

06/05/21 02:32:08 /home/ana/Desktop/proj/code/Bender/wavefunction\_animation.py

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1  # PHS3350
2  # Week 5 - Energy levels of a family of non-Hermitian Hamiltonians
3  # "what I cannot create I do not understand" - R. Feynman.
4  # Ana Fabela Hinojosa, 16/05/2021
5
6  import numpy as np
7  import matplotlib
8  import matplotlib.pyplot as plt
9  from scipy.integrate import quad
10 from scipy.optimize import fsolve
11 from scipy.special import gamma
12 import scipy.special as sc
13 from scipy import linalg
14 from odhobs import psi as cpsi_blank
15
16 plt.rcParams['figure.dpi'] = 200
17 np.set_printoptions(linewidth=200)
18
19 ##### eigenvalues & eigenvectors #####
20
21 Energies_2 = np.load("Energies_unbroken.npy")
22
23 def linear_algebra(epsilons):
24
25     eigenvalues_list = []
26     eigenvectors_list = []
27     for i, e in enumerate(epsilons):
28         matrix = np.load(f'matrices/matrix_{i:03d}.npy')
29         eigenvalues, eigenvectors = linalg.eig(matrix)
30         eigenvalues_list.append(eigenvalues)
31         eigenvectors_list.append(eigenvectors)
32
33         e_list = np.full(len(eigenvalues), e)
34
35     return np.array(eigenvalues_list), np.array(eigenvectors_list)
36
37 ##### sorting Eigenvectors #####
38
39 def filtering_and_sorting(evals, evecs):
40     mask = (0 < evals.real) & (evals.real < 20)
41     # print(mask)
42     evals = evals[mask]
43     evecs = evecs[:, mask]
44
45     # sorting
46     order = np.argsort(np.round(evals.real, 3) + np.round(evals.imag, 3) / 1e6)
47     # print(order)
48     evals = evals[order]
49     evecs = evecs[:, order]
50
51     # print(evals)
52
53     return evals[1:3], evecs[:, 1:3]
54

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55 ##### Eigenvectors plot #####
56
57 def spatial_wavefunctions(N, x, epsilons, evals, evecs):
58     # calculating basis functions
59     x[x == 0] = 1e-200
60     PSI_ns = []
61     for n in range(N):
62         psi_n = cpsi_blank(n, x)
63         PSI_ns.append(psi_n)
64     PSI_ns = np.array(PSI_ns)
65
66     # plt.plot(x, PSI_ns[1])
67     # plt.show()
68     np.save(f"PSI_ns.npy", PSI_ns)
69
70
71     for i, e in enumerate(epsilons):
72
73         eigenvalues, c = filtering_and_sorting(evals[i], evecs[i])
74
75         if c.shape[1] < 2:
76             print(i, "continuing")
77             continue
78         eigenstates = []
79         for j in range(2):
80             # print(len(evecs))
81             d = c[:, j]
82             psi_jx = np.zeros(x.shape, complex)
83             # for each H.O. basis vector relevant to the filtered and sorted
eigenvectors
84             for n in range(N):
85                 psi_jx += d[n] * PSI_ns[n]
86             # normalise
87             psi_jx /= np.sqrt(np.sum(abs(psi_jx) ** 2 * delta_x))
88             # impose phase convention at ~ x = 0
89             psi_jx *= np.exp(-1j * np.angle(psi_jx[Nx // 2]))
90
91             eigenstates.append(psi_jx)
92
93         fig, ax = plt.subplots()
94         # # probability density
95         # plt.plot(x, abs(eigenstates[0])**2, "-", color='blue', linewidth=1,
label=fr"$|\psi_1|^2$") # first excited state
96         # plt.plot(x, abs(eigenstates[1])**2, "-", color='orange', linewidth=1,
label=fr"$|\psi_2|^2$") # second excited state
97
98         # spatial wavefunctions
99         plt.plot(x, np.real(eigenstates[0]), "-", color='blue', linewidth=1,
label=fr"real $\psi_1$") # first excited state
100         plt.plot(x, np.real(eigenstates[1]), "-", color='orange', linewidth=1,
label=fr"real $\psi_2$") # second excited state
101         plt.plot(x, np.imag(eigenstates[0]), "--", color='blue', linewidth=0.4,
label=fr"imaginary $\psi_1$") # first excited state
102         plt.plot(x, np.imag(eigenstates[1]), "--", color='orange',
linewidth=0.4, label=fr"imaginary $\psi_2$") # second excited state
103
104         plt.legend(loc="upper right")

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105     plt.xlabel(r'$x$')
106     # plt.ylabel(r'$|\psi_n|^2$')
107     plt.ylabel(r'$\psi_n$')
108     textstr = '\n'.join((
109         fr'$E_1 = {eigenvalues[0]:.03f}$',
110         fr'$E_2 = {eigenvalues[1]:.03f}$',
111         fr'$\epsilon = {\epsilon:.03f}$'
112     ))
113
114     # place a text box in upper left in axes coords
115     ax.text(0.02, 1.15, textstr, transform=ax.transAxes,
116            verticalalignment='top')
116     plt.savefig(f"density_spatial_wavefunctions/wavefunction_{i:03d}.png")
117     plt.savefig(f"spatial_wavefunctions/wavefunction_{i:03d}.png")
118     plt.clf()
119     return eigenvalues, eigenstates
120
121
122 ##### Function calls #####
123
124 N = 100
125 Ne = 100
126 Nx = 1024
127 epsilons = np.linspace(-1.0, 0, Ne)
128 xs = np.linspace(-10, 10, Nx)
129 delta_x = xs[1] - xs[0]
130
131 evals, evecs = linear_algebra(epsilons)
132
133 eigenvalues, eigenstates = spatial_wavefunctions(N, xs, epsilons, evals, evecs)

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