

```
1: import matplotlib.animation as animation
2: import numpy as np
3: import pylab
4:
5: L = 5e-10
6: hb = 1.054571800e-34
7: mass = 9.1094e-31
8: # a = 0
9: a = 1.60218e-18
10: PSI = None
11:
12:
13: def simpson(func, a, b, n=50):
14:     """Approximates integral using simpson method"""
15:     h = abs(b - a) / n
16:     return (h / 3.0) * (
17:         func(a) + func(b) +
18:         (4.0 * sum([func(a + (k * h)) for k in range(1, n, 2)])) +
19:         (2.0 * sum([func(a + (k * h)) for k in range(2, n - 1, 2)])))
20:
21:
22: def H(n, m, v):
23:     """Generates n.m element of H matrix"""
24:     n += 1
25:     m += 1
26:     pre_1 = ((hb**2) * (n**2) * (np.pi**2)) / (mass * (L**3))
27:     pre_2 = 2 / L
28:     int_1 = simpson(
29:         lambda x: np.sin(m * np.pi * x / L) * np.sin(n * np.pi * x / L), 0, L)
30:     int_2 = simpson(
31:         lambda x: v(x) * np.sin(m * np.pi * x / L) * np.sin(n * np.pi * x / L),
32:         0, L)
33:     return pre_1 * int_1 + pre_2 * int_2
34:
35:
36: def phi(n, x):
37:     return np.sqrt(2 / L) * np.sin(n * np.pi * x / L)
38:
39:
40: def psi(p, A):
41:     return lambda x: sum(A[n] * phi(n, x) for n in range(len(A)))
42:
43:
44: def B(F_Psi, f_psi):
45:     return simpson(lambda x: F_Psi(x) * f_psi(x), 0, L)
46:
47:
48: def PSI_init(x):
49:     if 0 < x < L / 2:
50:         return np.sqrt(12 / L**3) * x
51:     elif L / 2 < x < L:
52:         return np.sqrt(12 / L**3) * (L - x)
53:     else:
54:         return 0
55:
56: X = np.linspace(0, L, 50)
57: T = np.linspace(0, 1.17e-16, 40)
58:
59: fig, ax = pylab.subplots()
60: plot, = pylab.plot(X, [np.nan] * len(X), animated=True)
61:
62:
63: def initialize():
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64:     ax.set_xlim(0, L)
65:     plot.set_ydata([np.nan] * len(X))
66:     plot.set_xdata(X)
67:     return plot,
68:
69:
70: def animate(t):
71:     # print(t)
72:     y_vals = [np.fabs(np.real(PSI(x, t)))**2 for x in X]
73:     pylab.title("{:e}".format(t))
74:     plot.set_ydata(y_vals)
75:     plot.set_xdata(X)
76:     # print(simpson(lambda x: PSI(x, 0)**2, 0, L, 500))
77:     return plot,
78:
79:
80: def main():
81:     global PSI
82:     V = lambda x: a * x / L
83:     eigen_1 = []
84:     eigen_2 = []
85:     vec_1 = []
86:     vec_2 = []
87:
88:     def cd():
89:         arr1 = np.array([[H(x, y, V) for x in range(0, 11)] for y in range(0, 11)])
90:         arr2 = np.array([[H(x, y, V) for x in range(0, 30)] for y in range(0, 30)])
91:         E1, Vec1 = np.linalg.eigh(arr1)
92:         E2, Vec2 = np.linalg.eigh(arr2)
93:         E1 /= 1.6022e-19
94:         E2 /= 1.6022e-19
95:         count = 0
96:         Vec1 = np.transpose(Vec1)
97:         Vec2 = np.transpose(Vec2)
98:         for i in range(len(E1)):
99:             if np.fabs(E1[i]) > 1e-10:
100:                 eigen_1.append(E1[i])
101:                 vec_1.append(Vec1[i])
102:                 count += 1
103:             if count == 10:
104:                 break
105:         count = 0
106:         for i in range(len(E2)):
107:             if np.fabs(E2[i]) > 1e-10:
108:                 eigen_2.append(E2[i])
109:                 vec_2.append(Vec2[i]);
110:                 count += 1
111:         print(eigen_1)
112:         print(eigen_2)
113:         print("The much larger matrix makes very little difference to the accuracy")
114:
115:     def e():
116:         psis = [psi(p, vec_2[p]) for p in range(3)]
117:         X = np.linspace(0, L, 100)
118:         pylab.plot(X, [psis[0](x)**2 for x in X])
119:         pylab.plot(X, [psis[1](x)**2 for x in X])
120:         pylab.plot(X, [psis[2](x)**2 for x in X])
121:         pylab.show()
122:         # PSI = lambda x, t: sum([B(init, psi(n, Vec[n]))*np.exp(-1j*E[n]*t/hb)*psi(n, V
ec[n])(x) for n in range(len(E))])
123:         # pass
124:
125:     cd()

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126:     # e()
127:     # V = lambda x: 0
128:     # Vec = np.transpose(Vec)
129:     # E /= 1.6022e-19
130:     # print(E)
131:     # psis = [psi(p, Vec[p]) for p in range(len(E))]
132:     init = lambda x: np.sqrt(12 / L**3) * x if x < L / 2 else np.sqrt(12 / L**3) * (L -
x)
133:     PSI = lambda x, t: sum([B(init, psi(n, vec_2[n]))*np.exp(-1j*eigen_2[n]*t/hb)*psi(n
,vec_2[n])(x) for n in range(len(eigen_2))])
134:     # PSI = lambda x, t: sum([B(init, psi(n, vec_1[n]))*np.exp(-1j*eigen_1[n]*t/hb)*psi
(n,vec_1[n])(x) for n in range(len(eigen_1))])
135:     pylab.plot(X, [PSI(x, 0)**2 for x in X])
136:
137:     # print(PSI(L/2, 0))
138:     # print(simpson(lambda x: PSI(x, 0)**2, 0, L, 500))
139:     # pylab.show()
140:     #
141:     # print(T)
142:     for i, t in enumerate(T):
143:         print(i, t)
144:         pylab.plot(X, [np.abs(PSI(x, t))**2 for x in X])
145:         # print(simpson(lambda x: np.abs(PSI(x, t))**2, 0, L, 100))
146:         pylab.savefig("anim/{}.png".format(i))
147:         pylab.clf()
148:         # pylab.show()
149:     # ani = animation.FuncAnimation(
150:     #     fig, animate, init_func=initialize, interval=60, blit=True, frames=T)
151:     # ani.save("anim.mp4")
152:     # pylab.show()
153:
154:
155: if __name__ == "__main__":
156:     main()
```