This is an exercise that will help you practise both analytical and numerical skills. We are going to attempt solving the inclined particle-in-a-box (PIB) problem by using the familiar PIB eigensolutions as a basis. We know that the PIB Hamiltonian is

$$H_{PIB} = \frac{p^2}{2m} + V(x) \tag{1}$$
$$p^2 = \frac{d^2}{dx^2} \tag{2}$$
$$V(x) = 0 \text{ if } 0 \leq x \leq L \tag{3}$$
$$= \infty \text{ otherwise }, \tag{4}$$

where $\hbar = 1$ is assumed for this exercise. The inclined PIB will have $V(x) = \alpha x$ instead of being 0, where α is a parameter to be specified later while actually solving the problem. We call the inclined PIB Hamiltonian as H_{in}.

(1) Our first step is to write down the H_{in} in the basis of PIB solutions. Write down the eigen-solutions $\{\phi\}$ of H_{PIB} in terms of the parameters defined above.

(2) To think about the new solutions clearly that we have to find (namely that of H_{in}) let's stick to using the two lowest PIB eigensolutions. Write down the 2×2 matrix representation of the H_{in} using the $\phi_1(x)$ and $\phi_2(x)$ basis functions. You should evaluate all the elements in the matrix

$$\mathbf{H}_{in} = \begin{bmatrix} \langle\phi_1|H_{in}|\phi_1\rangle & \langle\phi_1|H_{in}|\phi_2\rangle \\ \langle\phi_2|H_{in}|\phi_1\rangle & \langle\phi_2|H_{in}|\phi_2\rangle. \end{bmatrix} \tag{5}$$

Write down explicit expressions for these.

(3) Generalize your results to H_{ij} notation where it can be a diagonal element $i = j$ or off-diagonal element $i \neq j$.

(4) Approach 1 (numerical): Use MATLAB to write a code that finds the eigenenergies and eigensolutions of H_{in} using the *eig* intrinsic function. Attach your code and the eigenenergies assuming $\alpha = -0.1, m = 1, L = 10$ and for different number of PIB functions- namely choose 2, 3, 6, 7, 10, 12 and 20. Attach your code.

(5) Approach 2 (analytical): You have expressions for H_{in}^{11}, H_{in}^{22}, H_{in}^{12} and H_{in}^{21}. We represent an eigenfunction of the H_{in} as a linear combination of the PIB solutions

$$\Phi(x) = \sum_n c_n \phi_n(x). \tag{6}$$

(i) Write down the expression for the expectation value of the energy $\langle E\rangle$ using the above $\Phi(x)$. Make sure you define your symbols clearly.

(ii) A necessary but not sufficient condition for the minimization of any multivariate function is that all the partial derivatives are zero

$$\frac{\partial\langle E\rangle}{\partial c_k} = 0, \text{ for all } k. \tag{7}$$

Differentiate the expression you derived for $\langle E\rangle$ with respect to c_1 and c_2 and set them to zero to get 2 linear equations involving the unknowns c_1, c_2 and $\langle E\rangle$. The third equation that will give a unique solution for the 3 variables is the normalization condition $c_1^2 + c_2^2 = 1$. Using all this information, get an expression for $\langle E\rangle$ analytically, plug in the parameters used in the MATLAB code and compare your answer with the lowest energy eigenvalue from diagonalizing (i.e., using the *eig* function) the $\mathbf{H}_{in}$ matrix. What is the value you obtain by this method?