? Do you expect crystalline salt to behave like a metal or an insulator? Justify your answer. (Note, the atomic numbers of Na and Cl are respectively 11 and 17)

Na^+: $1s^2\ 2s^2\ 2p^6$ — 0 valence electrons

Cl^-: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$ — 8 valence electrons

fcc structure with 2 ions per primitive cell

no. valence electrons = $8 \times 2 = 16$ = even

though NaCl is an insulator we cannot make this call without considering the band structure.