Exercise 6 - Basis Sets

In order to solve any partial differential equation on a computer, we need to “discretize” it. In quantum mechanics, such a discretisation is usually referred to as a “basis set expansion”.

1. **Infinite potential well with an electric field**

   We consider a charged particle (charge $e$) in an infinite quantum well exposed to an electric field $F$. The particle is therefore exposed to a potential given by

   \[
   V(x) = \begin{cases} 
   eF(x - \frac{L}{2}) & 0 \leq x \leq L \\
   \infty & \text{elsewhere}
   \end{cases} \tag{1}
   \]

   a) Construct the Hamilton operator $H$ in dimensionless units for this problem. Use dimensionless quantities such as the energy $\eta_n = \frac{E_n}{E_0}$ with $E_0 = \frac{\hbar^2 \pi^2}{2mL^2}$, the length $\xi = \frac{x}{L}$, and the dimensionless field $\phi = \frac{F}{F_0}$ with $F_0 = \frac{E_0}{eL}$.

   b) On the last exercise sheet you have calculated the eigenfunctions for the zero-field problem. Show that dimensionless eigenfunctions can be written as $\psi_n(\xi) = \sqrt{2} \sin(n \pi \xi)$.

   **Reminder:** The dimensionless eigenfunctions fulfill the orthogonality condition

   \[
   \int_0^1 \psi_n^*(\xi) \psi_m(\xi) d\xi = \delta_{mn}. \tag{2}
   \]

   c) The solution $\Psi_n(\xi)$ for the problem with field is now expanded into a so called finite basis set

   \[
   \Psi_n(\xi) = \sum_{j=1}^{N} \alpha_n^j \psi_j(\xi). \tag{3}
   \]

   Show that this expansion can be used to map the problem to the eigenvalue problem

   \[
   H \vec{\alpha}_n = \eta_n \vec{\alpha}_n \tag{4}
   \]

   with $H_{ij} = \frac{1}{L} \int_0^L \psi_i^*(\xi) H \psi_j(\xi) d\xi$ and $\vec{\alpha}_n = (\alpha_{n1}, \ldots, \alpha_{nj}, \ldots, \alpha_{nN})^T$ is the vector of the expansion coefficients for the $n$.th eigenvalue.

   d) Use a computer to calculate the matrix elements of $H$ for an electrical field $\phi = 4$. Take as basis the lowest three eigenfunctions of the zero-field system. Solve the resulting 3x3 eigenproblem.

   e) Use the eigenvector for the lowest eigenvalue and construct an approximate solution for the true eigenfunction. Visualize this eigenfunction and compare it to the lowest eigenfunction of the zero-field system. What has changed?

   **Note:** The eigenfunctions for this problem are known exactly as Airy functions in the literature.

   f) Compare the lowest eigenvalue to the numerically “exact” value of 0.831810. How does it change if you take the lowest four eigenfunctions as basis expansion?