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FY2045 Problem set 9 fall 2023

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Problem 1

Find an approximate solution of the equation

$$x^3 - 4x + \lambda = 0, \tag{1}$$

where λ is assumed small by expanding

$$x = x_0 + \lambda x_1 + \lambda^2 x_2 + \dots, \tag{2}$$

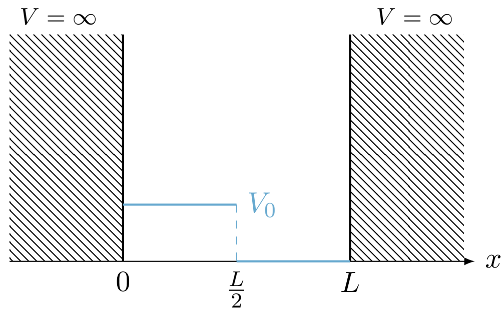
and inserting into the equation. Find the roots to second order in λ. For $\lambda = 0.1$ you can compare your results to the approximate roots $x \approx 0.0250$, $x \approx 1.9874$ and $x \approx -2.0124$.

Problem 2

In the lectures we considered a perturbation δV to the infinite square well potential

$$V(x) \to V(x) + \lambda \delta V \equiv V(x) + \lambda V_0 \Theta\left(\frac{L}{2} - x\right), \tag{3}$$

where $\Theta(x)$ is the Heaviside step function, as illustrated below.



Without the perturbation ($\lambda = 0$), the eigenenergies and eigenfunctions are

$$E_n^0 = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \equiv E_1^0 n^2, \tag{4}$$

$$\psi_n^0(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}, \tag{5}$$

with $n = 1, 2, 3, \ldots$. In the lectures, we showed that with the perturbation ($\lambda > 0$) the first order correction to the energies was $E_n^{(1)} = \frac{V_0}{2}$ for all states.

a) The second order corrections to the energies are given by

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m|\delta V|n\rangle|^2}{E_n^0 - E_m^0}. \tag{6}$$

Show that the *matrix elements* can be written

$$\langle m|\delta V|n\rangle = \frac{2V_0}{L} \int_0^{\frac{L}{2}} dx \ \sin \frac{\pi m x}{L} \cdot \sin \frac{\pi n x}{L} \tag{7}$$

in the position representation.

b) Solve the integral, and show that it results in

$$\langle m|\delta V|n\rangle = \frac{V_0}{\pi} \left[\frac{\sin \frac{\pi(m-n)}{2}}{m-n} - \frac{\sin \frac{\pi(m+n)}{2}}{m+n} \right]. \tag{8}$$

c) For what m and n are the matrix elements zero? Why do you think this is the case?

d) Assume that $n = 1$ and write down the non-zero matrix elements with $m \leq 10$, and compare the contribution to the sum in eq. (6) from the term with $m = 2$ and $m = 10$. Does it seem necessary to include *all* terms in the sum to get a good approximation for $E_n^{(2)}$?

e) It's possible to numerically determine the (approximate) eigenenergies and wavefunctions of the perturbed system. Using this example code (or this one) from `www.numfys.net`, determine the ground state energy as a function of the parameter V_0/E_1^0 (with $\lambda = 1$) and compare it with the result from perturbation theory to second order in λ including terms with $m \leq 10$ in the sum in eq. (6).

f) Calculate and plot the ground state wavefunction, and compare it to the approximate wavefunction from first-order perturbation theory,

$$\psi_n(x) \approx \psi_n^0(x) + \lambda \sum_{m \neq n} \frac{\langle m|\delta V|n\rangle}{E_n^0 - E_m^0} \psi_m^0(x). \tag{9}$$

Does the change to the ground state wavefunction seem reasonable?

g) What is the ground state energy in the limit $V_0 \to \infty$?