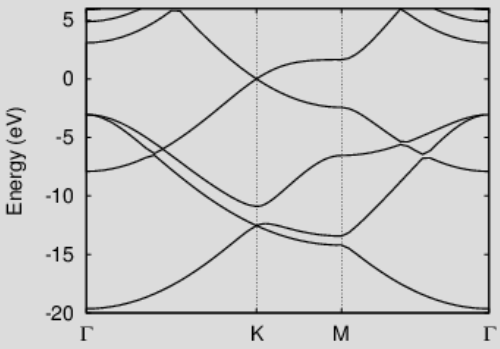
Computational Physics Course

Learn to use software packages

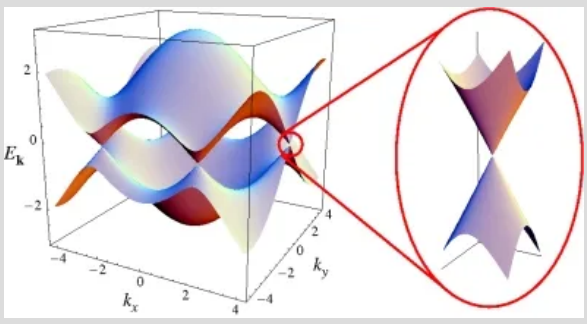
Now let us use "gnuplot" to finally draw the band.

```
#!/usr/local/bin/gnuplot -persist
# Last modified: 2014/01/03 02:33
set terminal postscript eps enhanced 28 lw 2
set output "band.eps"
set ylabel 'Energy (eV)'

set xtics ("{/Symbol G}" 0, "K" 0.666666, "M" 1, "{/Symbol G}" 1.5773)
set ytics 5

ymin=-20
ymax=6
set xrange [0:1.5773]
set yrange [ymin:ymax]
unset key

set arrow 1 nohead from 0.66666,ymin to 0.66666,ymax lt 2
set arrow 2 nohead from 1,ymin to 1,ymax lt 2

plot graphene.band.gnu' using 1:2 w l
```



Make the file "band.plt" using the lines shown in the above and type
$gnuplot band.plt
to get the band as shown in the right.

The Fermi level is -0.4661 eV as you can confirm by looking at the output file of the scf calculation. Fermi level is located at the point denoted as K.



http://faraday.fc.up.pt/cfp/Members/evcastro/figs/imag.jpg/view

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Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso

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