Demo 4 Cheat Sheet: Kinetic energy operator

Numpy (np.) and scipy.integrate

Usage	Purpose	Inputs
x=np.zeros(5) x =np.zeros((5,5))	Return a new array of given shape and type, filled with zeros.	shape = number or numbers
x = np.arange(-1.0,1.0, 0.1)	Return an array evenly spaced values within a given interval according to a step size.	start, stop, step_size
x = np.linspace(-1.0,1.0, 100)	Return an array of evenly spaced numbers over a specified interval.	start, stop, number of points
np.double(3)	Convert a number or integer into a floating number (decimals).	Scalar
simps(f_x, x) (as imported from scipy.integrate)	Integrate a function f(x) represented as an array (f_x) defined on the grid x using Simpson's rule.	f_x = vector with function values , x= vector representing the grid of x values
np.sqrt(x)	Calculate the square root of x	Scalar or vector
np.sin(x)	Calculate the sine of x	Scalar or vector

Matplotlib : Plotting (plt)

Usage	Purpose	Inputs
plt.figure(figsize=(10,8))	Setup parameter for a graphic, in this case we will use it change size.	figsize= (inches width, inches height)
plt.plot(x,y)	Plot lines	x, y = vectors
plt.hist(x)	Plot a histogram.	X =vector
plt.xlabel("Axis x name")	Set the *x* axis label of the current plot.	Name = string
plt.xlim([xmin,xmax])	Set the *x* limits of the current axes.	xmin,xmax = scalars
plt.title("Plot name")	Set a title of the current plot.	Name = string
plt.show()	Display a figure.	

Demo Specific - Common variables:

x == array with x values
L == length of the box
n, n1, n2 == used for the quantum number for the 1D particle in a box eigenstates
psi_x, psi_12 == wavefunctions.
T_to_psi (and similar) == kinetic energy operator applied to the wavefunction.
m == mass of the particle. 1 by default.
h_bar == value of h bar. Defined as 1 by default.
T_expectation (and similar) == expectation value of the kinetic energy operator
c1, c2 == coefficients in the superposition

Function	Purpose	Inputs
box_1D_eigenfunctiont(x,L,n)	Return the n-th eigenstate of a 1D particle in a box (as an array) system with the box defined between 0 and L.	x = vector of positions from 0 to L , L=length of the box, n = quantum number
kinetic_energy_operator(x,psi_x, h_bar=1,m=1)	Return the function (as an array) obtained from applying the kinetic energy operator to the wavefunction using finite differences.	x = vector of positions, psi_x= vector with wavefunction values in the range of x, m=mass of the particle
analytical_T_n(n,L,h_bar,m)	Return the analytical value of the kinetic energy for the n-th eigenstate of a 1D particle in a box	n=quantum number, L=length of the box, m=mass of the particle