Bands with plane waves

IMPRS Solid State Physics
May 2017

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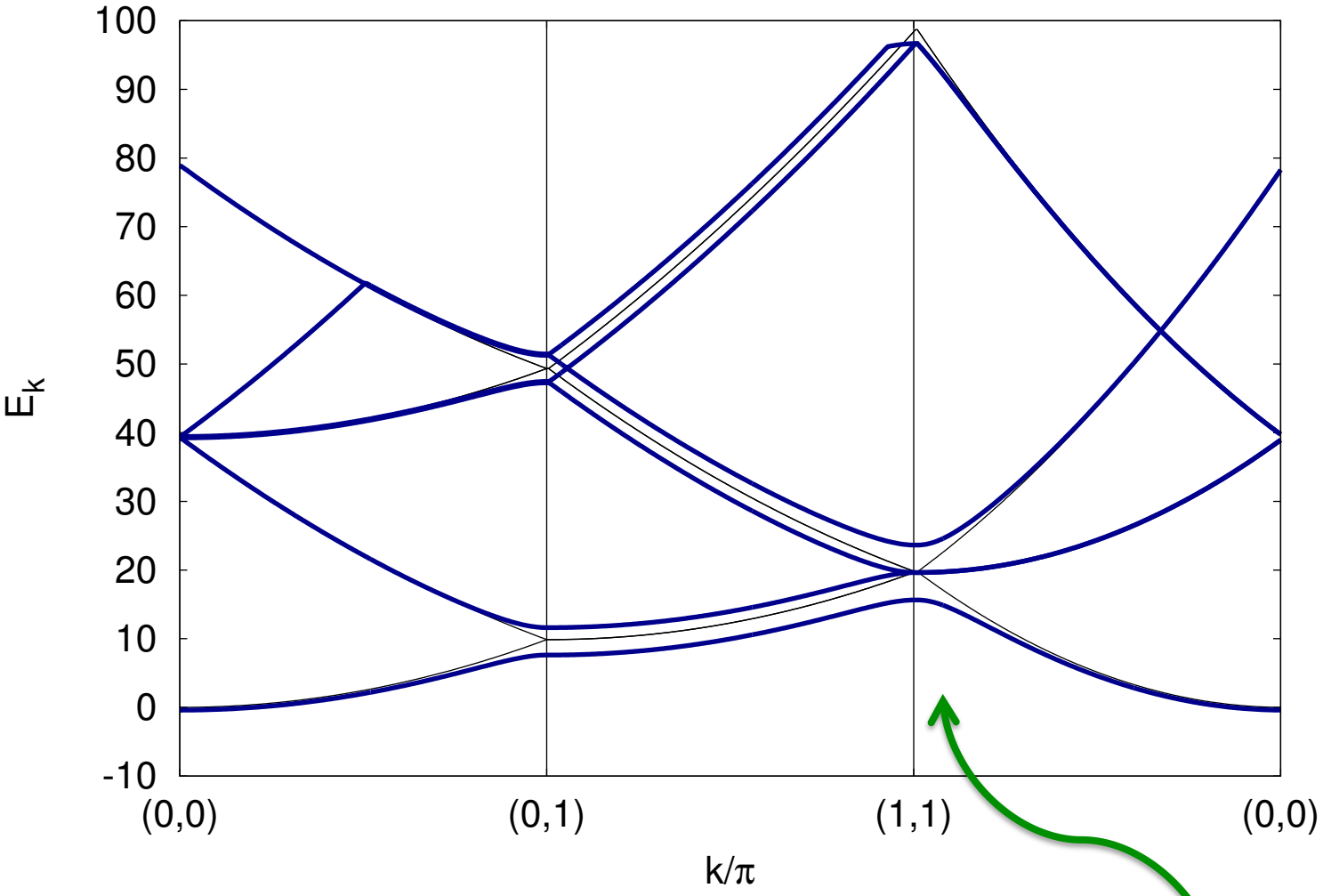
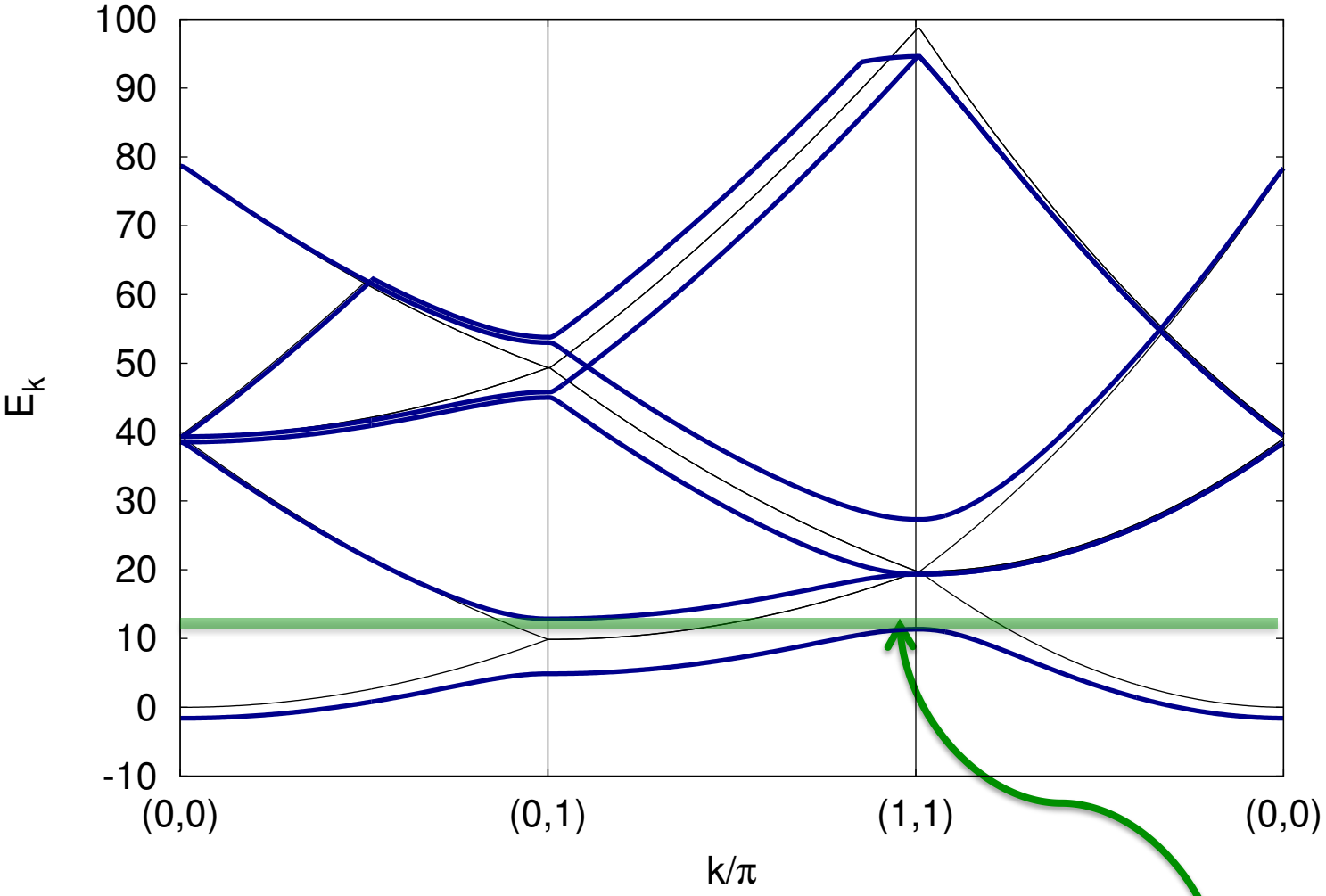
$V_0 = 4$, $V_1 = 0$; Black: free, Blue: N=3



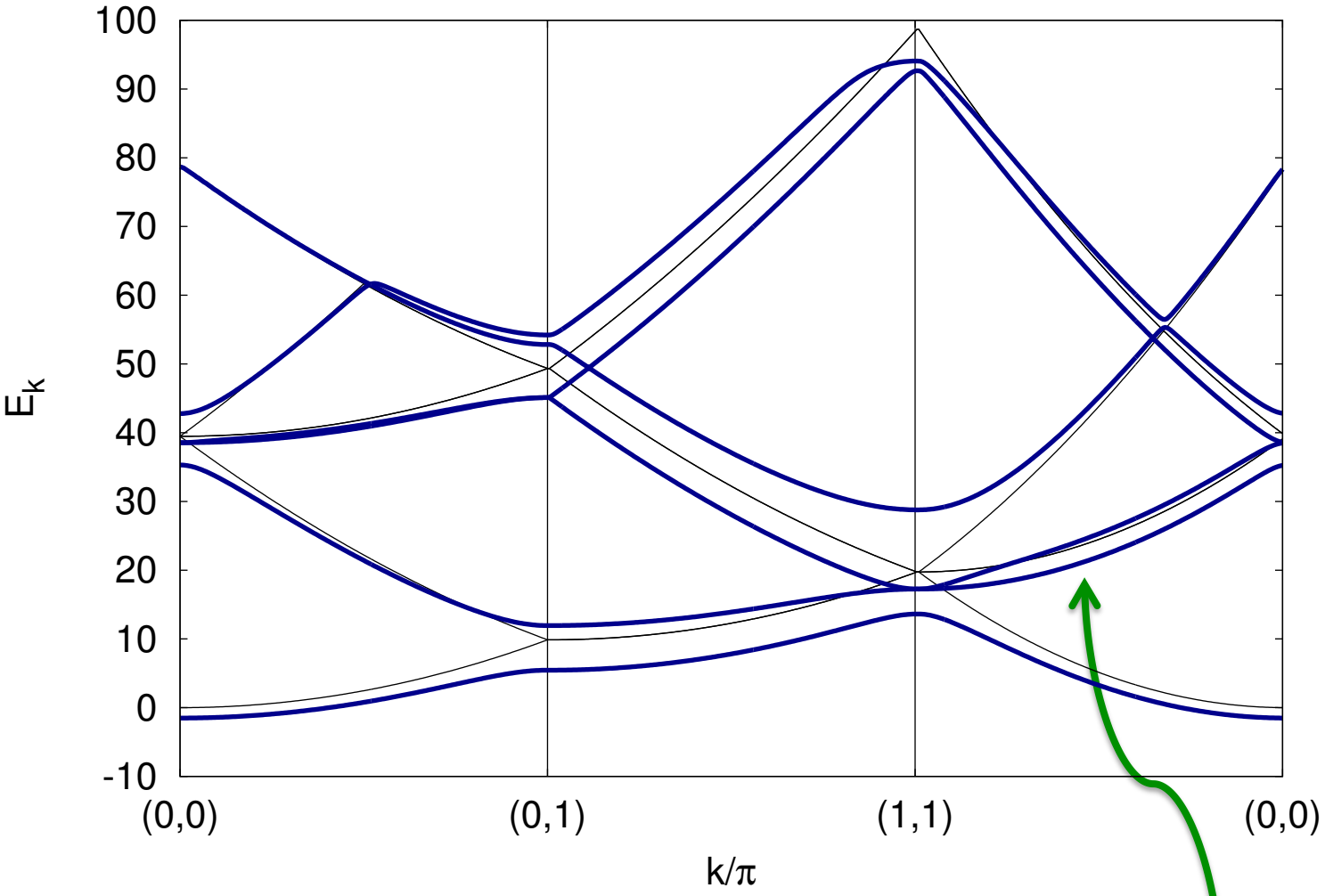
Degeneracies lifted but still metallic
Fermi surface: Hole and electron pockets
for 2 electrons per unit cell

$V_0 = 8$, $V_1 = 0$; Black: free, Blue: N=3



Insulator: Indirect band gap
for 2 electrons per unit cell

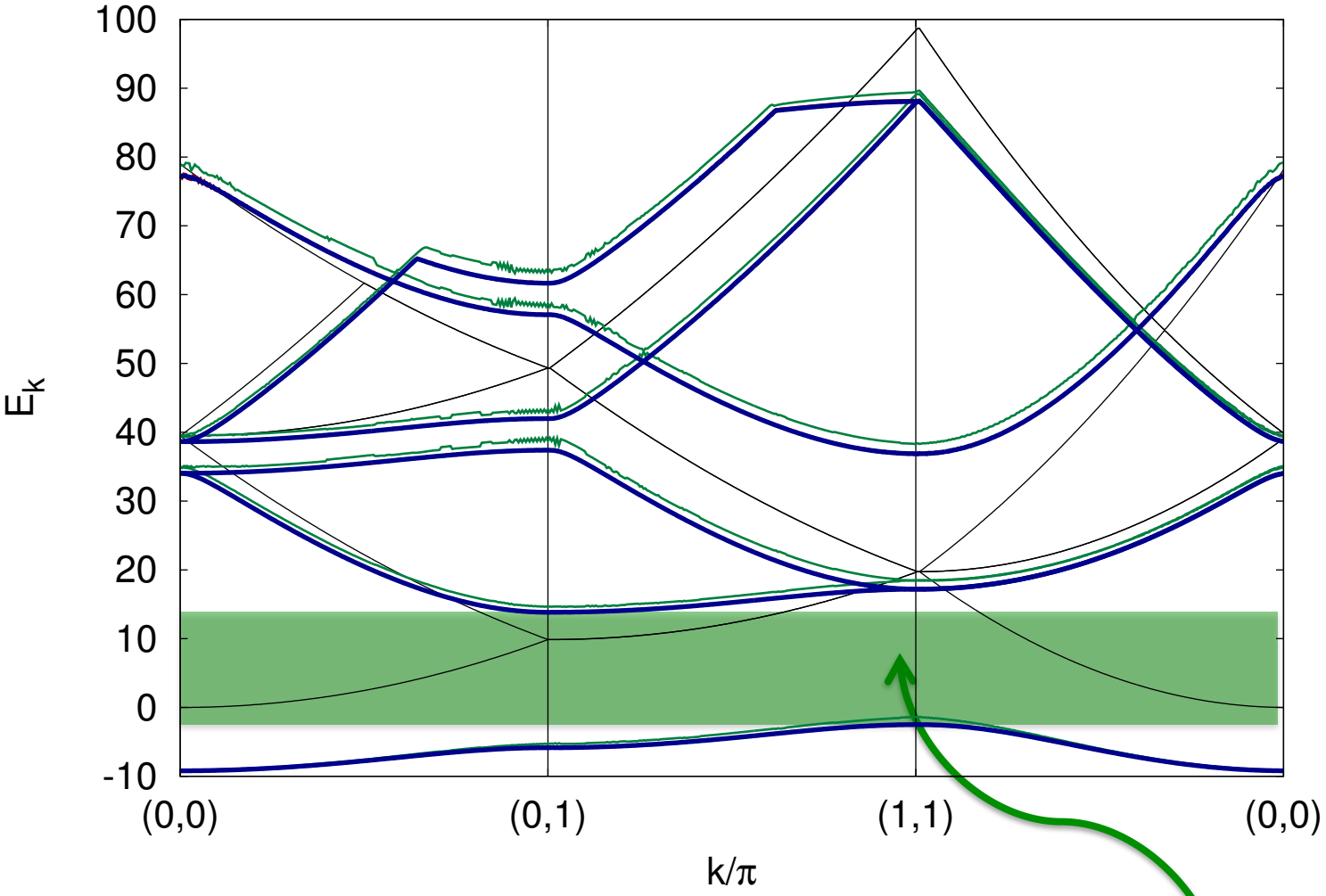
$V_0 = 8$, $V_1 = 4$; Black: free, Blue: N=3



Lifting of degeneracies in 1st order perturbation theory due to V1>0

$V_0 = 20$, $V_1 = 0$; Black: free, Green: N=1, Red: N=2, Blue: N=3

Check convergence with N = #plane waves



Strong potential: Lowest band becomes flat
tight-binding limit, see below

Insulator: Indirect band gap
for 2 electrons per unit cell