Solution_TI-01

January 11, 2023

[1]:
```
import sisl
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
import functools
```

1 Quantum Hall Effect

In this exercise, we will build on **TB_07** and **A_03** to simulate the quantum Hall effect. In **A_03**, we learned how to created a Hall bar device and in **TB_07**, how to deal with magnetic fields.

Here, we will extract the Hall resistance from the transmissions calculated with `TBtrans` using the Landauer-Büttiker formalism.

1.1 Exercise Overview:

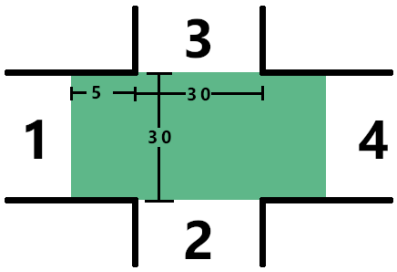
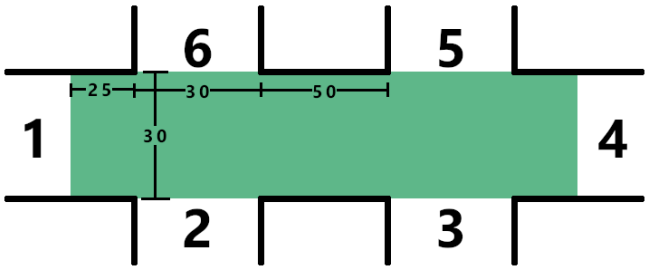
1. Create a Hall bar (see **A_03**)
2. Construct Hamiltonians and add magnetic fields (see **TB_07**)
3. Calculate the transmission with `TBtrans`
4. Extract the Hall resistance (R_H).
5. Extract the logitudinal resistance (R_L).

1.2 Exercise

1.2.1 1. Create a Hall bar

In order to be able to observe the quantum Hall effect, the size of the Hall bar needs to be big enough. For a 4(6) lead device reasonable dimensions are: 1. 4-lead device (square lattice): - Width of electrodes (perpendicular to the semi-infinite axis): 30 atoms - Offset of the electrodes 2(3) from the corner of the central part: >= 5 atoms

2. 6-lead device (square lattice):
   - Width of electrodes (perpendicular to the semi-infinite axis): 30 atoms
   - Spacing between electrodes on the same side: 50 atoms
   - Offset of the electrodes 2(3,5,6) from the corner of the central part: > 25 atoms
3. 6-lead Graphene Hall bar:
   - Width of electrodes (perpendicular to the semi-infinite axis): ~30 Å
   - Spacing between electrodes on the same side: ~50 Å
   - Offset of the electrodes 2(3,5,6) from the corner of the central part: ~ 15 Å

4-lead device	6-lead device
	

[2]:
```
sq = sisl.Geometry([.5] * 3,
                   sisl.Atom(1, R=1.),
                   sc=sisl.SuperCell([1., 1., 10.], nsc=[3, 3, 1]))
```

[3]:
```
el_width = 30 # Width of the electrode (perpendicular to semi-inf. direction)
el_length = 1 # Length of the electrode (in the semi-inf. direction)
el_offx = 25  # Offset along x-axis of electrodes from the corners of the␣
 ↪device
el_offy = 0   # Offset along y-axis of electrodes from the corners of the device
el_pad = 50   # Distance between electrodes (only for 6-lead device)


el_x = sq.tile(el_width, 1).tile(el_length, 0)
el_y = sq.tile(el_width, 0).tile(el_length, 1)
```

4-lead device

[4]:
```
nx = 1 * el_width + 2 * el_offx
ny = 1 * el_width + 2 * el_offy
center = sq.tile(nx, 0).tile(ny, 1)

# Create space for the electrode regions
dev = center.prepend(el_x.sc, axis=0).prepend(el_x.sc, axis=0)
dev = dev.prepend(el_y.sc, axis=1).prepend(el_y.sc, axis=1)
dev = dev.move(el_x.cell[0]+el_y.cell[1])

# These help find atomic indices by their grid position
dev_idx = np.arange(dev.no).reshape((nx,ny), order='F')
el_x_idx = np.arange(el_x.no).reshape((el_length, el_width), order='C')
el_y_idx = np.arange(el_y.no).reshape((el_width, el_length), order='F')

# Attach the electrodes
print("1) Elec.Left\n\t electrode-position", dev.no+1)
dev = dev.attach(dev_idx[0,el_offy], el_x, el_x_idx[-1,0], dist=[-1,0,0])

print("2) Elec.Bottom\n\t  electrode-position", dev.no+1)
```

```
dev = dev.attach(dev_idx[el_offx, 0], el_y, el_y_idx[0,-1], dist=[0,-1,0])

dev = dev.attach(dev_idx[el_offx, -1], el_y, el_y_idx[0,0], dist=[0,1,0])
print("3) Elec.Top\n\t  electrode-position end", dev.no)

dev = dev.attach(dev_idx[-1,el_offy], el_x, el_x_idx[0,0], dist=[1,0,0])
print("4) Elec.Right\n\t  electrode-position end", dev.no)

dev_final = dev
```

```
1) Elec.Left
        electrode-position 2401
2) Elec.Bottom
         electrode-position 2431
3) Elec.Top
         electrode-position end 2490
4) Elec.Right
         electrode-position end 2520
```

6-lead device

[5]:
```
nx = 2 * el_width + 1 * el_pad + 2 * el_offx
ny = 1 * el_width + 2 * el_offy
center = sq.tile(nx, 0).tile(ny, 1)

# Create space for the electrode regions
dev = center.prepend(el_x.sc, axis=0).prepend(el_x.sc, axis=0)
dev = dev.prepend(el_y.sc, axis=1).prepend(el_y.sc, axis=1)
dev = dev.move(el_x.cell[0]+el_y.cell[1])

# These help find atomic indices by their grid position
dev_idx = np.arange(dev.no).reshape((nx,ny), order='F')
el_x_idx = np.arange(el_x.no).reshape((el_length, el_width), order='C')
el_y_idx = np.arange(el_y.no).reshape((el_width, el_length), order='F')

# Attach the electrodes
print("1) Elec.Left\n\t  electrode-position", dev.no+1)
dev = dev.attach(dev_idx[0,el_offy], el_x, el_x_idx[-1,0], dist=[-1,0,0])

print("2) Elec.BottomLeft\n\t  electrode-position", dev.no+1)
dev = dev.attach(dev_idx[el_offx, 0], el_y, el_y_idx[0,-1], dist=[0,-1,0])

print("3) Elec.BottomRight\n\t  electrode-position", dev.no+1)
dev = dev.attach(dev_idx[-1-el_offx, 0], el_y, el_y_idx[-1,-1], dist=[0,-1,0])

dev = dev.attach(dev_idx[-1,el_offy], el_x, el_x_idx[0,0], dist=[1,0,0])
print("4) Elec.Right\n\t  electrode-position end", dev.no)
```

```
dev = dev.attach(dev_idx[-1-el_offx, -1], el_y, el_y_idx[-1,0], dist=[0,1,0])
print("5) Elec.TopRight\n\t  electrode-position end", dev.no)

dev = dev.attach(dev_idx[el_offx, -1], el_y, el_y_idx[0,0], dist=[0,1,0])
print("6) Elec.TopLeft\n\t  electrode-position end", dev.no)

dev_final = dev
```

```
1) Elec.Left
          electrode-position 4801
2) Elec.BottomLeft
          electrode-position 4831
3) Elec.BottomRight
          electrode-position 4861
4) Elec.Right
          electrode-position end 4920
5) Elec.TopRight
          electrode-position end 4950
6) Elec.TopLeft
          electrode-position end 4980
```

1.2.2 2. Construct Hamiltonian and add magnetic fields

The required field strengths may vary depending on the size of the Hall bar. We should start with a corse grid, and create a finer grid once we have identified the correct range. A good starting point might by `B = 1 / np.arange(10,31)`.

[6]:
```
def peierls(self, ia, atoms, atoms_xyz=None, B=None):
    idx = self.geometry.close(ia, R=[0.1, 1.01], atoms=atoms,␣
 ↪atoms_xyz=atoms_xyz)
    # Onsite
    self[ia, idx[0]] = 4

    # Hopping
    if B == 0:
        self[ia, idx[1]] = -1
    else:
        xyz = self.geometry.xyz[ia]
        dxyz = self.geometry[idx[1]]
        self[ia, idx[1]] = - np.exp(-0.5j * B * (dxyz[:, 0] - xyz[0])*(dxyz[:
 ↪,1] + xyz[1]))
```

[7]:
```
# Create hamiltonian for the electrodes
H_el = sisl.Hamiltonian(el_x, dtype=np.float64)
H_el.set_nsc([3,1,1])
H_el.construct(functools.partial(peierls, B=0.))
H_el.write('ELEC_x.nc')
```

```
H_el = sisl.Hamiltonian(el_y, dtype=np.float64)
H_el.set_nsc([1,3,1])
H_el.construct(functools.partial(peierls, B=0.))
H_el.write('ELEC_y.nc')
```

[8]:
```
# Create device hamiltonian without magnetic field
H_dev = sisl.Hamiltonian(dev_final, dtype=np.float64)
H_dev.set_nsc([1,1,1])
H_dev.construct(functools.partial(peierls, B=0))
H_dev.write('DEVICE.nc')
```

[9]:
```
# Calculate device hamiltonian with magnetic field and store dH
dH = sisl.Hamiltonian(dev_final, dtype=np.complex128)
dH.set_nsc([1,1,1])

# Rec_phis: reciprocal phis, reciprocal mesh is advantages because steps scale␣
 ↪with 1/B and phi ~ B
rec_phis = np.linspace(10,30,21)
for rec_phi in rec_phis:
    dH.construct(functools.partial(peierls, B=1/rec_phi))
    dH = dH - H_dev
    with sisl.get_sile('M_{}.dH.nc'.format(rec_phi), mode='w') as fh:
        fh.write_delta(dH)
```

[10]:
```
# plt.figure(figsize=(4,4), dpi=400)
# plt.imshow(dH.Hk(format='array').imag, interpolation='None')
# plt.colorbar()
```

1.2.3 3. Calculate the transmission with TBtrans

The folder of this exercise contains the skeleton of an input file for a 4-lead (RUN-4.fdf) and 6-lead device (RUN-6.fdf), as well as a script to run TBtrans for all values of the magnetic field (run.sh).

Depending on the size of the Hall bar, this step might require a considerable amount of time.

1.2.4 4. Extract the Hall resistance (R_H)

In Hall effect we measure the build up of a potential difference between the measurement electrodes as response to an electric current. The Hall resistance (R_H) in a 4 lead Hall bar like the one shown above is given by

$$R_H = \left.\frac{V_2 - V_3}{I_1}\right|_{I_2=I_3=0}.$$

In `TBtrans` the chemical potentials of all electrodes can be specified and the currents are calculated as a response to the biases. Rather than trying many combinations of chemical potentials to find the Hall resistance, we use transmission curves to calculate R_H.

To start, we express the lead currents I_i in terms of applied biases V_i and the transmissions T_{ij} between leads i and j

$$I_i = \sum_j G_{ij}(V_i - V_j) \quad \text{where} \quad G_{ij} = \frac{2e^2}{h} T_{ij}.$$

We rewrite this relation as

$$\mathbf{I} = \mathcal{G}\mathbf{V} \quad \text{, where} \quad \mathcal{G}_{ii} = \sum_{i \neq j} G_{ij} \quad \text{and} \quad \mathcal{G}_{ij} = -G_{ij}.$$

Since the currents only depend on bias differences, we can set one of them to zero without loss of generality (here $V_4 = 0$). Further, Kirchhoff's current law allow us to eliminate one of current (here $I_4 = -I_1 - I_2 - I_3$). This leaves us with an invertible 3×3 matrix equation.

Using the inverse $\mathbf{R}$ of $\mathcal{G}$, we can express V_2 and V_3 in terms of the lead currents I_i and calculate the Hall conductance:

$$\mathbf{V} = \mathcal{G}^{-1}\mathbf{I} = \mathbf{R}\mathbf{I} \quad \Rightarrow \quad V_i = R_{i1}I_1 + R_{i2}I_2 + R_{i3}I_3,$$

and finally, we find the Hall resistance:

$$R_H = \left. \frac{R_{21}I_1 + R_{22}I_2 + R_{23}I_3 - (R_{31}I_1 + R_{32}I_2 + R_{33}I_3)}{I_1} \right|_{I_2 = I_3 = 0} \tag{1}$$

$$= R_{21} - R_{31} \tag{2}$$

The derivation for the 6-lead device is analogous and yields:

$$R_H = R_{21} - R_{61}$$

If everything is set up correctly, the quantization of the Hall resistance should be visible.

$$R_H = \frac{h}{2ne^2} \qquad \text{for square lattice Hall bar} \qquad n \in \mathbb{N} \tag{3}$$

$$R_H = \frac{h}{2(2n-1)e^2} \qquad \text{for graphene Hall bar} \qquad n \in \mathbb{N} \tag{4}$$

1.2.5 5. Extract longitudinal resistance R_L

The longitudinal resistance can be extracted using the same approach used for the Hall resistance. With a 6-lead Hall bar we can replace the V_3 with V_6 and get it immediately.

$$R_L = R_{21} - R_{31}$$

With a 4-lead Hall bar we need to create a new device with electrodes 2 and 3 on the same side of the Hall bar.

If the energy mesh in TBTrans and the mesh for magnetic field strength are fine engough, spikes in R_L should be observable at each step of R_H.

[11]:
```
# Create short-hand function to open files
gs = sisl.get_sile
# No magnetic field
tbt0 = gs('M_0/siesta.TBT.nc')
# All magnetic fields in increasing order
tbts = [gs('M_{}/siesta.TBT.nc'.format(rec_phi)) for rec_phi in rec_phis]
```

[12]:
```
# Create matrix G
def Tmatrix (tbtsile, n, E_idx, ref_idx):
    mT = np.zeros((E_idx, n, n))
    for i in range(n):
        for j in range(n):
            if i == j: continue
            Tij = tbtsile.transmission(i,j)
            mT[:,i,j] = -Tij
            mT[:,i,i] += Tij
    return np.delete(np.delete(mT, ref_idx, axis=2), ref_idx, axis=1)

E = tbt0.E
n, E_idx, ref_idx = 6, E.shape[0], 3
T0 = Tmatrix(tbt0, n, E_idx, ref_idx)

T = np.zeros((len(rec_phis), E_idx, n-1, n-1))
for i, tbt in enumerate(tbts):
    T[i] = Tmatrix(tbt, n, E_idx, ref_idx)
```

[13]:
```
# Calculate inverse of G
R0 = np.linalg.inv(T0)
R = np.linalg.inv(T)

# Extract RH (and longitudial resistance for 6-lead device (R_L))
RH = R0[:,1,0] - R0[:,4,0]
RL = R0[:,1,0] - R0[:,2,0]
RH = R[:,:,1,0] - R[:,:,4,0]
RL = R[:,:,1,0] - R[:,:,2,0]
```

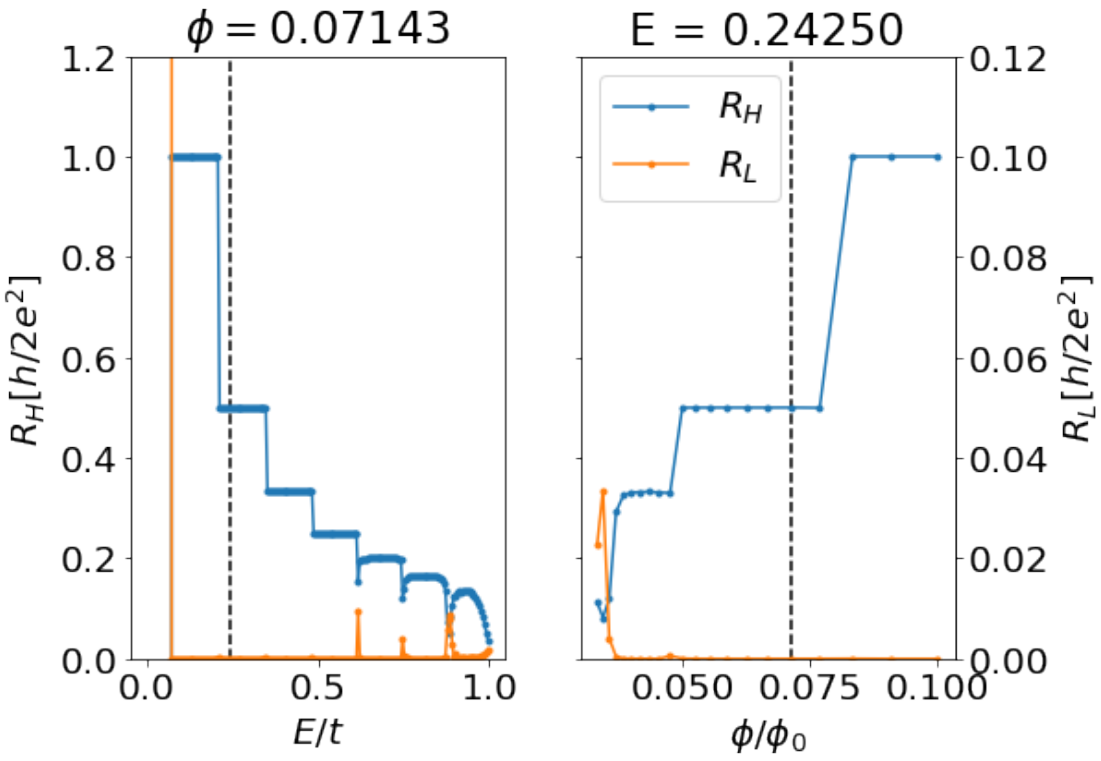
[15]:
```
# Plot the results
E_idx = 48
phi_idx = 4
plt.rcParams.update({'font.size':20})
fig, axs = plt.subplots(1,2, sharey=True, figsize=(8,6))#, dpi=300)
axs[0].set_title('$\phi = {:.5f}$'.format(1/rec_phis[phi_idx]))
axs[0].axvline(x=E[E_idx], ls='--', c='k')
axs[0].plot(E, RH[phi_idx,:], '.-', label='$R_{H}$')
axs[0].plot(E, 10*RL[phi_idx,:], '.-', label='$R_{L}$')
axs[0].set_ylim(0,1.2)
# axs[0].set_xlim(00.1,0.3)
```

```
axs[1].set_title(f'E = {E[E_idx]:.5f}')
axs[1].axvline(x=1/rec_phis[phi_idx], ls='--', c='k')
axs[1].plot(1/rec_phis, RH[:,E_idx], '.-', label='$R_{H}$')
axs[1].plot(1/rec_phis, 10*RL[:,E_idx], '.-', label='$R_{L}$')

secax = axs[1].secondary_yaxis('right', functions=(lambda y: 0.1*y, lambda y:␣
↪10*y))

axs[0].set_ylabel(r'$R_H \left[h/2e^2\right]$')
axs[0].set_xlabel('$E/t$')
axs[1].set_xlabel('$\phi/\phi_0$')
secax.set_ylabel(r'$R_L \left[h/2e^2\right]$')

axs[1].legend()
plt.show()
```



[ ]: