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Abstract

Problems to review concepts on the VARIATIONAL PRINCIPLE: its introductory theory and how to find upper bounds to the exact ground-state energy level. You can use a symbolic computation software (such as Mathematica) when/if needed.

1. Apply the Rayleigh-Ritz variational method to a particle in a box of width L (when needed) to find:
   (a) The ground state energy using a second-degree polynomial as trial function.
   (b) The ground state energy using a fourth-degree polynomial.
   (c) The energy of the first excited state using the simplest appropriate polynomial as a trial function.

   Note: In each case choose your trial function to satisfy the correct boundary conditions at the walls.
2. Griffiths' Problem 8.30: [Part c) is a coding problem. You can code it on any programming language of your choice (Mathematica, Matlab, Python, Julia, or any other you want). Attach to your HW solution also the files of the code and plot scripts and indicate in which language it runs.] Performing a variational calculation requires finding the minimum of the energy, as a function of the variational parameters. This is, in general, a very hard problem. However, if we choose the form of our trial wave function judiciously, we can develop an efficient algorithm. In particular, suppose we use a linear combination of functions $\phi_n(x)$:

   $$\psi(x) = \sum_{n=1}^{N} c_n \phi_n(x)$$

   where the c_n are the variational parameters. If the ϕ_n are an orthonormal set ($\langle \phi_m | \phi_n \rangle = \delta_{nm}$), but $\psi(x)$ is not necessarily normalized, then $\langle H \rangle$ is

   $$\varepsilon = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\sum_{m,n} c_m^* H_{mn} c_n}{\sum_n |c_n|^2}$$

   where $H_{mn} = \langle \phi_m | H | \phi_n \rangle$. Taking the derivative with respect to c_j^* (and setting the result equal to 0) gives

   $$\sum_n H_{jn} c_n = \varepsilon c_j,$$

recognizable as the j-th row in an eigenvalue problem:

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & \cdots & H_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & \cdots & H_{NN} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = \varepsilon \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$$

The smallest eigenvalue of this matrix H gives a bound on the ground state energy and the corresponding eigenvector determines the best variational wave function of the proposed form (linear combination of our basis).

(a) Verify the equation $\sum_n H_{jn} c_n = \varepsilon c_j$.

(b) Now take the derivative of the equation $\varepsilon = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{m,n} c_m^* H_{mn} c_n}{\sum_n |c_n|^2}$ with respect to c_j and show that you get a result redundant with the equation $\sum_n H_{jn} c_n = \varepsilon c_j$.

(c) Consider a particle in an infinite square well of width a, with a sloping floor:

$$V(x) = \begin{cases} \infty & x < 0, \\ V_0 x/a, & 0 \le x \le a, \\ \infty, & x > a \end{cases}$$

Using a linear combination of the first ten stationary states of the infinite square well as the basis functions,

$$\phi_n = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a}),$$

determine a bound for the ground state energy in the case $V_0 = 100\hbar^2/ma^2$. Make a plot of the optimized variational wave function. [Note: The exact result is $39.9819\hbar^2/ma^2$.] [Second note: footnote (26) from Griffiths': Each c_j, being complex, stands for two independent parameters (its real and imaginary parts). One could take derivatives with respect to the real and imaginary parts,

$$\frac{\partial}{\partial \Re\{c_j\}} E = 0, \quad \text{and}$$

$$\frac{\partial}{\partial \Im\{c_j\}} E = 0,$$

but it is also legitimate (and simpler) to treat c_j and c_j^* as the independent parameters:

$$\frac{\partial}{\partial c_j} E = 0, \quad \text{and}$$

$$\frac{\partial}{\partial c_j^*} E = 0.$$

You get the same result either way.]