Lecture_04

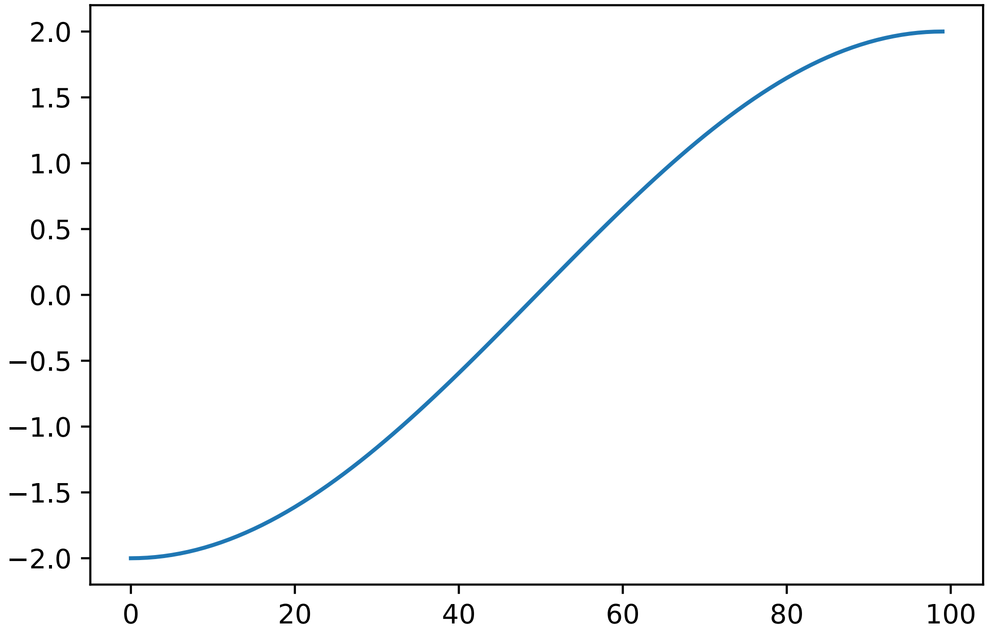
October 28, 2022

[1]:
```
import numpy as np  # for numerics (matrix math)
from scipy.sparse import diags  # for numerics (creating diagonal matrix)
from scipy.stats import gaussian_kde  # for numerics (DOS)
import matplotlib.pyplot as plt  # for plotting

# for vector plots:
import matplotlib_inline.backend_inline
matplotlib_inline.backend_inline.set_matplotlib_formats('svg')
```

[2]:
```
def make_disp(E0, t, a):
    def f(k):
        return E0 + 2*t*np.sum(np.cos(k * a), axis=1)
    return f

E = make_disp(0, -1, np.pi)  # E = E(k)
```

[3]:
```
k_path = np.linspace((0,),(1),100)
plt.plot(E(k_path))
```

[3]:
```
[<matplotlib.lines.Line2D at 0x19956d5bcd0>]
```

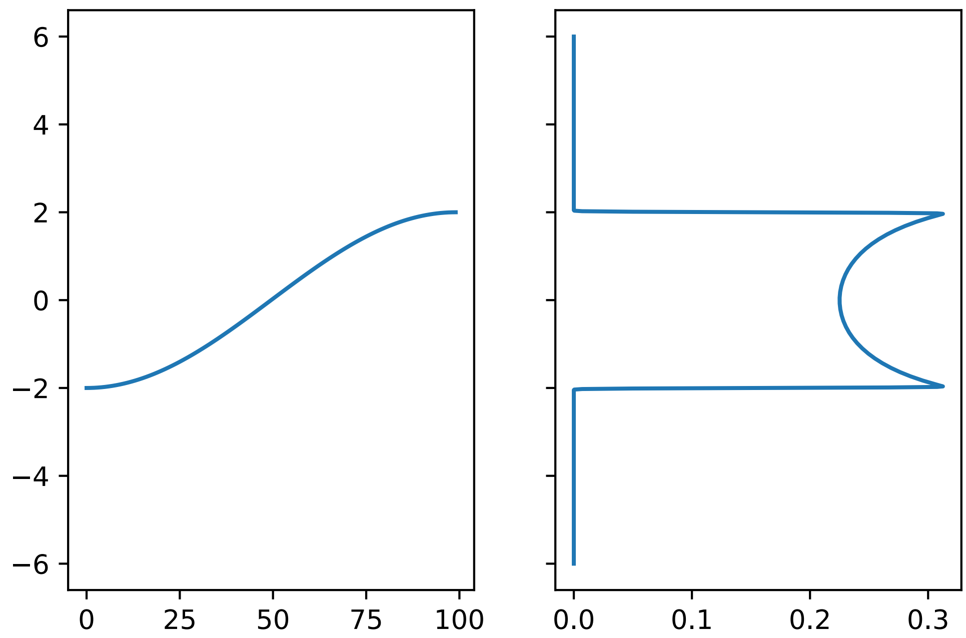


[4]:

```
fig, axs = plt.subplots(ncols=2, sharey=True)
k_mesh = np.mgrid[0:1:1000j].reshape(2,-1).T
es = E(k_mesh)

xrange = np.linspace(-6, 6, 1000)
axs[1].plot(gaussian_kde(es, 0.01).pdf(xrange), xrange)
axs[0].plot(E(k_path))
```

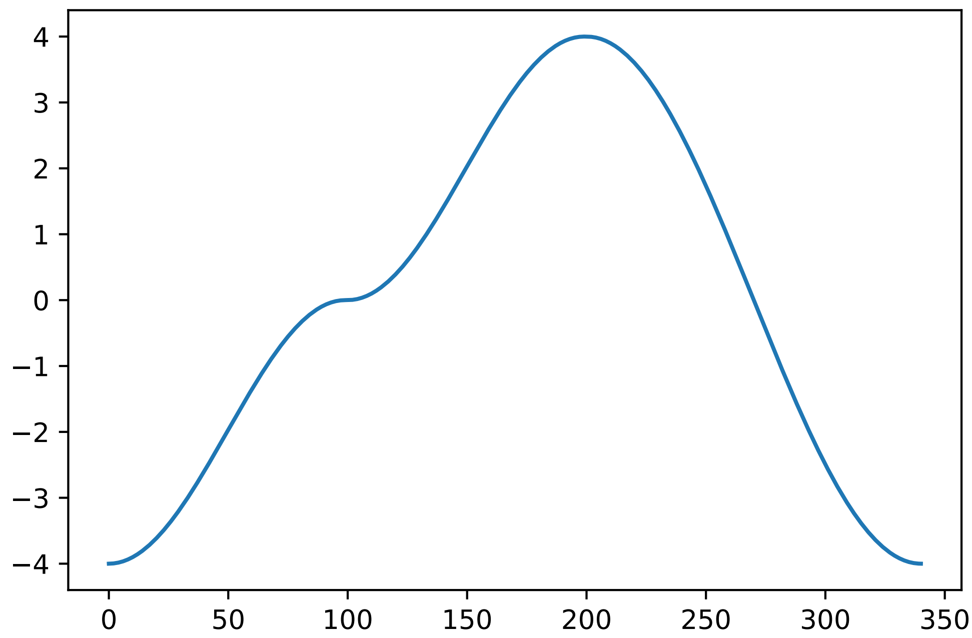
[4]:

```
[<matplotlib.lines.Line2D at 0x19958e942b0>]
```



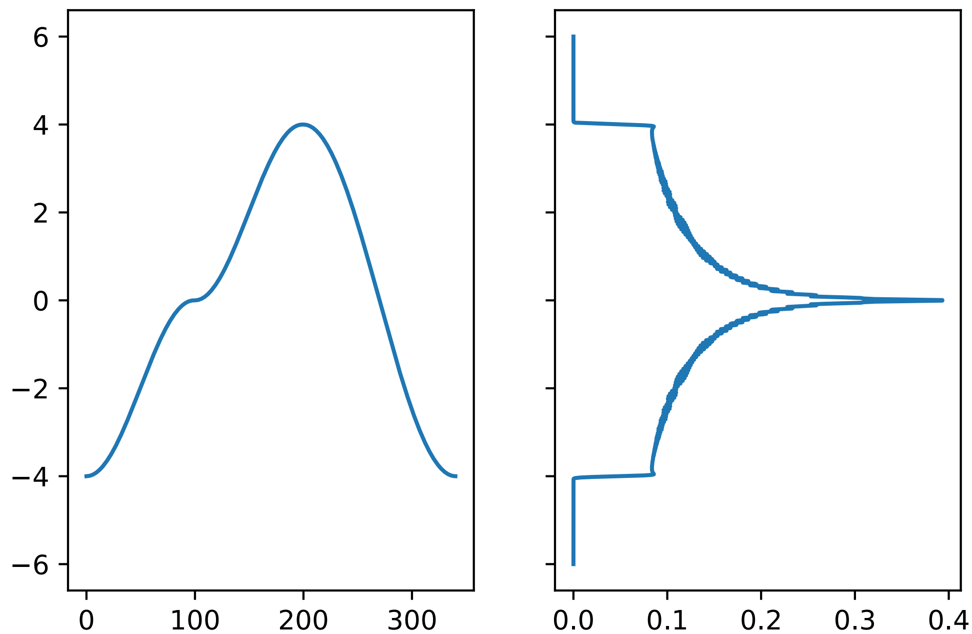
[5]:
```
k_path = np.vstack([np.linspace((0,0),(1,0),100),
                    np.linspace((1,0),(1,1),100),
                    np.linspace((1,1),(0,0),int(np.sqrt(2)*100)),
                  ])
plt.plot(E(k_path))
```

[5]: `[<matplotlib.lines.Line2D at 0x19958f3a2b0>]`



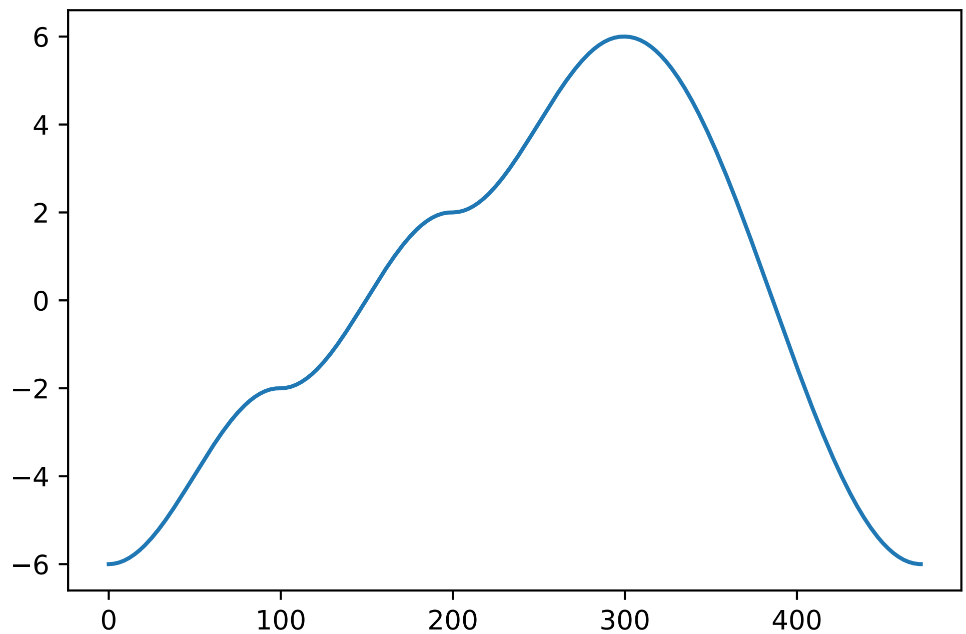
[6]:
```
fig, axs = plt.subplots(ncols=2, sharey=True)
axs[0].plot(E(k_path))
k_mesh = np.mgrid[0:1:100j, 0:1:100j].reshape(2,-1).T
es = E(k_mesh)
axs[1].plot(gaussian_kde(es, 0.01).pdf(xrange), xrange)
```

[6]: [<matplotlib.lines.Line2D at 0x19958fdc970>]



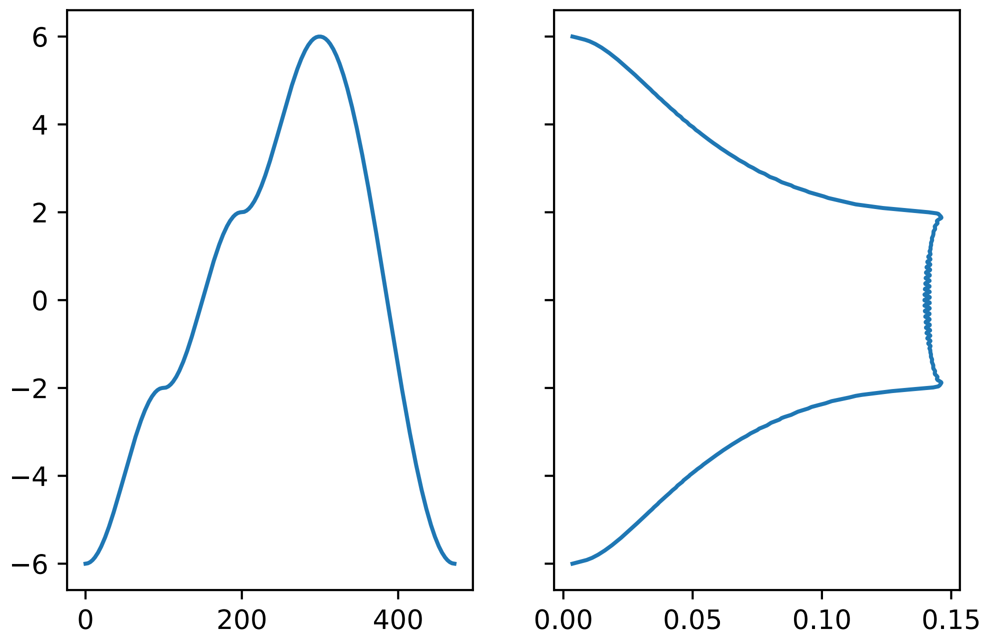
[7]:
```
k_path = np.vstack([np.linspace((0,0,0),(1,0,0),100),
                    np.linspace((1,0,0),(1,1,0),100),
                    np.linspace((1,1,0),(1,1,1),100),
                    np.linspace((1,1,1),(0,0,0),int(np.sqrt(3)*100)),
                  ])
plt.plot(E(k_path))
```

[7]: [<matplotlib.lines.Line2D at 0x199590aee50>]



[8]:
```
fig, axs = plt.subplots(ncols=2, sharey=True)
axs[0].plot(E(k_path))
k_mesh = np.mgrid[0:1:50j, 0:1:50j, 0:1:50j].reshape(3,-1).T
es = E(k_mesh)
axs[1].plot(gaussian_kde(es, 0.02).pdf(xrange), xrange)
```

[8]: [<matplotlib.lines.Line2D at 0x1995916d5b0>]



[9]:
```
def chain(N, E0, t):
    return diags([(N-1)*[t], N*[E0], (N-1)*[t]], (-1, 0, 1)).todense()
```

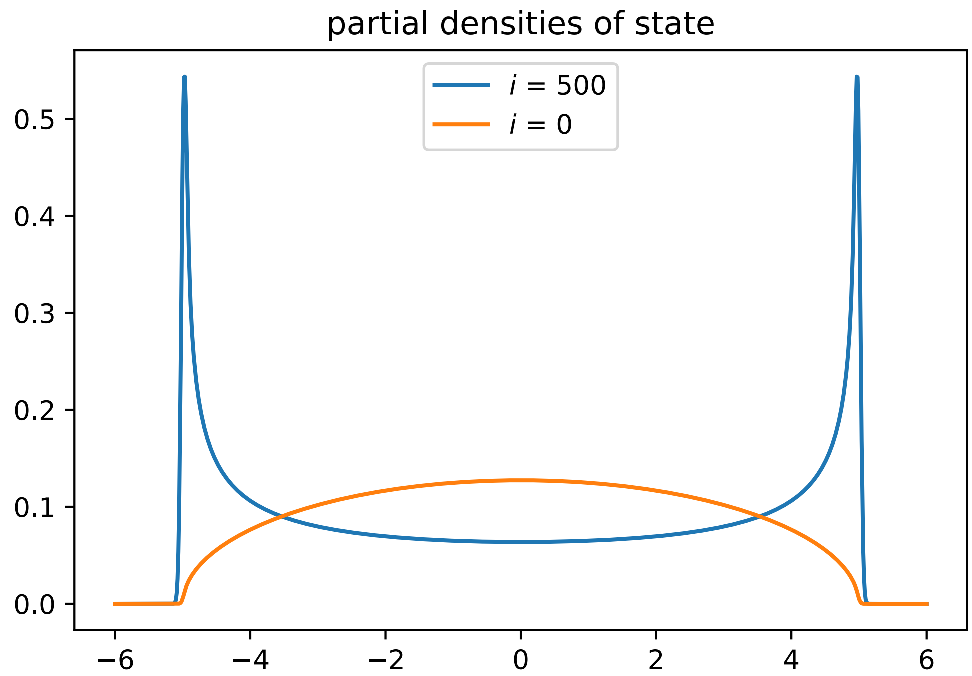
1 No impurity

[10]:
```
H_chain = chain(1001, 0, 2.5)
```

[11]:
```
ew, ev = np.linalg.eigh(H_chain)
```

[12]:
```
weight1 = np.abs(ev.A[500])**2
weight2 = np.abs(ev.A[0])**2

xrange = np.linspace(-6, 6, 1000)
pdos1 = gaussian_kde(ew, 0.01, weights=weight1).pdf(xrange)
pdos2 = gaussian_kde(ew, 0.01, weights=weight2).pdf(xrange)

plt.plot(xrange, pdos1,
         label='$i$ = 500')
plt.plot(xrange, pdos2,
         label='$i$ = 0')
plt.title('partial densities of state')
plt.legend()
```

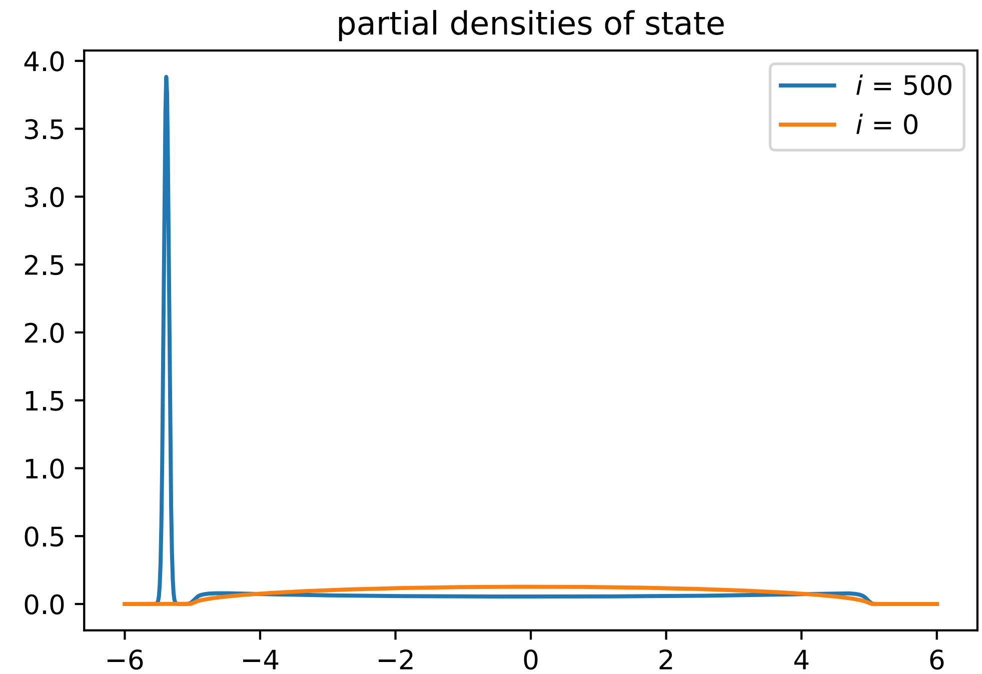
[12]: <matplotlib.legend.Legend at 0x199594dc640>



2 Impurity at site N/2

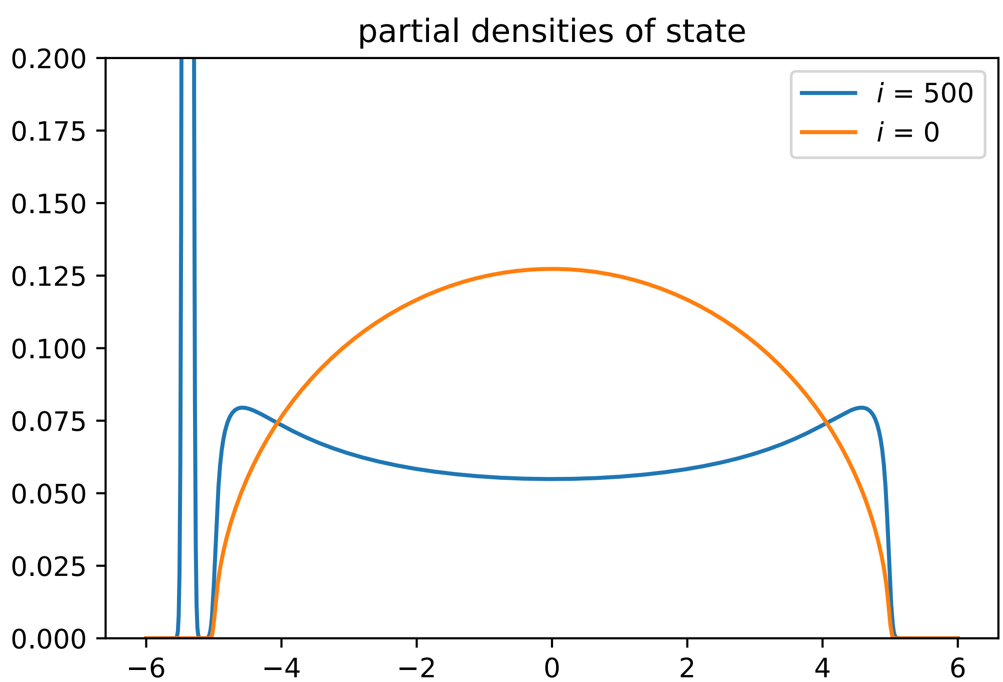
[13]:
```
H_chain = chain(1001, 0, 2.5)
i_imp = 500
H_chain[i_imp, i_imp] = -2
ew, ev = np.linalg.eigh(H_chain)
```

[14]:
```
weight1 = np.abs(ev.A[500])**2
weight2 = np.abs(ev.A[0])**2

pdos1 = gaussian_kde(ew, 0.01, weights=weight1).pdf(xrange)
pdos2 = gaussian_kde(ew, 0.01, weights=weight2).pdf(xrange)

plt.plot(xrange, pdos1,
         label='$i$ = 500')
plt.plot(xrange, pdos2,
         label='$i$ = 0')
plt.title('partial densities of state')
plt.legend()
f, ax = plt.gcf(), plt.gca()
```



[15]:
```
ax.set_ylim(0, 0.2)
f
```

[15]:



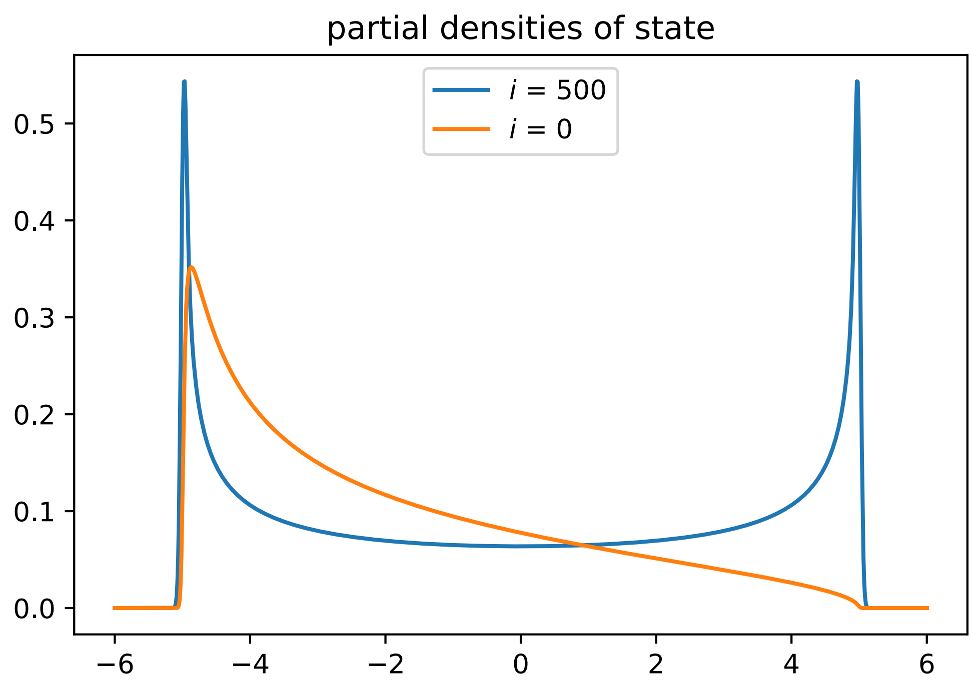
3 Impurity at site 0

[16]:
```python
H_chain = chain(1001, 0, 2.5)
i_imp = 0
H_chain[i_imp, i_imp] = -2
ew, ev = np.linalg.eigh(H_chain)
H_chain
```

[16]:
```
matrix([[-2. ,  2.5,  0. , …,  0. ,  0. ,  0. ],
        [ 2.5,  0. ,  2.5, …,  0. ,  0. ,  0. ],
        [ 0. ,  2.5,  0. , …,  0. ,  0. ,  0. ],
        …,
        [ 0. ,  0. ,  0. , …,  0. ,  2.5,  0. ],
        [ 0. ,  0. ,  0. , …,  2.5,  0. ,  2.5],
        [ 0. ,  0. ,  0. , …,  0. ,  2.5,  0. ]])
```

[17]:
```python
weight1 = np.abs(ev.A[500])**2
weight2 = np.abs(ev.A[0])**2

xrange = np.linspace(-6, 6, 1000)
pdos1 = gaussian_kde(ew, 0.01, weights=weight1).pdf(xrange)
pdos2 = gaussian_kde(ew, 0.01, weights=weight2).pdf(xrange)

plt.plot(xrange, pdos1,
         label='$i$ = 500')
plt.plot(xrange, pdos2,
         label='$i$ = 0')
plt.title('partial densities of state')
plt.legend()
```

[17]:
```
<matplotlib.legend.Legend at 0x19959d2d580>
```




```
[18]: def imp(delta, i_imp=0):
          H_chain = chain(1001, 0, 2.5)
          H_chain[i_imp, i_imp] = delta
          ew, ev = np.linalg.eigh(H_chain)

          weight1 = np.abs(ev.A[500])**2
          weight2 = np.abs(ev.A[0])**2

          xrange = np.linspace(-6, 6, 1000)
          pdos1 = gaussian_kde(ew, 0.01, weights=weight1).pdf(xrange)
          pdos2 = gaussian_kde(ew, 0.01, weights=weight2).pdf(xrange)

          plt.plot(xrange, pdos1,
                   label='$i$ = 500')
          plt.plot(xrange, pdos2,
                   label='$i$ = 0')
          plt.title(f'partial densities of state\nBound state energy difference:␣
       ↪{ew[1]-ew[0]:.2f}eV')
          plt.legend()
```

```
[19]: from ipywidgets import interact, FloatSlider, IntSlider
      i = interact(imp,
                   delta=FloatSlider(-2, min=-5, max=2, step=0.25,␣
       ↪continuous_update=False),
```

```
              i_imp=IntSlider(0, min=0, max=500, step=1,␣
↪continuous_update=False))
```

```
interactive(children=(FloatSlider(value=-2.0, continuous_update=False,␣
↪description='delta', max=2.0, min=-5.0,…
```

[ ]:

```

```