Quantum Mechanics: Worksheet 1

Non-degenerate perturbation theory and the variational method

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When we cannot solve a quantum mechanical problem exactly, we can use perturbative methods to obtain approximate results. In this worksheet, we consider the most simple approximation methods: non-degenerate perturbation theory and the variational method.

1 Harmonic oscillator – frequency change as a perturbation

Consider the Hamiltonian $H = H_0 + \lambda V$ with

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2, \quad V = \frac{1}{2} m\omega^2 x^2.$$

(a) Calculate the spectrum exactly, expand it about $\lambda = 0$ to second order:

$$E_n(\lambda) \simeq E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)},$$

and identify the coefficients $E_n^{(1)}$ and $E_n^{(2)}$.

(b) Calculate the first and second order coefficients $E_n^{(1)}$ and $E_n^{(2)}$ with non-degenerate perturbation theory. Also find the first-order correction to the eigenstates.

2 Hydrogen atom trial wave function

The Hamiltonian for the relative motion of the electron of the hydrogen atom is (in Gaussian units)

$$H = \frac{p^2}{2m_e} - \frac{e^2}{r},$$

and can be solved exactly with ground-state energy $E_0 = -\frac{e^2}{2a_0}$, where $a_0 = \frac{\hbar^2}{m_e e^2}$ is the Bohr radius. Use a trial wave function $\psi_\alpha(r) = e^{-\frac{\alpha}{2} r^2}$ to approximate the energy and determine the best approximation. How does it compare with the exact result?

3 Infinite potential well with a delta-function barrier

Consider a particle in a one-dimensional infinite potential well:

$$V(x) = \begin{cases} 0 & -a < x < a \\ \infty & \text{elsewhere,} \end{cases}$$

Give the energy together with the even and odd parity eigenfunctions of the unperturbed well and calculate the effect of the perturbation $W(x) = wa\,\delta(x)$ on the energy levels

(a) up to first order for all levels and,

(b) up to second order for the four lowest levels.

Why are odd-parity solutions not affected in any order of perturbation? Finally, solve this problem exactly for comparison.

4 Harmonic oscillator trial wave function

Approximate the ground-state energy of the harmonic oscillator with the following trial wave functions ($a, \alpha > 0$)

$$\psi_a(x) = \frac{1}{x^2 + a}, \qquad \psi_\alpha(x) = e^{-\frac{\alpha}{2}|x|}.$$

Useful identities

1. Non-degenerate perturbation theory:

$$E_n^{(k)} = \langle \psi_n^{(0)} | V | \psi_n^{(k-1)} \rangle, \qquad |\psi_n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | V | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle.$$

2. Harmonic oscillator:

$$\langle m | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle m | \hat{a} + \hat{a}^\dagger | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\sqrt{n}\, \delta_{m,n-1} + \sqrt{n+1}\, \delta_{m,n+1} \right).$$

3. Variational method (E_0 is the true ground-state energy):

$$E_0 \leq \langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle},$$

$$\int_{-\infty}^{\infty} dx\, \psi^* \frac{d^2}{dx^2} \psi = \left[\psi^* \frac{d}{dx} \psi \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx \left| \frac{d\psi}{dx} \right|^2.$$

4. Telescoping series (k is a positive integer):

$$\sum_{m=1}^{\infty} \frac{k}{m(m+k)} = \sum_{m=1}^{\infty} \left(\frac{1}{m} - \frac{1}{m+k} \right) = \sum_{m=1}^{k} \frac{1}{m}.$$

5. Differentiation under the integral sign (a and b are constants):

$$\boxed{\frac{d}{dt} \int_a^b dx\, f(x,t) = \int_a^b dx\, \frac{\partial}{\partial t} f(x,t).}$$