

Quantum Chemistry

Seminar 6

Approximate methods II
Perturbation methods

Exercise 1 (unassigned)

Find the solution of the illustrative example (lesson 6, page 6) for $y_0 = 0$ up to the 6th order and evaluate the values of the left-hand side of the solved equation for $\varepsilon = 0.1$ and for the solutions of 4th to 6th order. Compare the results with page 7 of lesson 6.

Exercise 2 (unassigned)

Find the solution of the illustrative example (lesson 6, page 6) for $y_0 = 1$ up to the 3rd order and evaluate the values of the left-hand side of the solved equation for $\varepsilon = 0.1$ and for the solutions of 0th to 3rd order.

Exercise 3 (Shaho)

Using the known solution ([wiki](#)) of the time-independent Schrödinger equation for the linear harmonic oscillator, $\hat{H}_0 = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2x^2$, find, within the 1st order perturbation approximation, the ground-state energy of a linear anharmonic oscillator, $\hat{H} = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2x^2 + \varepsilon x^4$, $\varepsilon > 0$, and compare it with the value obtained for the linear harmonic oscillator.