Topological properties with WannierTools

Tutorial IV: Landau level spectrum

Hands-on session

Wannier 2022 Summer School Trieste

Hands-on based on WannierTools v2.6.2

Useful information about WannierTools:
Documentation: www.wanniertools.com
Forum: www.wanniertools.org
Open source: https://github.com/quanshengwu/wannier_tools
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Tips: Open file.eps, file.pdf file in Linux, you can use command "evince". such as

```
$ evince file.eps
```

Open file.png file in Linux, you can use command "eog". such as

```
$ eog file.png
```

In this session we will study Landau level spectrum using WannierTools.

1 Hofstadter butterfly of Graphene

When the magnetic field is applied to the perpendicular direction of a two-dimensional lattice, then then energy bands will split into the Landau levels. When increasing the magnetic field from zero-flux to 2π flux per unit cell, the evolution of the energy levels will form the Hofstadter butterfly.

In this tutorial, we will study the Hofstadter butterfly (HB) of graphene instead of twisted bilayer graphene since there are only 2 orbitals in the unit cell of graphene. The procedure to obtain Landau level spectrum of TBG system is the same but needs much much more computational resource. Woking direction for this section is

```
$ git clone https://github.com/wannier-developers/wannier-tutorials.git
$ cd wannier-tutorial/2022_05_Trieste/DAY4_AM_1_WannierTools/ex2/Graphene-LL
```

There are two ways to obtain the HB spectrum. The first one is to exactly diagonalize the magnetic Hamiltonian for a given flux Magp/Nslab$*\phi_0$ by setting tag "LandauLevel_B_calc=T" in "CONTROL" namelist. The second one is to use Lanczos method by setting tag "LandauLevel_B_dos_calc=T". Some important tags that can be set during the HB spectrum calculations.

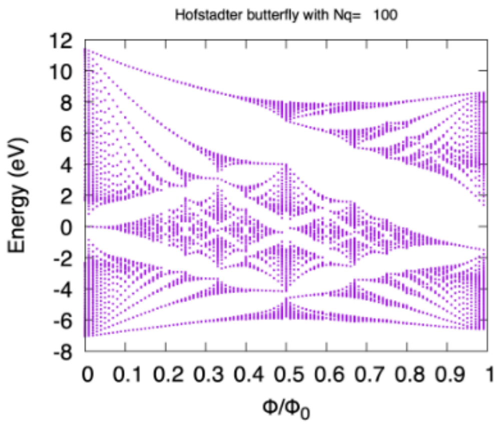
1. SURFACE card, The first line of this card is used to set direction of magnetic field. In this case, B//[0,0,1].
2. Nslab: size of magnetic supercell.
3. Magp: WannierTools will calculate LLs from flux 0 to Magp/Nslab*$*\phi_0$. There are Magp+1 fluxes. If you use MPI to run WannierTools, number_of_tasks should be less than Magp+1 in the "LandauLevel_B_calc=T" mode and less than (Magp+1)*NumRandomConfs in the "LandauLevel_B_dos_calc=T" mode.

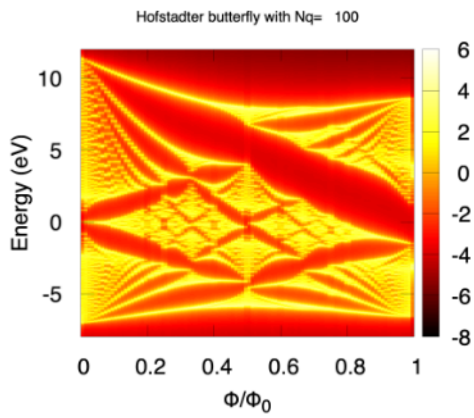
Now let's run WannierTools to obtain HB spectrum of Graphene.

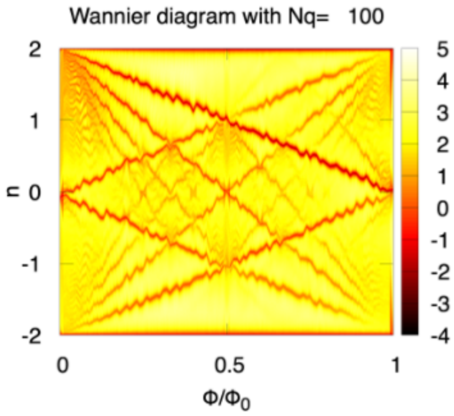
```
$cp wt.in-landaulevel-ED wt.in
$mpiexec -np 4 wt.x
$gnuplot LandauLevel_B.gnu0
$eog landaulevel_B.png

$cp wt.in-landaulevel-Lanczos wt.in
$mpiexec -np 4 wt.x
$gnuplot LandauLevel_B_dos.gnu0
$eog landaulevel_B_dos.png
$gnuplot wannierdiagram.gnu0
$eog wannierdiagram.png
```

If everything works smooth, you will get the following plots







▶ Excercise

1. Read reference *Wannier Phys.Stat.Sol (1978)* to understand the relation between Wannier diagram and Hofstadter butterfly.

2. Try to setup HB spectrum calculation for TBG systems on supercluster after this summer school. PhysRevLett.126.056401 this paper could be useful as a guide.

2 Landau level and HB of a Weyl semimetal toy model

2.1 LL along a k-path parallel to magnetic field

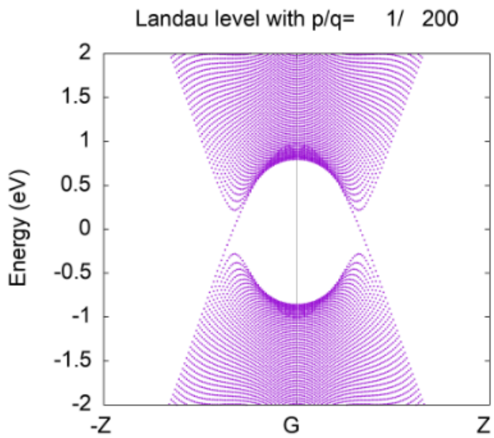
When applying magnetic field in a 3D Weyl semimetal, there will be chiral Landau level states linking the conduction LLs and the valence LLs (Ref. PhysRevB.94.121105). Although the energy bands

perpendicular to the magnetic field are quantized into LLs, there still be translation symmetry along the magnetic field. So let's first study the LLs along the k-path parallel to magnetic field.
Woking direction for this section is

```
$ git clone https://github.com/wannier-developers/wannier-tutorials.git
$ cd wannier-tutorial/2022_05_Trieste/DAY4_AM_1_WannierTools/ex2/3DWeyl-model-LL
```

```
$cp wt.in-landaulevel-kpath wt.in
$mpiexec -np 4 wt.x
$gnuplot landaulevel_k.gnu0
$eog landaulevel_k.png
```

Then you will obtain a plot.



▶ Excercise

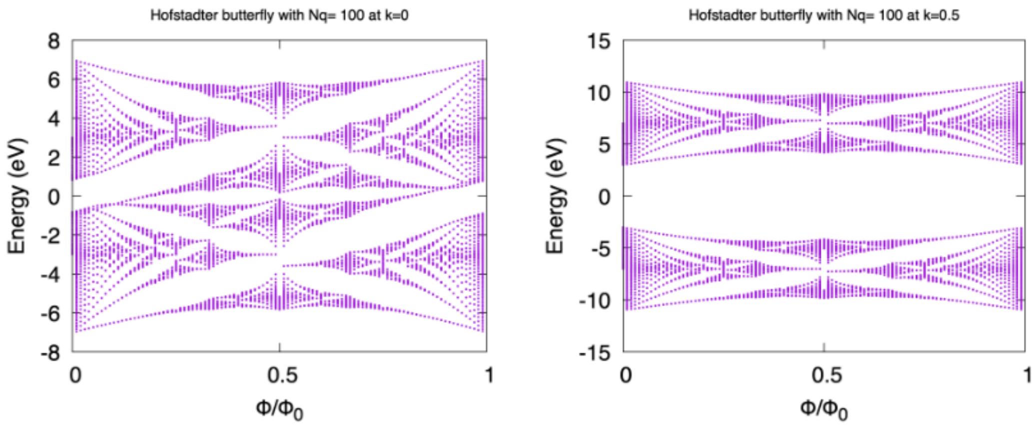
1. Change the direction of magnetic field in the SURFACE card to recalculate the LLs.
2. change the k-path in "KPATH_BULK" to check whether there is enery dispersion along a k-path that perpendicular to the magnetic field.

2.2 HB at different k point

From the above subsection, we know that there is energy dispersion along the k-path parallel to magnetic field. So the HB plot should be k dependent. In WannierTools, we use use a "SINGLEKPOINT_3D" card to control the k point.

```
$cp wt.in-landaulevel-B wt.in
$mpiexec -np 4 wt.x
$gnuplot landaulevel_B.gnu
$eog landaulevel_B.png
```

Here we give two HB plots when k=(0,0,0) and k=(0.5,0,0).



- Excercise

1. Find the location of Weyl point using "FindNodes_calc = T", and set the "SINGLEKPOINT_3D" to the k point, and recalculate the HB.

Notes: The unit in KPATH_BULK and SINGLEKPOINT_3D is not the primitive unit cell of the cell defined in LATTICE card but the magnetic supercell. The first(second) lattice vector of the magnetic supercell is the first(second) vector defined in SURFACE card, while the third vector is the Nslab times the third vector defined in SURFACE card. Eventually, for small magnetic field, i.e. Magp/Nslab-¿0, only the first value of a k vector in the primitive unit cell of magnetic supercell will affect the HB plots.

If the Weyl point is (0,0,kc), B//[001] and you want to set SINGLEKPOINT_3D at the Weyl point, then SINGLEKPOINT_3D should set as
SINGLEKPOINT_3D
Direct
kc 0 0