Lecture_11

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')
```

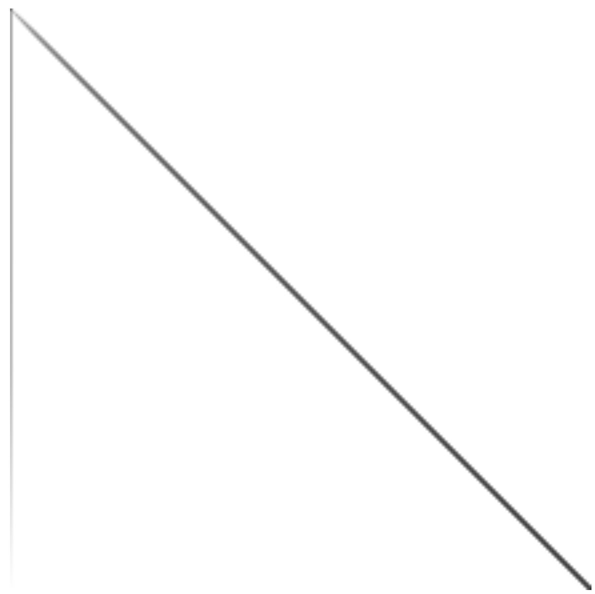
0.1 Setting up the Hamiltonian

[2]:
```
def make_H_W(Ef0, t, D, N):
    H = np.eye(N+1)
    H[0, 0] = Ef0
    host_band = np.linspace(0, D, N)
    H[1:, 1:] *= host_band
    w = np.cos(np.pi/2 * np.arange(N)/N)
    H[1:, 0] = w*t
    W = np.insert(w, 0, 1.)
    return H, W
```

[3]:
```
Ef0 = 1.
#E1 = .001
N = 1250  # number of host states
D = 2.5  # "bandwidth" of host states (note: this is not the real bandwidth as␣
 ↪it scales the number of states)
t = 0.02251 # hybridization
H, W = make_H_W(Ef0, t, D, N)
```

[4]:
```
from matplotlib.colors import SymLogNorm
plt.imshow(H, cmap='gist_yarg', norm=SymLogNorm(linthresh=t/10),␣
 ↪rasterized=True)
plt.axis('off')
```

[4]: (-0.5, 1250.5, 1250.5, -0.5)



[5]:

```
ew, ev = np.linalg.eigh(H)
print(ew)
```

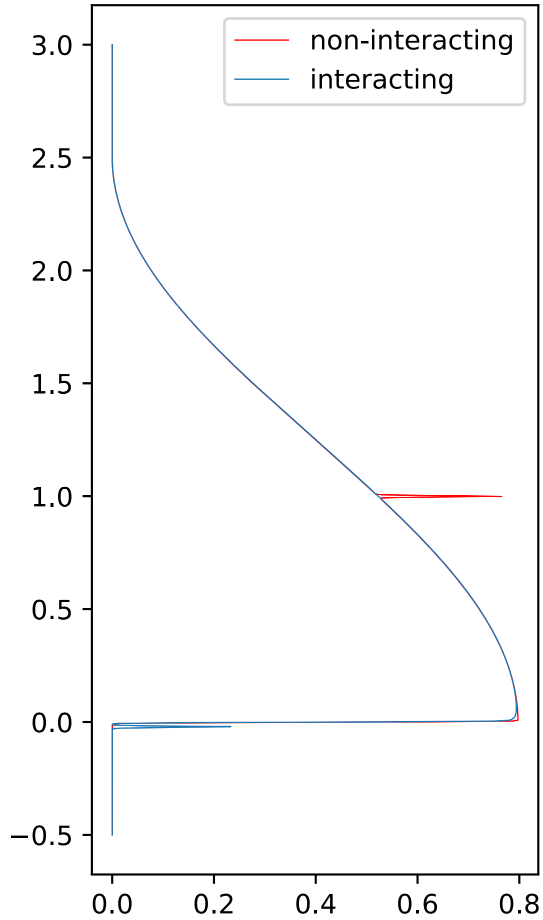
```
[-2.09052344e-02  5.66814316e-04  2.67966114e-03 …  2.49599680e+00
  2.49799840e+00  2.50000000e+00]
```

[6]:

```
dos_ni = gaussian_kde(H.diagonal(), 0.005, weights=W**2)
dos_i = gaussian_kde(ew, 0.005, weights=W**2)

plt.figure(figsize=(3.0, 6.0))
xrange = np.linspace(-0.5, 3, 1000)
plt.plot(dos_ni.pdf(xrange), xrange, color='red', lw=0.5, label='non-interacting')
plt.plot(dos_i.pdf(xrange), xrange, lw=0.5, label='interacting')
plt.legend()
```

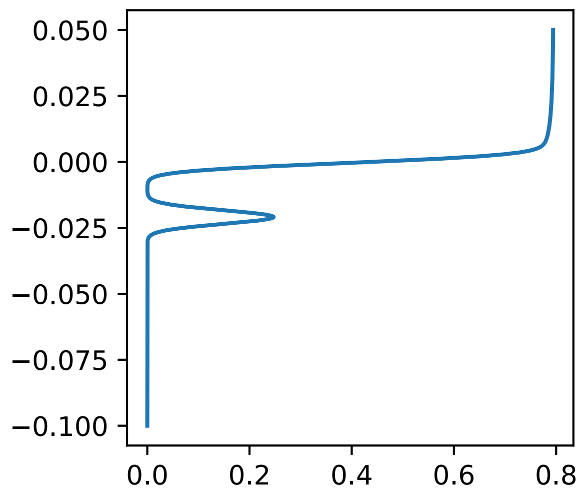
[6]:

```
<matplotlib.legend.Legend at 0x29c35908a00>
```



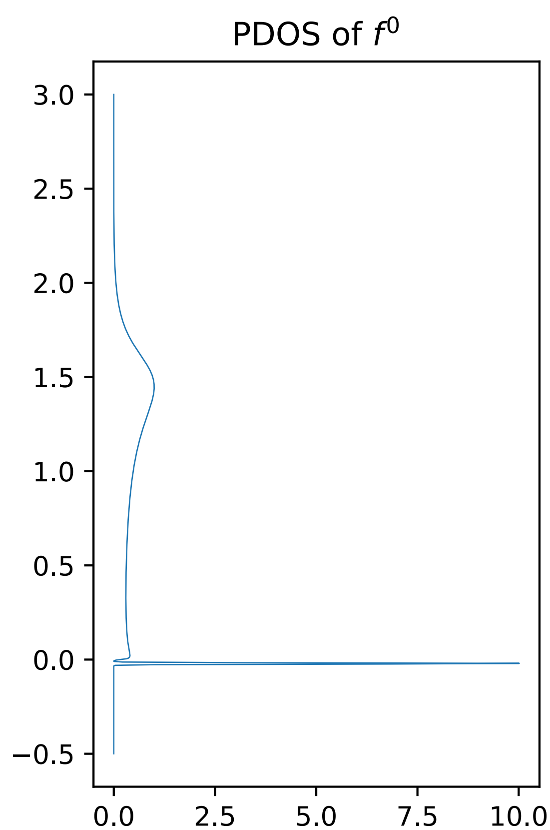
[7]:
```
plt.figure(figsize=(3.0, 3.0))
xrange_zoom = np.linspace(-0.1, 0.05, 1000)
plt.plot(dos_i(xrange_zoom), xrange_zoom)
```

[7]: `[<matplotlib.lines.Line2D at 0x29c3599bc40>]`



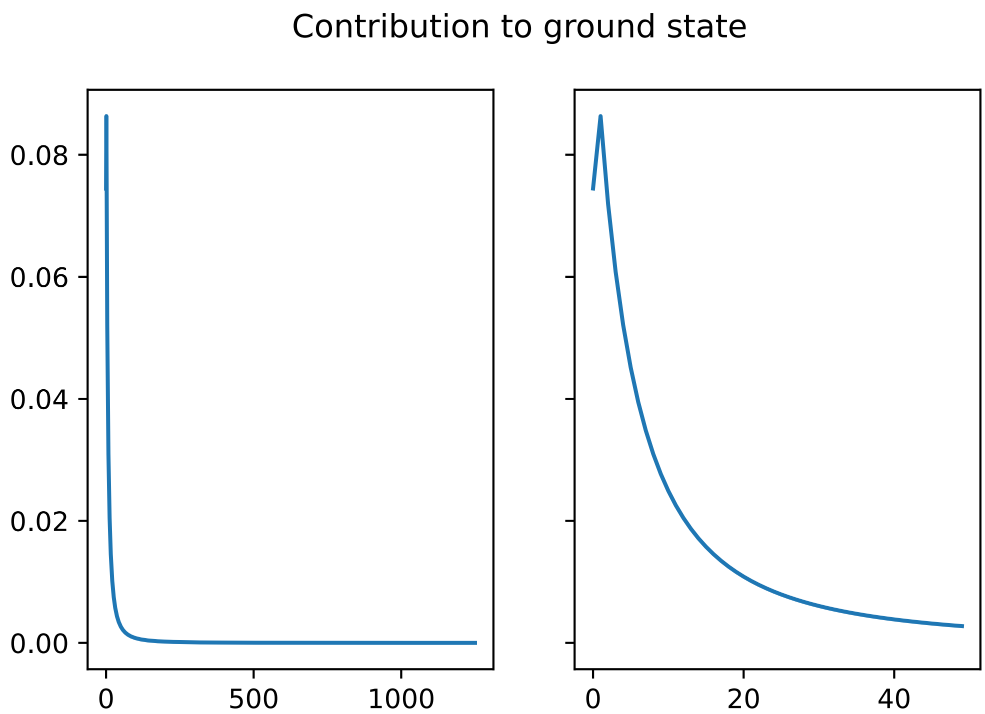
[8]:
```
plt.figure(figsize=(3.0, 5.0)); plt.title('PDOS of $f^0$')
w_f0 = ev[0]**2
plt.plot(gaussian_kde(ew, 0.005, weights=w_f0).pdf(xrange), xrange, lw=0.5)
```

[8]:
```
[<matplotlib.lines.Line2D at 0x29c35a17ee0>]
```



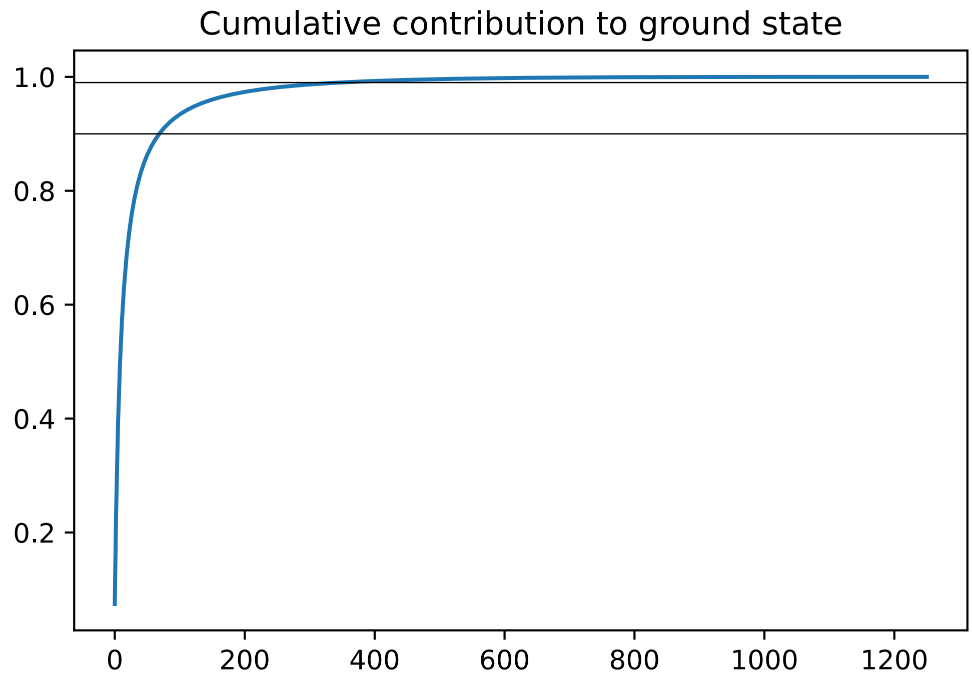
[9]:
```
fig, axs = plt.subplots(ncols=2, sharey=True)
axs[0].plot(ev[:, 0]**2)
axs[1].plot(ev[:50, 0]**2)
plt.suptitle('Contribution to ground state')
```

[9]:
```
Text(0.5, 0.98, 'Contribution to ground state')
```



[10]:
```
plt.plot(np.cumsum(ev[:, 0]**2))
plt.axhline(0.9, color='k', lw=0.5)
plt.axhline(0.99, color='k', lw=0.5)
plt.title('Cumulative contribution to ground state')
```

[10]:
```
Text(0.5, 1.0, 'Cumulative contribution to ground state')
```

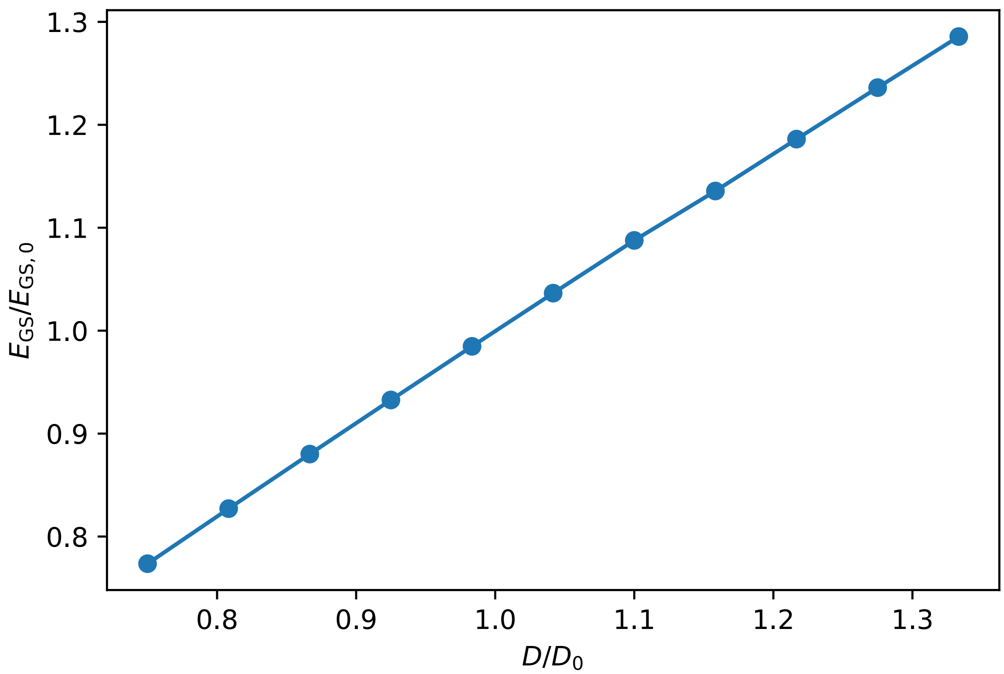


0.2 Influence of parameter D

[11]:
```
factors = np.linspace(3/4, 4/3, 11)
H_seriesD = [make_H_W(Ef0, t, a*D, int(a*N))[0] for a in factors]
gs_ews = [np.linalg.eigvalsh(H)[0] for H in H_seriesD]
```

[12]:
```
plt.plot(factors, gs_ews/ew[0], '-o')
plt.ylabel(r"$E_\mathrm{GS} / E_{\mathrm{GS},0} $")
plt.xlabel("$D / D_0 $")
```

[12]:
```
Text(0.5, 0, '$D / D_0 $')
```

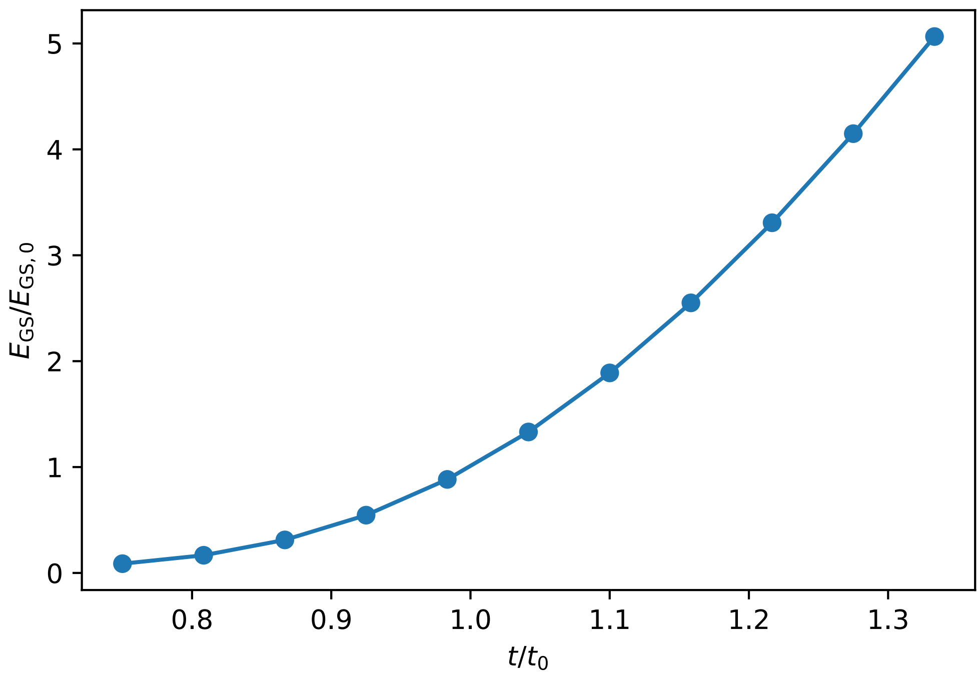


0.3 Influence of parameter t

[13]:
```
factors = np.linspace(3/4, 4/3, 11)
H_seriest = [make_H_W(Ef0, a*t, D, N)[0] for a in factors]
gs_ews = [np.linalg.eigvalsh(H)[0] for H in H_seriest]
```

[14]:
```
plt.plot(factors, gs_ews/ew[0], '-o')
plt.ylabel(r"$E_\mathrm{GS} / E_{\mathrm{GS},0} $")
plt.xlabel("$t / t_0 $")
```

[14]:
```
Text(0.5, 0, '$t / t_0 $')
```

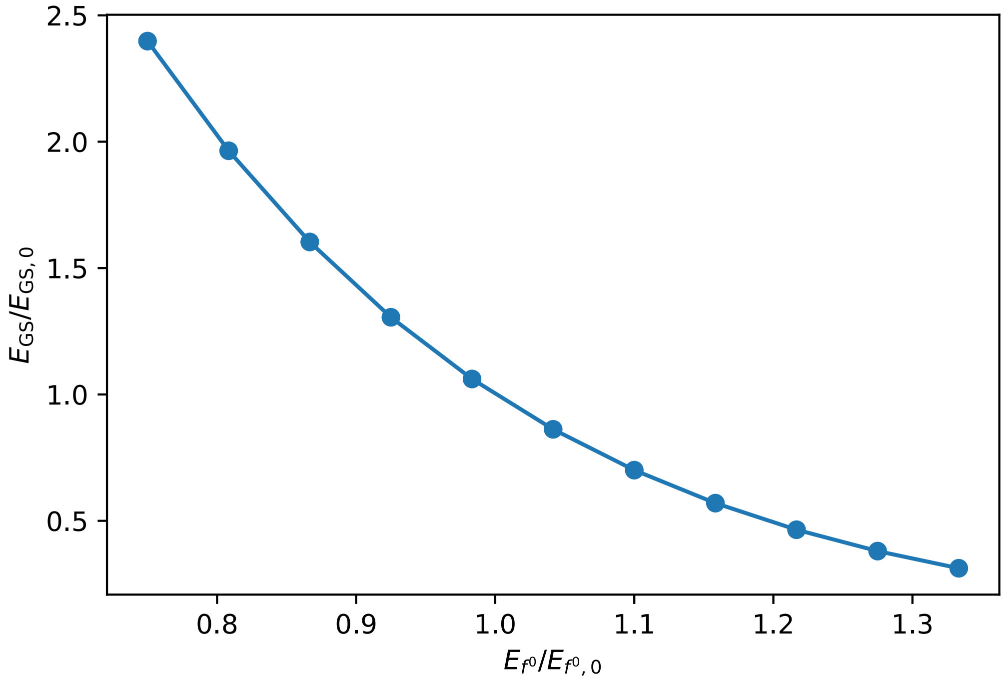


0.4 Influence of parameter E_{f^0}

[15]:
```
factors = np.linspace(3/4, 4/3, 11)
H_seriesEf0 = [make_H_W(a*Ef0, t, D, N)[0] for a in factors]
gs_ews = [np.linalg.eigvalsh(H)[0] for H in H_seriesEf0]
```

[16]:
```
plt.plot(factors, gs_ews/ew[0], '-o')
plt.ylabel(r"$E_\mathrm{GS} / E_{\mathrm{GS},0} $")
plt.xlabel("$E_{f^0} / E_{f^0,0} $")
```

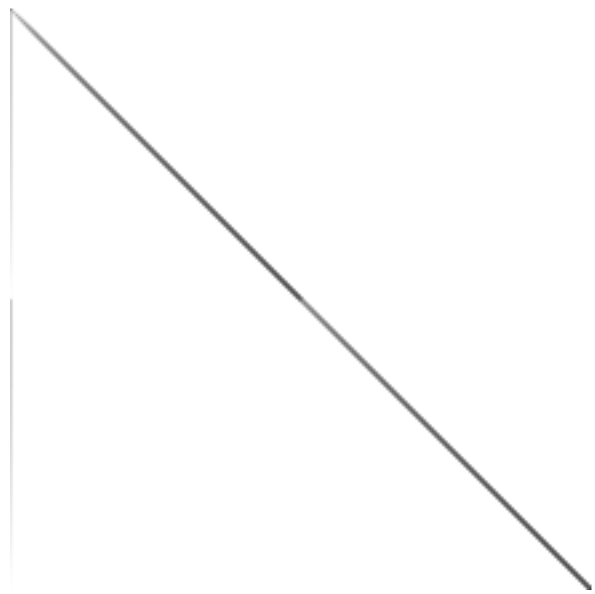
[16]:
```
Text(0.5, 0, '$E_{f^0} / E_{f^0,0} $')
```



1 Adding a second band (CEF, SO, ...)

[17]:
```
H_new, W_new = make_H_W(Ef0, 0.01918, D, N)  # change t to maintain same T_K
H2 = np.eye(2*N + 1)
H2[:N+1, :N+1] = H_new
delta_so = 0.3  # 300meV SO split
host_band = H_new.diagonal()[1:]
H2[N+1:, N+1:] *= host_band + delta_so
H2[N+1:, 0] = H_new[1:N+1, 0]

W2 = np.hstack([W_new[0], W_new[1:], W_new[1:]])
```

[18]:
```
plt.imshow(H2, cmap='gist_yarg', norm=SymLogNorm(linthresh=t/10),␣
 ↪rasterized=True)
plt.axis('off');
```

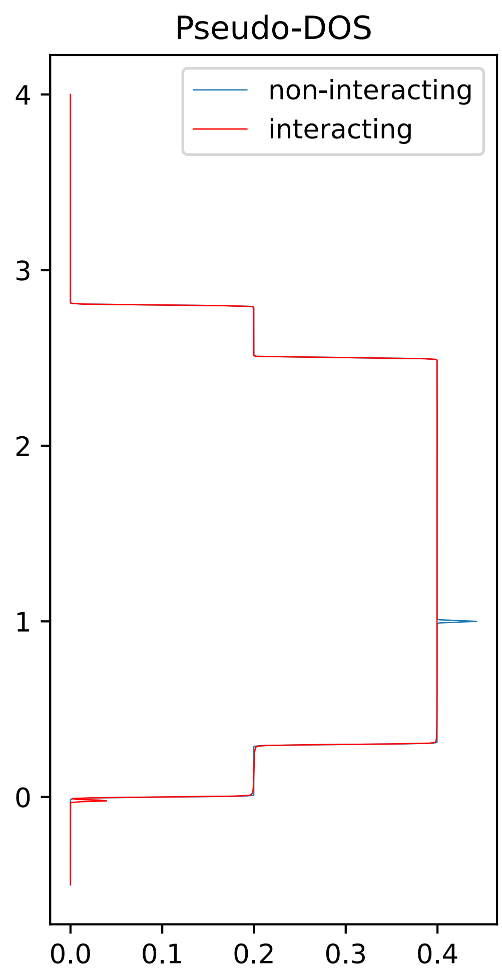


[19]:
```
ew, ev = np.linalg.eigh(H2)
print(ew)
```

```
[-2.08972726e-02  5.55812280e-04  2.66475635e-03 …  2.79599680e+00
  2.79799840e+00  2.80000000e+00]
```

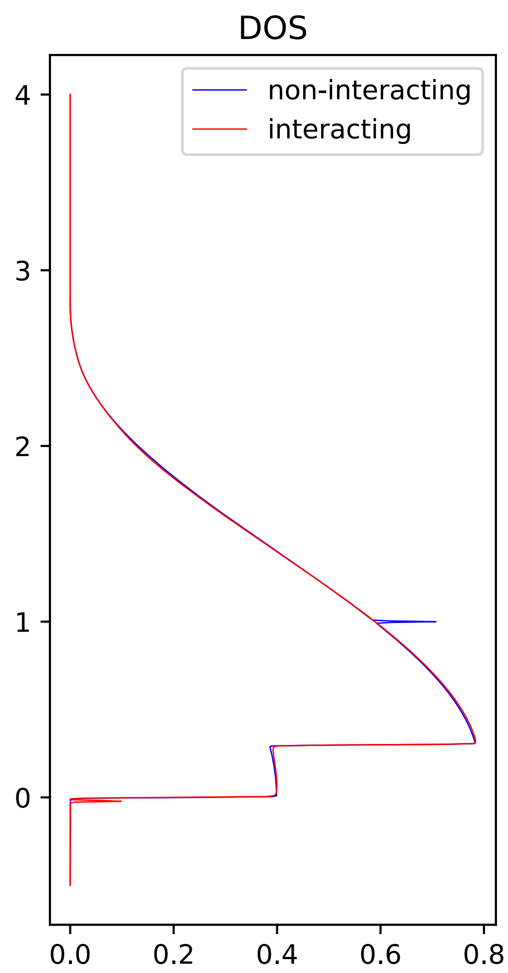
[20]:
```
plt.figure(figsize=(3.0, 6.0)); plt.title('Pseudo-DOS')
xrange = np.linspace(-0.5, 4, 1000)

dos_ni = gaussian_kde(H2.diagonal(), 0.005).pdf(xrange)
dos_i = gaussian_kde(ew, 0.005).pdf(xrange)

plt.plot(dos_ni, xrange, lw=0.5, label='non-interacting')
plt.plot(dos_i, xrange, color='red', lw=0.5, label='interacting')
plt.legend()
```

[20]: <matplotlib.legend.Legend at 0x29c364214f0>



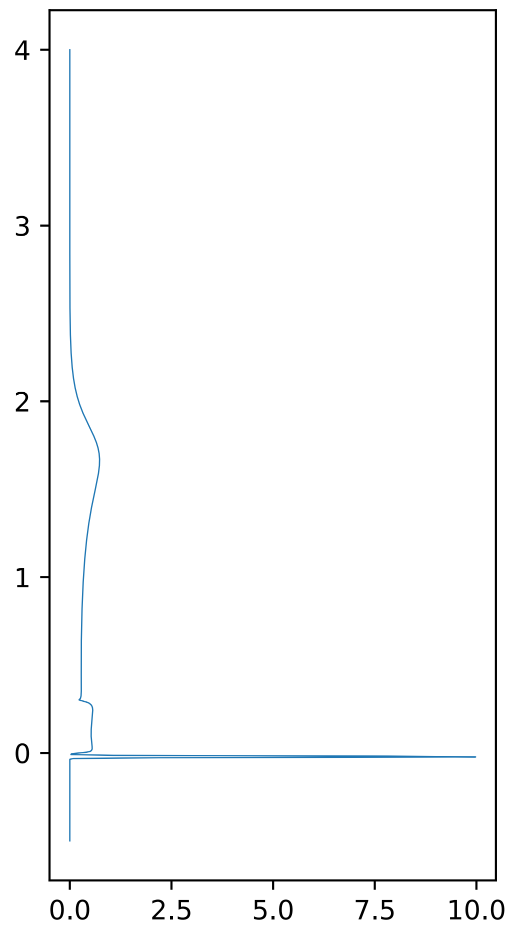
[21]:
```
plt.figure(figsize=(3.0, 6.0)); plt.title('DOS')
plt.plot(gaussian_kde(H2.diagonal(), 0.005, weights=W2**2).pdf(xrange), xrange,␣
 ↪color='blue', lw=0.5, label='non-interacting')

W2_final = np.dot(W2, ev**2)  # ev: initial -> final representation
plt.plot(gaussian_kde(ew, 0.005, weights=W2_final**2).pdf(xrange), xrange,␣
 ↪color='red', lw=0.5, label='interacting')
plt.legend()
```

[21]: <matplotlib.legend.Legend at 0x29c59293640>



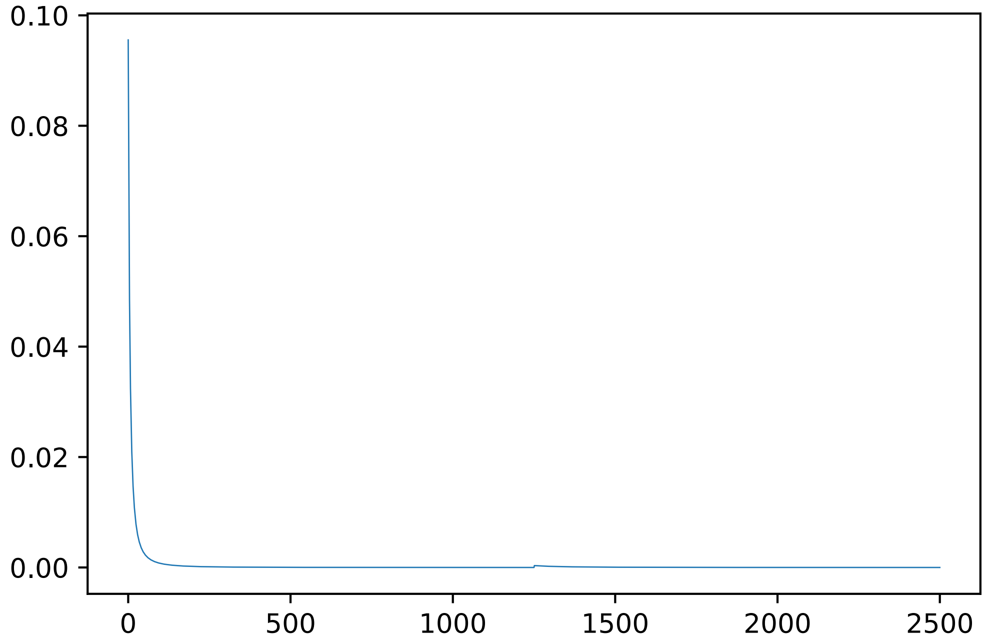
[22]:
```
plt.figure(figsize=(3.0, 6.0))

w_f0 = ev[0]**2  #  equal to [1 0 0 0 0 ...] . ev**2, i.e. PDOS of initial f0␣
 ↪state
pdf = gaussian_kde(ew, 0.005, weights=w_f0).pdf(xrange)
plt.plot(pdf, xrange, lw=0.5)
print(ev[0]**2)
```

```
[9.55467200e-02 6.94601177e-04 8.55041828e-04 … 2.25996771e-09
 1.00121962e-09 2.49506884e-10]
```



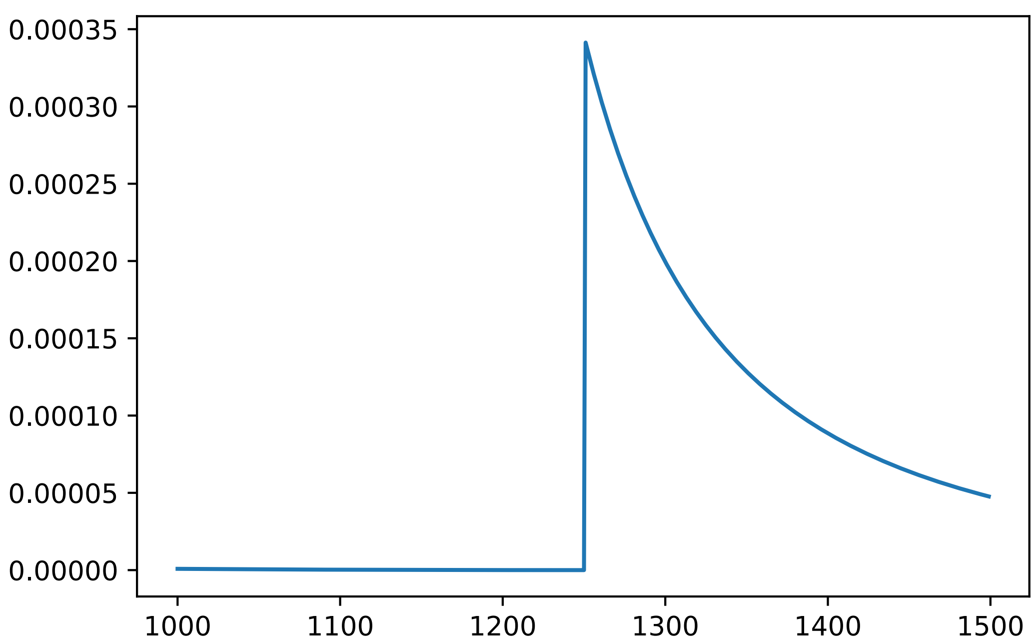
[23]:
```
contrib_gs = ev[:, 0]**2  # weights of new ground state in terms of initial␣
↪state
plt.plot(contrib_gs, lw=0.5)
```

[23]: [<matplotlib.lines.Line2D at 0x29c386e3f10>]



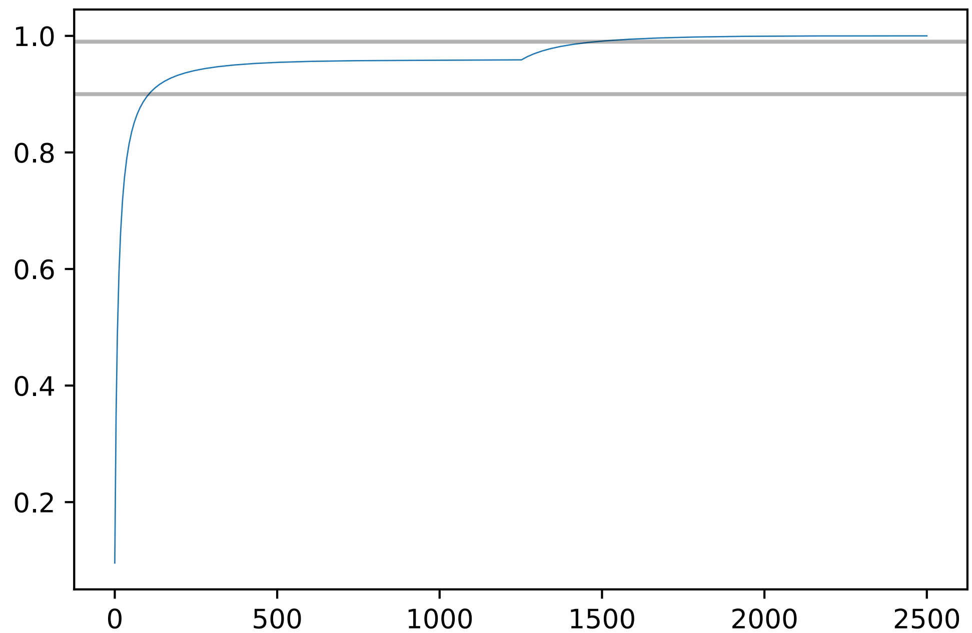
[24]:
```
plt.plot(range(1000, 1500), contrib_gs[1000:1500])
```

[24]: [<matplotlib.lines.Line2D at 0x29c38603670>]



[25]:
```
plt.plot(np.cumsum(contrib_gs), lw=0.5)
plt.axhline(0.9, alpha=0.3, color='k'); plt.axhline(0.99, alpha=0.3, color='k')
```

[25]: <matplotlib.lines.Line2D at 0x29c386a4640>



[ ]:
```

```