Lecture_03

October 28, 2022

[1]:

```python
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]:

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

[3]:

```python
def ring(N, E0, t):
    H = chain(N, E0, t).todense()
    H[0, N-1] = t
    H[N-1, 0] = t
    return H
```

[4]:

```python
# %timeit np.linalg.eigvalsh(ring(1001, 0, 2.5))  # 90ms
# %timeit np.linalg.eigvals(ring(1001, 0, 2.5))  # 900ms
H = ring(1001, 0, 2.5)
ev = np.linalg.eigvalsh(H)
print(H)
```

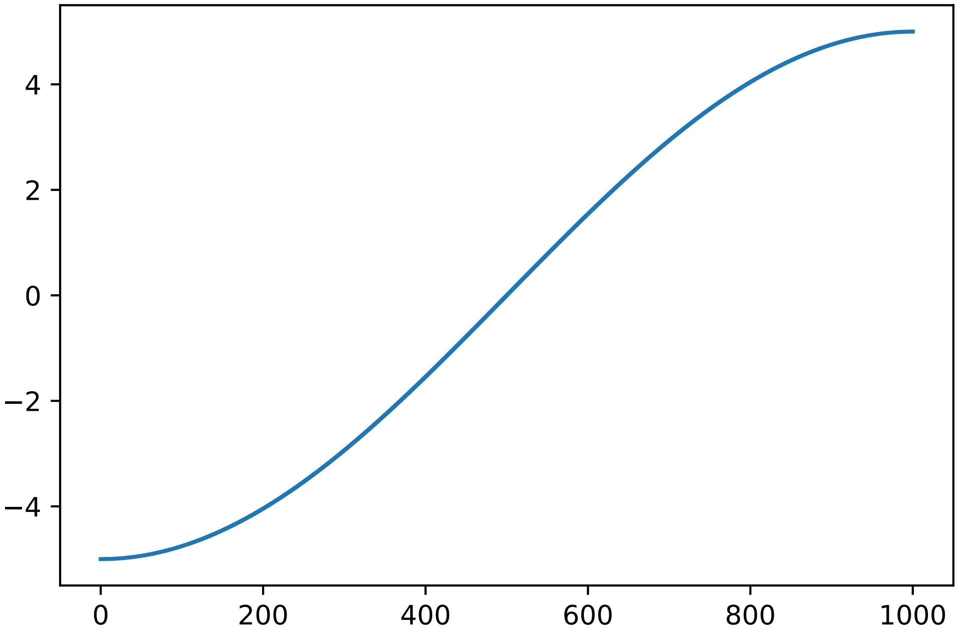
```
[[0.  2.5 0.  … 0.  0.  2.5]
 [2.5 0.  2.5 … 0.  0.  0. ]
 [0.  2.5 0.  … 0.  0.  0. ]
 …
 [0.  0.  0.  … 0.  2.5 0. ]
 [0.  0.  0.  … 2.5 0.  2.5]
 [2.5 0.  0.  … 0.  2.5 0. ]]
```

[5]:

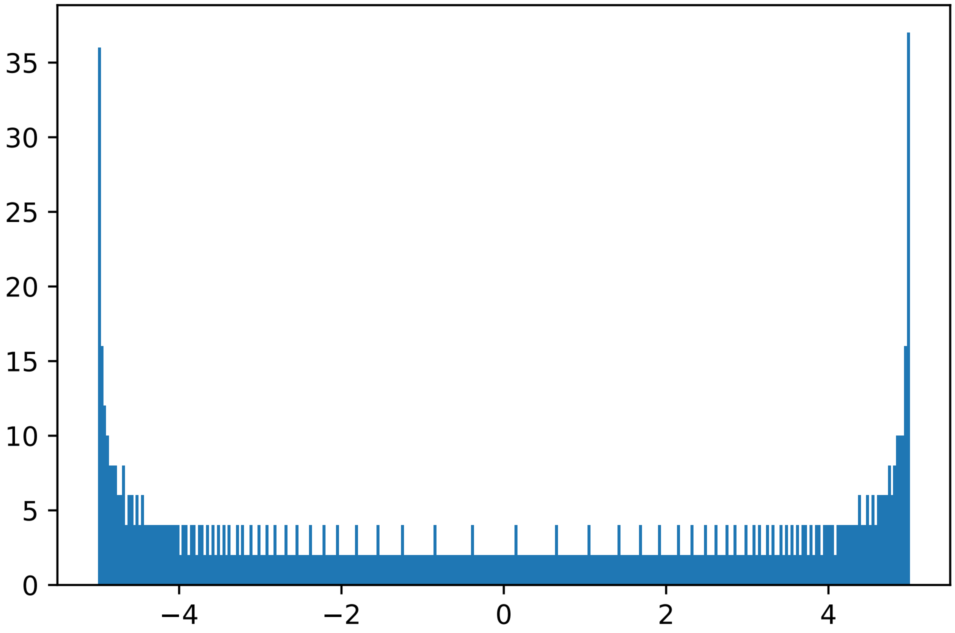
```python
plt.plot(ev)
```

[5]:

```
[<matplotlib.lines.Line2D at 0x18f917d7df0>]
```



[6]:
```
h = plt.hist(ev, bins=300)
```



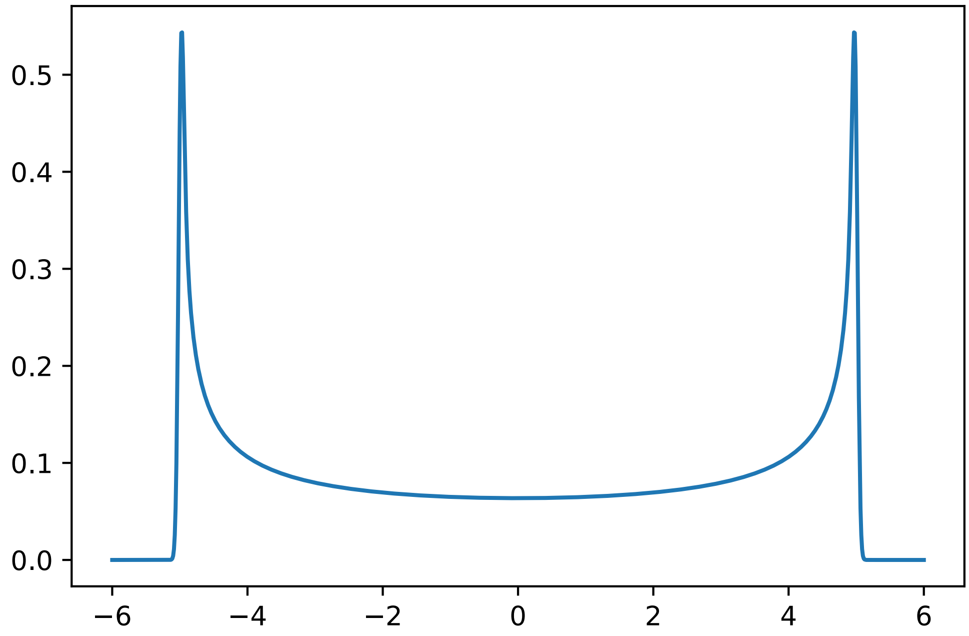
[7]:
```
kde = gaussian_kde(ev, 0.01)
```

[8]:

```
xrange = np.linspace(-6, 6, 1000)
plt.plot(xrange, kde.pdf(xrange))
```

[8]:

```
[<matplotlib.lines.Line2D at 0x18f91bc03d0>]
```



[9]:

```
H_imp = ring(1001, 0, 2.5)
i_imp = 500
H_imp[i_imp, i_imp] = -2
print(H_imp)
print()
print(H_imp[497:504, 497:504])
```

```
[[0.  2.5 0.  … 0.  0.  2.5]
 [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]
 [2.5 0.  0.  … 0.  2.5 0. ]]

[[ 0.   2.5  0.   0.   0.   0.   0. ]
 [ 2.5  0.   2.5  0.   0.   0.   0. ]
 [ 0.   2.5  0.   2.5  0.   0.   0. ]
 [ 0.   0.   2.5 -2.   2.5  0.   0. ]
 [ 0.   0.   0.   2.5  0.   2.5  0. ]
 [ 0.   0.   0.   0.   2.5  0.   2.5]]
 [ 0.   0.   0.   0.   0.   2.5  0. ]]
```

[10]:

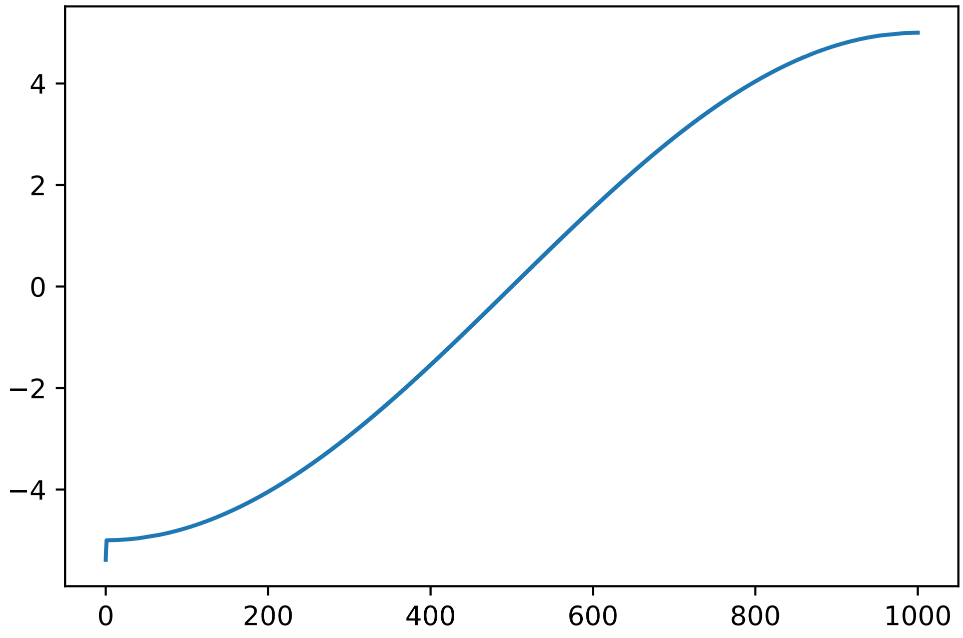
```
ev_imp = np.linalg.eigvalsh(H_imp)
```

[11]:

```
plt.plot(ev_imp)
```

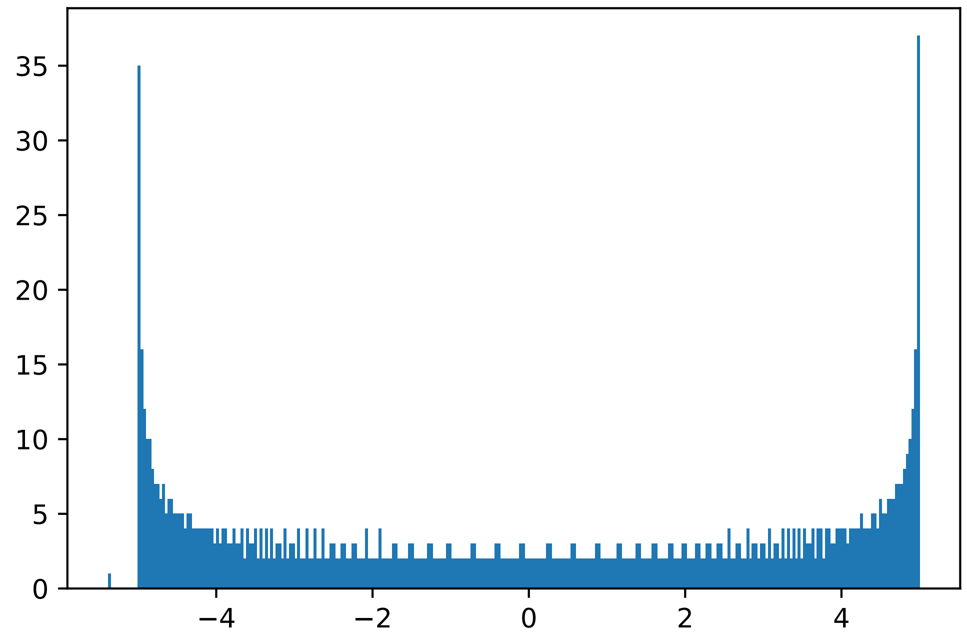
[11]:

```
[<matplotlib.lines.Line2D at 0x18f91c389d0>]
```



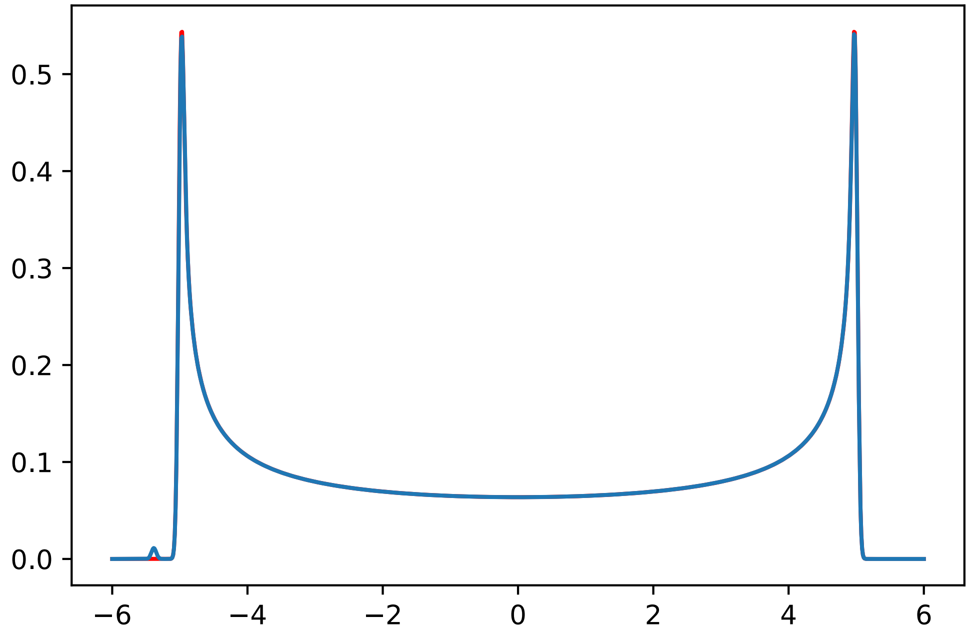
[12]:

```
h = plt.hist(ev_imp, bins=300)
```



```
[13]: plt.plot(xrange, kde.pdf(xrange), color='red')
      plt.plot(xrange, gaussian_kde(ev_imp, 0.01).pdf(xrange))
```

```
[13]: [<matplotlib.lines.Line2D at 0x18f94768970>]
```



[14]:

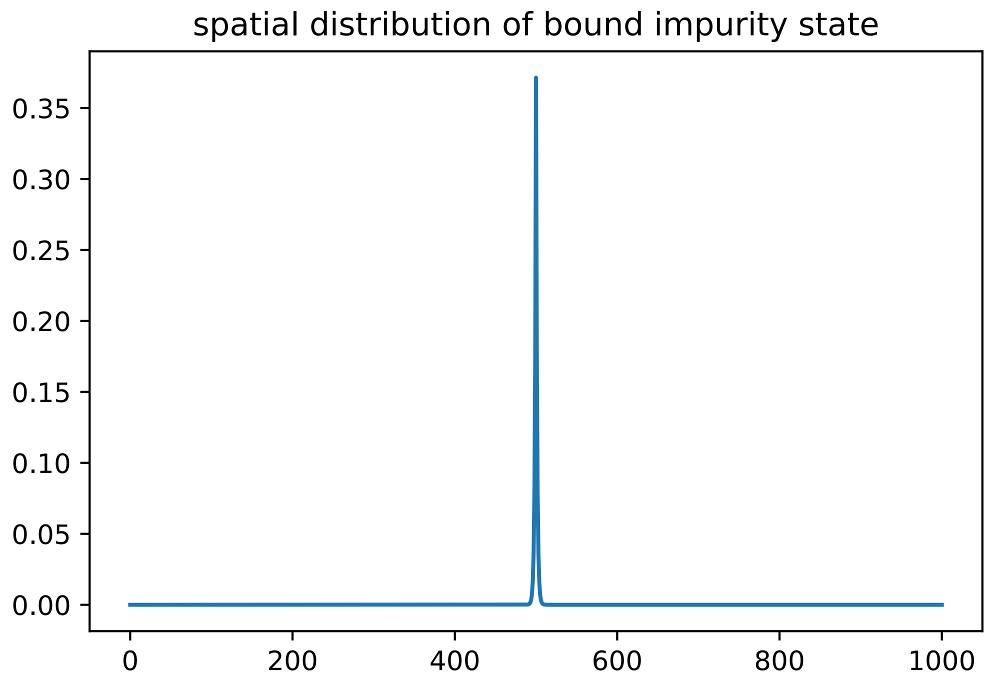
```
eval_imp, evec_imp = np.linalg.eigh(H_imp)
```

[15]:

```
# evec [input states, output eigenstates]
plt.title('spatial distribution of bound impurity state')
plt.plot((evec_imp.A[:, 0])**2)
```

[15]:

```
[<matplotlib.lines.Line2D at 0x18f94fa4ac0>]
```



[16]:

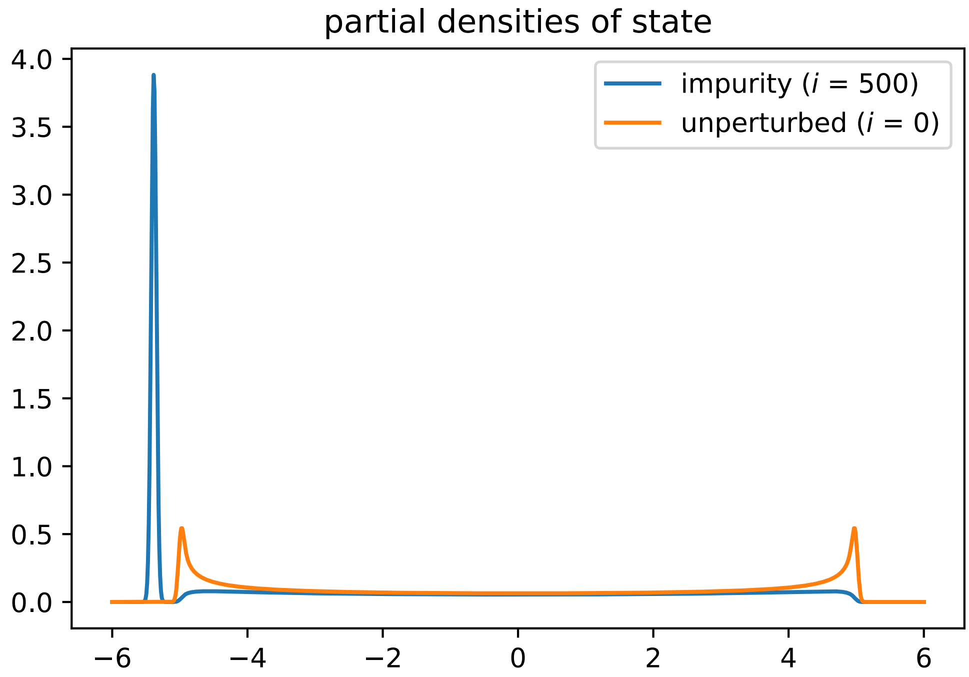
```
imp_weight = np.abs(evec_imp.A[i_imp])**2
oth_weight = np.abs(evec_imp.A[0])**2

pdos_imp = gaussian_kde(eval_imp, 0.01, weights=imp_weight).pdf(xrange)
pdos_oth = gaussian_kde(eval_imp, 0.01, weights=oth_weight).pdf(xrange)

plt.plot(xrange, pdos_imp,
         label='impurity ($i$ = 500)')
plt.plot(xrange, pdos_oth,
         label='unperturbed ($i$ = 0)')
plt.title('partial densities of state')
plt.legend()
```

[16]:

```
<matplotlib.legend.Legend at 0x18f94ffa5e0>
```


partial densities of state
impurity (i = 500)
unperturbed (i = 0)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−6
−4
−2
0
2
4
6

```
[ ]:
```