Take home exercise Quantum Physics (GEMF)

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The purpose of this exercise is to find the optimal linear combination of the polynomials $\phi_a = N_a x^a (L-x)^a$ to describe the ground state of a particle in a box. We will use the following trial wave function

$$\psi = c_1\phi_1 + c_2\phi_2 \tag{1}$$

The box is defined as $V(x) = 0$ for $0 \leq x \leq L$ and $V(x) = \infty$ everywhere else. For simplicity, $L = 1$. Use the standard integral

$$\int_0^1 x^a(1-x)^b dx = B(a+1,b+1) \qquad \text{with} \quad B(a+1,b+1) = \frac{(a)!(b)!}{(a+b+1)!} \tag{2}$$

where $B(a,b)$ is the beta function, closely related to the maybe more commonly known gamma function Γ:

$$B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} \tag{3}$$

Answer the following points one-by-one to find the solution. Correct answers to questions 1-12 give 0.833 points each. The rest of the questions give 0.5 points. The sum of all points has a maximum of 10.

1. Calculate the normalization constants N_1 and N_2
2. Give the general formula for N_a
3. Calculate the overlap of ϕ_1 and ϕ_2: $S_{12} = \langle\phi_1|\phi_2\rangle$
4. Write down the energy expectation value of ψ in terms of the functions ϕ_1 and ϕ_2 (don't forget the normalization!) From here on, we will derive the integrals $H_{ij} = \langle\phi_i|\hat{H}|\phi_j\rangle$ and $S_{ij} = \langle\phi_i|\phi_j\rangle$ that appear in the energy expression.
5. Express the overlap integral $S_{ab} = \langle\phi_a|\phi_b\rangle$ in terms of beta functions.

The Hamiltonian only consists of the kinetic energy operator since $V(x) = 0$ in the region where the wave function is defined. Instead of using the standard expression

involving the scalar product of the state vector with the second derivative of the state vector, we will use an alternative expression involving only first derivatives.

$$\begin{aligned}\langle\phi_a|\hat{H}|\phi_b\rangle &= \frac{-\hbar^2}{2m}\langle\phi_a|\frac{d^2}{dx^2}|\phi_b\rangle = \frac{-\hbar^2}{2m}\langle\phi_a|\frac{d}{dx}\frac{d}{dx}|\phi_b\rangle \\ &= \frac{-\hbar^2}{2m}\int_0^1 \left(\phi_a\frac{d}{dx}\right)^\dagger \frac{d}{dx}\phi_b dx = \frac{-\hbar^2}{2m}\int_0^1 -\frac{d}{dx}\phi_a\frac{d}{dx}\phi_b dx \\ &= \frac{\hbar^2}{2m}\langle\phi'_a|\phi'_b\rangle \end{aligned} \tag{4}$$

where ϕ'_a represents $\frac{d\phi_a}{dx}$. Note the minus sign due to the anti-hermitic character of d/dx.

6. Calculate $\frac{d}{dx}\phi_a$.

7. Calculate H_{11}. Express the final results in terms of $\frac{\hbar^2}{8m}$, which will be used as energy scale by putting it to 1.

Before continuing with the other matrix elements of the Hamiltonian, a general expression for H_{ij} must be derived

8. Start with the expression

$$\langle\phi_a|\hat{H}|\phi_b\rangle = \frac{\hbar^2}{2m}\int_0^1 \phi'_a\phi'_b dx = \frac{\hbar^2}{2m}\frac{N_a N_b}{N_{a-1}N_{b-1}}ab\int_0^1 \phi_{a-1}(1-2x)^2\phi_{b-1}dx \tag{5}$$

   to derive an expression for H_{ab} in terms of beta functions.

9. Calculate H_{11}, H_{12} and H_{22} using the general expression for H_{ab}.

10. Take the expression for the expectation value of the energy and derive the equations for which the partial derivatives with respect to c_1 and c_2 are equal to zero.

    [*Hint*: Multiply left- and right-hand-side of the energy expression by the denominator of the rhs term and derive lhs and rhs with respect to c_1 and c_2]

    [*Answer*: $\mathbf{Hc} = \mathbf{ESc}$, where $\mathbf{H}$ is the 2×2 H_{ab} matrix, $\mathbf{S}$ the 2×2 S_{ab} matrix, $\mathbf{c}$ the column vector with the coefficients c_1 and c_2 and $\mathbf{E}$ the diagonal matrix with the two energy eigenvalues.]

11. The equations that result from the previous question can be solved analytically, but the expressions for the energy become rather awkward and not easily extended to larger dimensions. A more versatile approach is to solve the equations numerically. Here we will use the linear algebra library of Python to find the optimal coefficients c_1 and c_2 and the corresponding eigenvalues. Follow these instructions:

(a) Open the webpage: https://www.pythonanywhere.com/try-ipython

(b) After a little while, a line starting with `[1]:` will appear. Type the following Python instructions:

```
[1] import numpy as np
[2] import scipy.linalg
[3] H = np.array([[H11,H12],[H12,H22]])
[4] S = np.array([[S11,S12],[S12,S22]])
[5] E,psi = scipy.linalg.eig(H,S)
[6] E
[7] psi
```

where you have to replace `Hab` and `Sab` by the numerical values that you have calculated before. Only type the text in red.

12. Compare the lowest energy eigenvalue with the exact energy of the ground state of a particle in a box of length 1.

13. Normalize the coefficients for the lowest eigenstate and write down the optimal approximation to the exact wave function as linear combination of ϕ_1 and ϕ_2.

14. Make a graph comparing the exact wave function, ϕ_1, ϕ_2 and ψ with the optimal expansion coefficients. Shortly comment the shape of the curves.

15. Which state is approximately represented by the second root? Compare the energy to the exact answer.

16. How does the energy of the trial wave function compare to the exact one when c_2 is made zero?

17. Solve the general eigenvalue problem by extending the linear combination with ϕ_3. Compare the energies of all roots to the exact ones. How much is the improvement for the second root?

18. As you might have noticed the current set of functions used to approximate the exact solutions only represent the even solutions of the particle-in-a-box problem. Suggest an extension of the basis set to extend the description to the odd solutions.