Quantum transport simulations using Kwant

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ICTP Summer School “Advances in Condensed Matter Physics”,
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I borrowed from a tutorial by J.B. Weston (CC-BY-SA), link at the end

Plan

1. How to solve a scattering problem?
2. How to define and solve it with Kwant?

Kwant

- An open source package for quantum transport
- `https://kwant-project.org`
- New version (1.4) released a couple of months ago
- Works with *tight binding* models
- Main focus on the scattering matrix formalism of quantum transport

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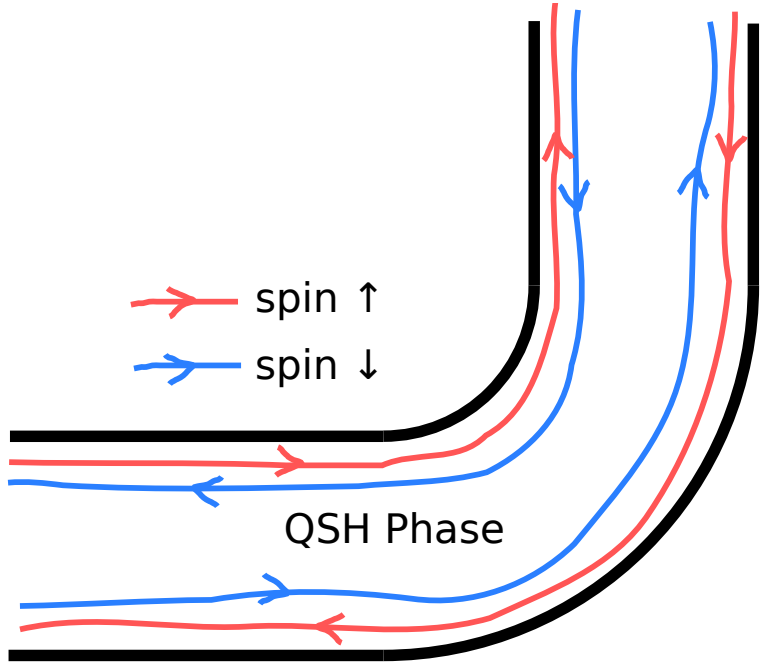
Case study: a bend in a quantum spin Hall insulator

- Topologically protected transmission across a bend
- $k \cdot p$ Hamiltonian

$$
\begin{aligned}
H(k_x, k_y) = & \\
& + \mu - D(k_x^2 + k_y^2) \\
& + [M - B(k_x^2 + k_y^2)]\tau_z \\
& + A[k_x \sigma_z \tau_x + k_y \tau_y]
\end{aligned}
$$



Discretize

- Kwant works with *tight-binding models* and a finite number of degrees of freedom
- $\Rightarrow$ discretize space onto a square lattice with lattice spacing a

$$k_x^2 \to \frac{\partial^2}{\partial x^2} \to \frac{1}{4a^2} \begin{pmatrix} \ddots & \ddots & & & \\ \ddots & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & \ddots & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

In Kwant

Discretize

```
import kwant

bhz_continuum = '''
    + mu * kron(sigma_0, sigma_0)
    + M * kron(sigma_0, sigma_z)
    - B * (k_x**2 + k_y**2) * kron(sigma_0, sigma_z) - D * (k_x**2 + k_y**2) * kron(sigma_0, sigma_0)
    + A * (k_x * kron(sigma_z, sigma_x) + k_y * kron(sigma_0, sigma_y))
'''
qshe_model = kwant.continuum.discretize(bhz_continuum)
```

Check the matrix elements

```
tb_matrix_elements, coords = kwant.continuum.discretize_symbolic(bhz_continuum)
tb_matrix_elements[0, 0]  # onsite
```

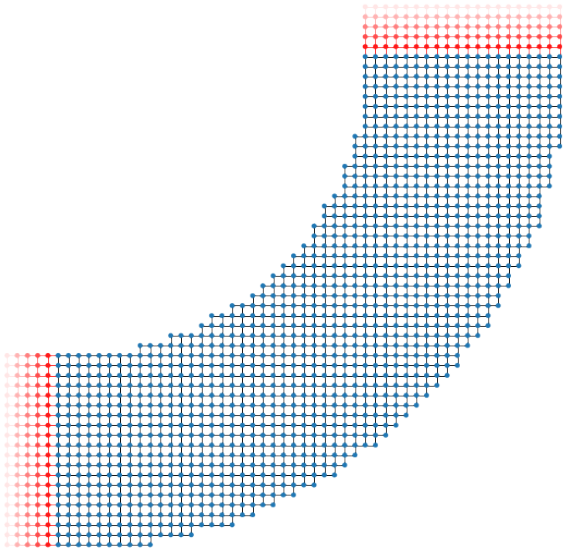
$$\begin{bmatrix} -\frac{2B}{a_y^2} - \frac{2B}{a_x^2} - \frac{2D}{a_y^2} - \frac{2D}{a_x^2} + M + \mu & 0 & 0 & 0 \\ 0 & \frac{2B}{a_y^2} + \frac{2B}{a_x^2} - \frac{2D}{a_y^2} - \frac{2D}{a_x^2} - M + \mu & 0 & 0 \\ 0 & 0 & -\frac{2B}{a_y^2} - \frac{2B}{a_x^2} - \frac{2D}{a_y^2} - \frac{2D}{a_x^2} + M + \mu & 0 \\ 0 & 0 & 0 & \frac{2B}{a_y^2} + \frac{2B}{a_x^2} - \frac{2D}{a_y^2} - \frac{2D}{a_x^2} - M + \mu \end{bmatrix}$$

Check the symmetries

```
symmetries = kwant.qsymm.find_builder_symmetries(qshe_model)
print(f"{len(symmetries)} symmetries found.")
```

```
17 symmetries found.
```

Infinite system



has the Hamiltonian:

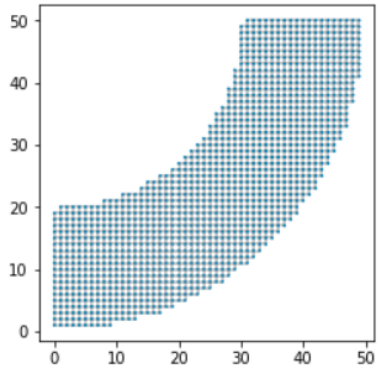
$$H = \begin{pmatrix} \ddots & V_L & & \\ V_L^\dagger & H_L & V_L & \\ & V_L^\dagger & H_L & V_L \\ & & V_L^\dagger & H_S \end{pmatrix}$$

(H_L and V_L are block-diagonal if there are many leads)

In Kwant

Scattering region

```
syst = kwant.Builder() # We'll fill this with the TB model of our scattering region

def scattering_region(site):
    x, y = site.tag  # position in integer lattice coordinates
    y = y - 50
    return (30**2 < (x**2 + y**2) < 50**2  # inside a ring
            and (x >= 0 and y <= 0))  # lower-right quadrant ofring

# Fill our scattering region with the BHZ model in a certain region of space
syst.fill(template=qshe_model, shape=scattering_region, start=(0, 10))

kwant.plot(syst);
```



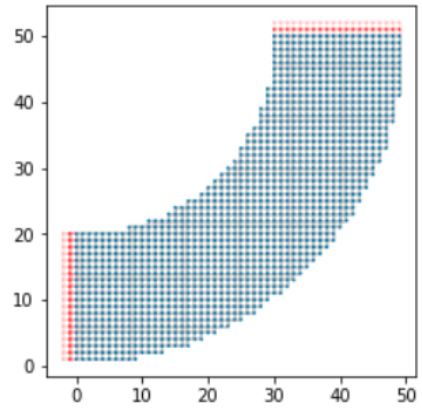
In Kwant

Make a lead

```
lead_x = kwant.Builder(
    symmetry=kwant.TranslationalSymmetry((-1, 0)),
    time_reversal=np.kron(1j * sigma_y, sigma_0),
    conservation_law=np.kron(-sigma_z, sigma_0),  # spin conservation
)

lead_x.fill(qshe_model, lambda site: 1 <= site.tag[1] <= 20, (0, 1))
```

Combine everything

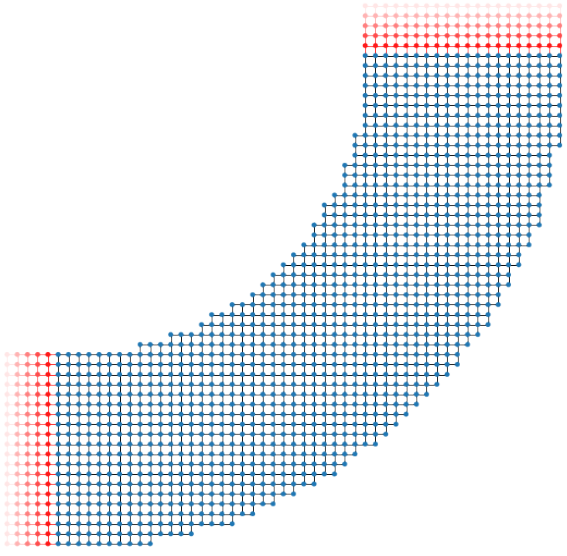
```
syst.attach_lead(lead_x)
syst.attach_lead(lead_y)

kwant.plot(syst);
```




```
fsyst = syst.finalized()  # Transform the system into an efficient form for numerics
print(fsyst)
```

```
<FiniteSystem with 1272 sites, 4888 hoppings, and parameters: ('M', 'B', 'D', 'A', 'mu')>
```

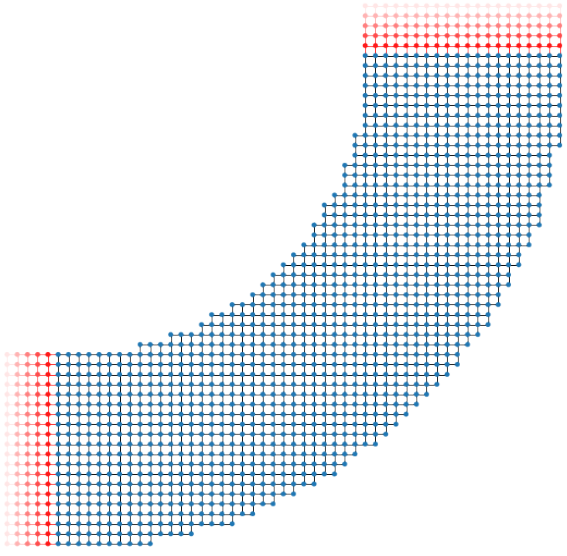
Scattering problem



Now to get conductance and other observables, we only need to calculate Σ_{lead}, G^R, $G^<$, and we're done.

(that is what one mostly hears)

Scattering problem



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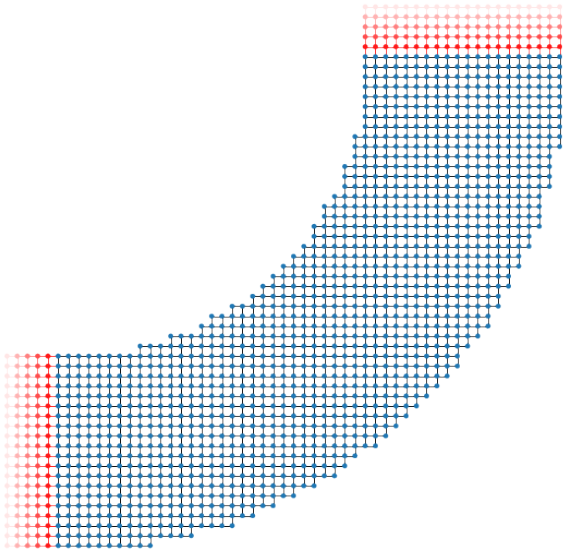
. . . But there is a more intuitive definition.

Scattering problem



Problem statement:

$$H = \begin{pmatrix} \ddots & V_L & & \\ V_L^\dagger & H_L & V_L & \\ & V_L^\dagger & H_L & V_L \\ & & V_L^\dagger & H_S \end{pmatrix}, \quad \psi = \begin{pmatrix} \vdots \\ \psi_2 \\ \psi_1 \\ \psi_S \end{pmatrix}$$

We are solving $(H - E)\psi = 0$ with a *fixed* E.

Modes in the lead

Since the leads are translationally invariant, we decompose the lead wave function into eigenvectors of translation (lead modes)

$$\psi_j = \lambda^j \psi_0,$$

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or in a matrix form:

$$\begin{pmatrix} -V_L^{-1} H_L & -V_L^{-1} \\ V_L^\dagger & 0 \end{pmatrix} \begin{pmatrix} \psi_0 \\ V_L^\dagger \psi_1 \end{pmatrix} = \lambda^{-1} \begin{pmatrix} \psi_0 \\ V_L^\dagger \psi_1 \end{pmatrix}$$

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. . . or in a more stable form and reduced basis:

$$\begin{pmatrix} iA^\dagger \tilde{H}^{-1} B & -A^\dagger \tilde{H}^{-1} B \\ -1 + iB^\dagger \tilde{H}^{-1} B & -B^\dagger \tilde{H}^{-1} B \end{pmatrix} \begin{pmatrix} \tilde{\psi}_0 \\ \tilde{\psi}_1 \end{pmatrix} = \lambda^{-1} \begin{pmatrix} A^\dagger \tilde{H}^{-1} A & -1 - iA^\dagger \tilde{H}^{-1} A \\ B^\dagger \tilde{H}^{-1} A & -iB^\dagger \tilde{H}^{-1} A \end{pmatrix} \begin{pmatrix} \tilde{\psi}_0 \\ \tilde{\psi}_1 \end{pmatrix},$$

$$\tilde{H} = H_L + iAA^\dagger + iBB^\dagger, \quad V_L = AB^\dagger, \quad \tilde{\psi}_0 = B^+ \psi_0, \quad \tilde{\psi}_1 = A^+ \psi_1$$

Separating the modes

Split all the eigenvectors into incoming, outgoing and evanecsent, such that:

$$\langle \psi_{\text{in}} | \hat{I} | \psi_{\text{in}} \rangle = 1$$

$$\langle \psi_{\text{out}} | \hat{I} | \psi_{\text{out}} \rangle = -1$$

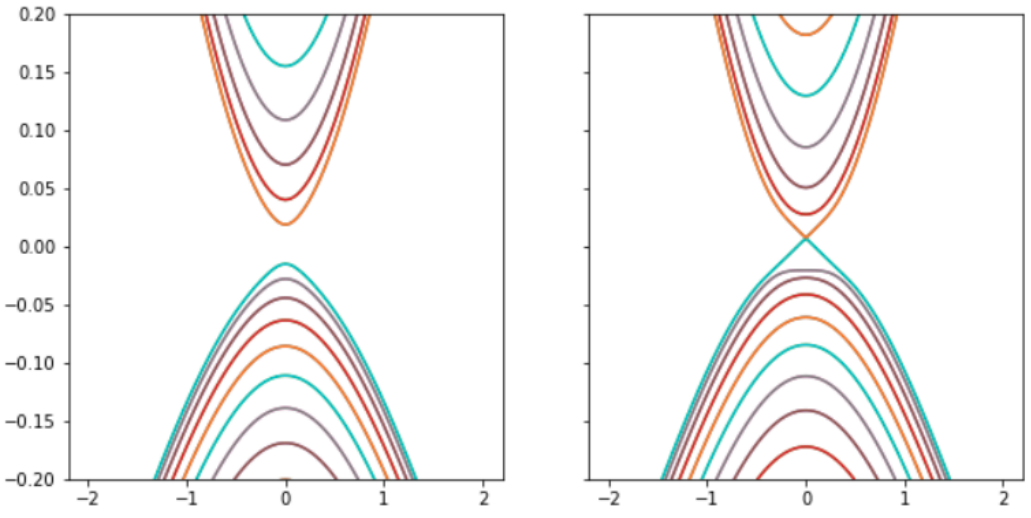
$$\langle \psi_{\text{evan}} | \hat{I} | \psi_{\text{out}} \rangle = 0, \quad |\lambda_{\text{evan}}| < 1$$

In Kwant

Dispersion

```
topo_params = dict(A=0.09, B=-0.18, D=-0.065, M=-0.02, mu=0)  # Parameters for topological phase
trivial_params = dict(A=0.09, B=-0.18, D=-0.065, M=0.01, mu=0)  # Parameters for trivial phase

fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 5), sharey=True)
kwant.plotter.bands(flead_x, momenta=np.linspace(-2, 2, 101), params=trivial_params, show=False, ax=ax1)
kwant.plotter.bands(flead_x, momenta=np.linspace(-2, 2, 101), params=topo_params, show=False, ax=ax2)
ax1.set_ylim(-.2, .2);
```



Modes at $E = 0$

```
propagating_modes, _ = flead_x.modes(energy=0, params=topo_params)

print(propagating_modes.wave_functions.shape)
print(propagating_modes.velocities)
print(propagating_modes.momenta)
```

```
(80, 4)
[-0.08354984 -0.08354984  0.08354984  0.08354984]
[ 0.08609145  0.08609145 -0.08609145 -0.08609145]
```

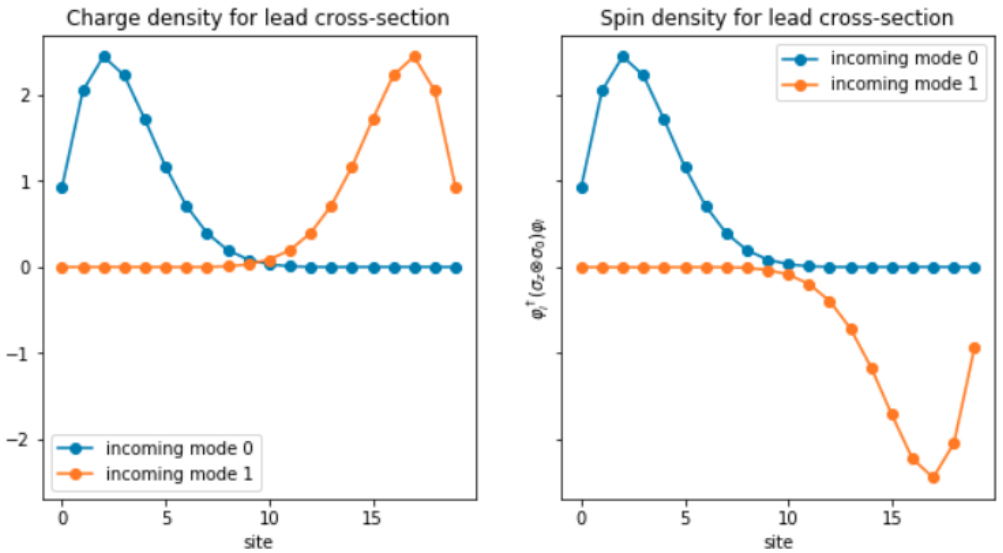
In Kwant

Mode wave functions

```
phi0, phi1 = propagating_modes.wave_functions[:, :2].transpose()

density = kwant.operator.Density(fsyst.leads[0]) # calculate |φ_i|**2 for each site (summing degrees of freedom)
spin_density = kwant.operator.Density(fsyst.leads[0], np.kron(sigma_z, sigma_0))

fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 5), sharey=True)
plot_densities(density(phi0), density(phi1), title='Charge', ax=ax1)
plot_densities(spin_density(phi0), spin_density(phi1), title='Spin', ax=ax2)
```



Equations to solve

Substitute the lead modes into the Hamiltonian and get a linear system:

$$\begin{pmatrix} -U_{\text{out}} & 1 \\ V_L^\dagger U_{\text{out}} \Lambda_{\text{out}} & H_{\text{S}} \end{pmatrix} \begin{pmatrix} \mathbf{S} \\ \psi_S \end{pmatrix} = \begin{pmatrix} U_{\text{in}} \\ -V_{\text{L}}^\dagger U_{\text{in}} \Lambda_{\text{in}}, \end{pmatrix} \tag{1}$$

with U_{in} and U_{out} wave functions of incoming and outgoing modes, and $\Lambda \equiv \text{diag}(\lambda_i)$.

Equations to solve

Substitute the lead modes into the Hamiltonian and get a linear system:

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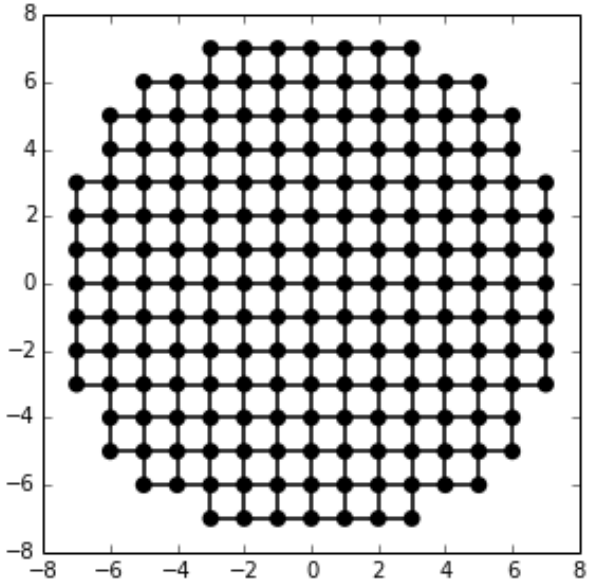
with $U_{\rm in}$ and $U_{\rm out}$ wave functions of incoming and outgoing modes, and $\Lambda \equiv \mathrm{diag}(\lambda_i)$.

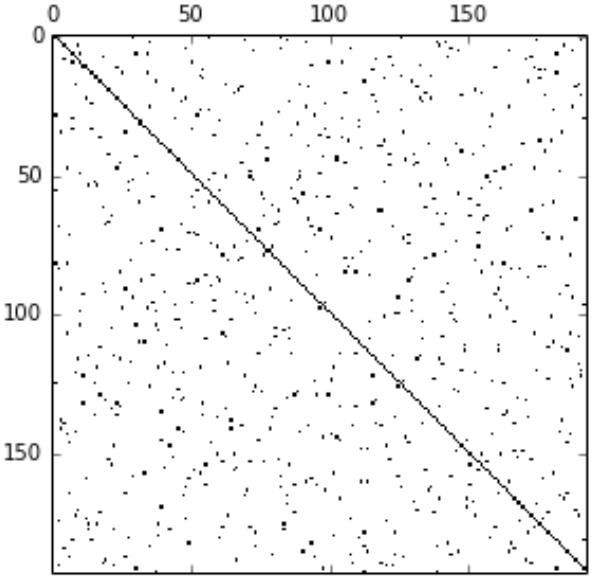
Next: write down these linear equations and solve them.

(NB: if we start by eliminating **S**, the rhs becomes $H_S + \Sigma$)

Solving a scattering problem

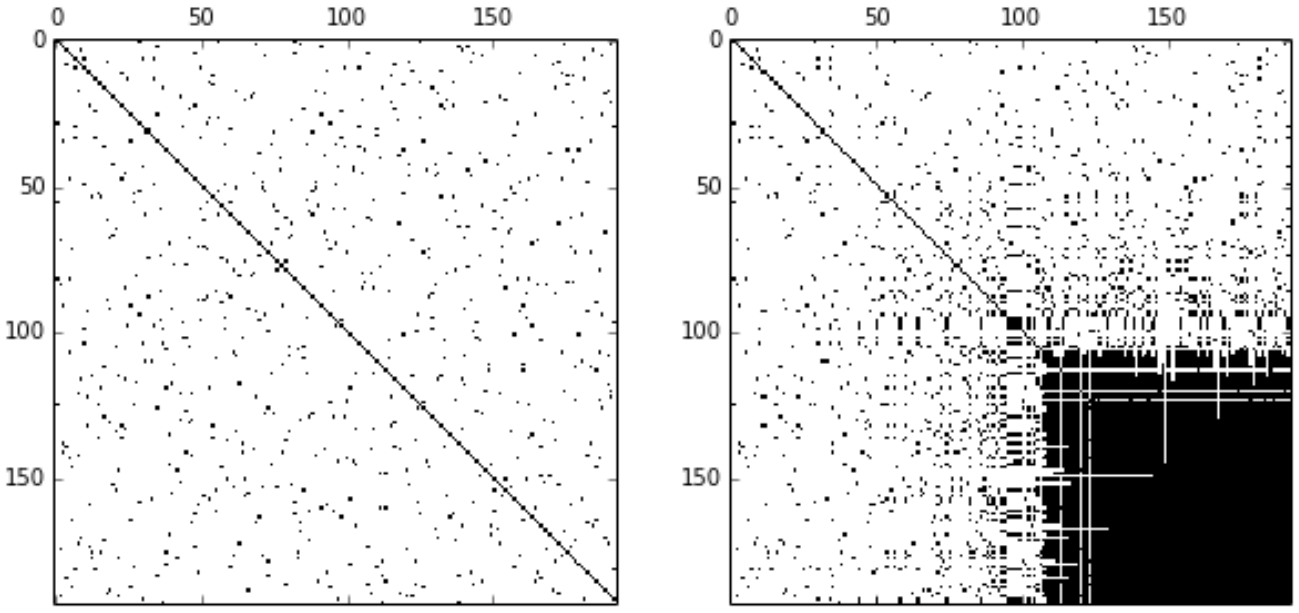
The scattering region is large and its Hamiltonian is sparse.





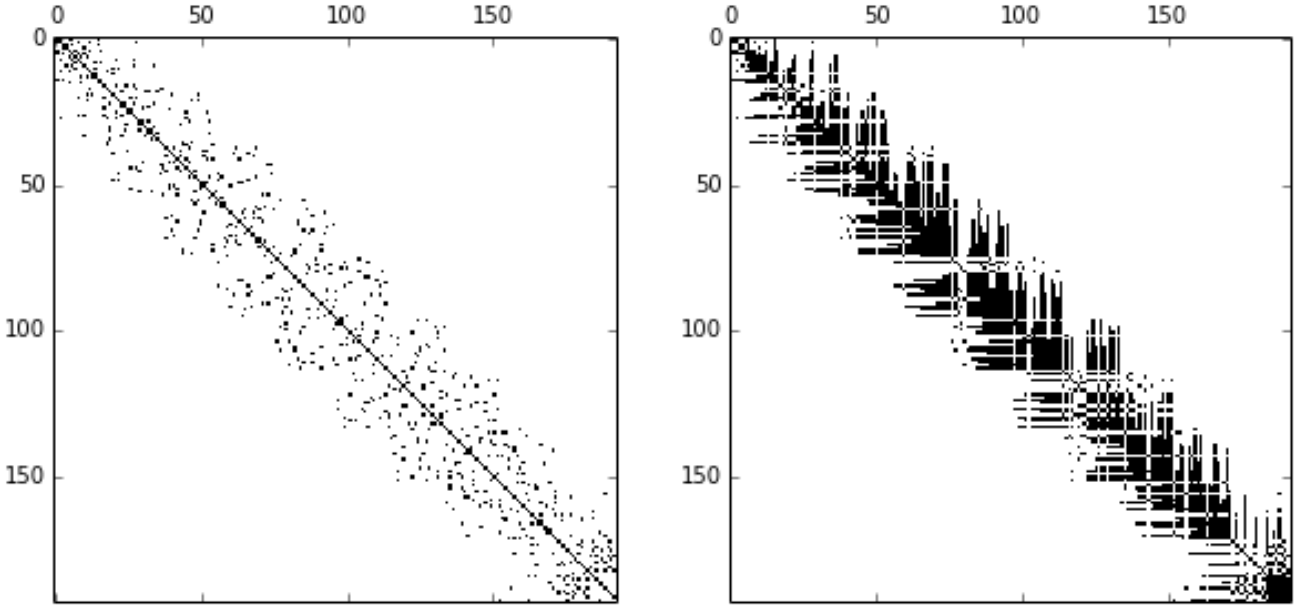
Solving a scattering problem

Naive solution: gaussian elimination
(dense LU decomposition, cost L^6)



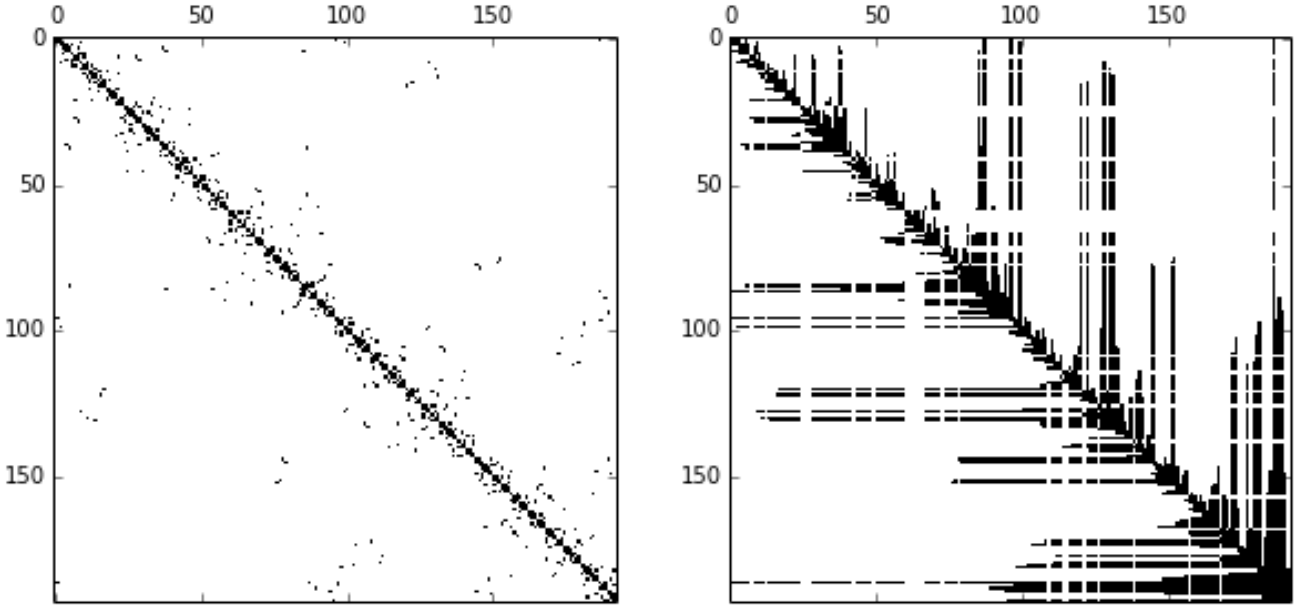
Solving a scattering problem

Better option: reshuffle to reduce bandwidth
("recursive Green's functions", cost L^4)



Solving a scattering problem

What specialized libraries do
(nested dissection, cost L^3, $\sim 10\times$ better):



In Kwant

Scattering matrix

```
S = kwant.smatrix(fsyst, energy=0, params=topo_params)

print(np.round(S.data, 2))
print(S.transmission(1, 0))  # Tr(t . t^†)
```

```
[[-0.  -0.j    0.  +0.j    0.27-0.96j  0.  +0.j  ]
 [-0.  +0.j   -0.  -0.j   -0.  +0.j    0.5 +0.86j]
 [ 0.5 +0.86j  0.  +0.j   -0.  -0.j    0.  +0.j  ]
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1.9999957932536172
```

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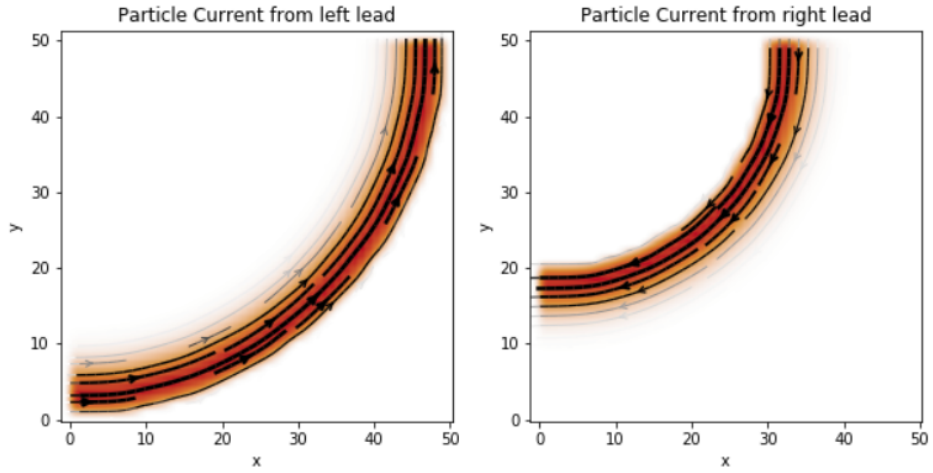
 [ 0.5 +0.86j  0.  +0.j   -0.  -0.j    0.  +0.j  ]
 [-0.  +0.j    0.27-0.96j -0.  +0.j   -0.  -0.j  ]]
1.9999957932536172
```

Current density

```
current = kwant.operator.Current(fsyst).bind(params=topo_params)

(ax0, ax1) = prepare_axes('Particle Current');
kwant.plotter.current(fsyst, current(sl0) , ax=ax0)
kwant.plotter.current(fsyst, current(sr0), ax=ax1)
```



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[[-0.  -0.j    0.  +0.j    0.27-0.96j  0.  +0.j  ]
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 [-0.  +0.j    0.27-0.96j -0.  +0.j   -0.  -0.j  ]]
1.9999957932536172
```
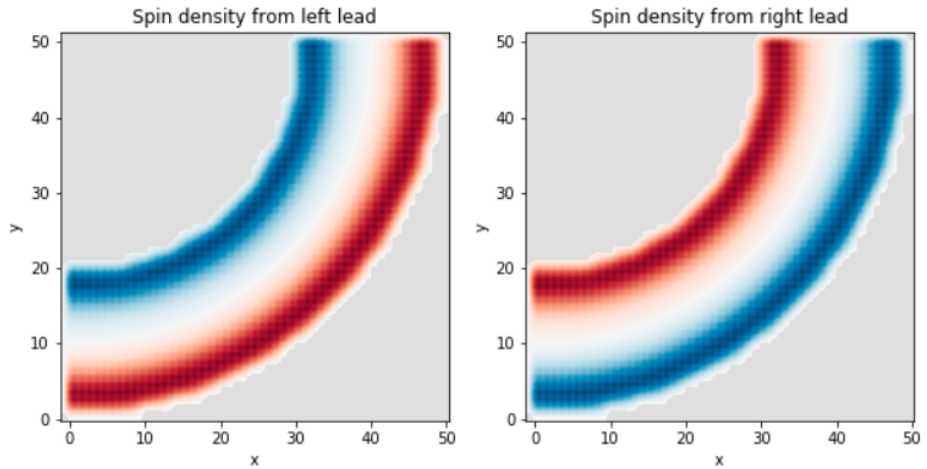

Spin density

```
spin_density = kwant.operator.Density(fsyst, spinz_operator).bind(params=topo_params)

(ax0, ax1) = prepare_axes('Spin density')
kwant.plotter.density(fsyst, spin_density(sl0) + spin_density(sl1), cmap='RdBu_r', ax=ax0)
kwant.plotter.density(fsyst, spin_density(sr0) + spin_density(sr1), cmap='RdBu_r', ax=ax1)
```



Conclusions

- Write down a problem + feed it to a good solver = problem solved
- Kwant does this with quantum transport
- Try a live version at
  `https://tiny.cc/maryland-kwant-tutorial`
  (I used code and images from it)

The end.
Questions?