Quantum Mechanics

Week 11

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Exercise Material

Webpage

Week 11

Review

Exercises

Review of Last Week

- Any questions on last week's topics?
- Feedback on the previous session?

Review

Perturbation Theory

- Tool for approximating complex quantum systems
- Introduces small modifications to simpler, solvable systems
- Starts with a well-established Hamiltonian $\hat{H}^{(0)}$

Hamiltonian Formulation

- New Hamiltonian:

$$\hat{H}_{new} = \hat{H}^{(0)} + \lambda \cdot \hat{H}'$$

- $\hat{H}_{new}$: Hamiltonian for the complex problem
- $\hat{H}^{(0)}$: Solvable Hamiltonian
- λ: Adjustable parameter (assumed to be one if not specified)
- $\hat{H}'$: Perturbation

Objective

- Solve the equation:

$$\hat{H}\psi_n = E_n\psi_n$$

- Using the solution of:

$$\hat{H}^{(0)}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$$

Power Series Expansion

- Energies and wavefunctions as second-order power series in λ

$$E_n = E_n^{(0)} + \lambda \cdot E_n^{(1)} + \lambda^2 \cdot E_n^{(2)}$$
$$\psi_n = \psi_n^{(0)} + \lambda \cdot \psi_n^{(1)} + \lambda^2 \cdot \psi_n^{(2)}$$

With a power series expansion we approximate with every order closer the solution.

Non-Degenerate Perturbation Theory

- Quantum systems with distinct energy levels
- $E_n^{(0)} \neq E_m^{(0)}$
- Unperturbed Hamiltonian $\hat{H}^{(0)}$
- Eigenvalues $E_n^{(0)}$ and eigenfunctions $\psi_n^{(0)}$
- Perturbation $\hat{H}'$ introduced

$$\hat{H}_{new} = \hat{H}^{(0)} + \lambda \hat{H}'$$

First-Order Energy Correction

$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle$$

- Quantifies the primary influence of the perturbation
- Really important and simple to use! We can know our disturbance of energy by only knowing the difference in Hamiltonian and the unperturbed state!

First-Order Wavefunction Correction

$$\psi_n^{(1)} = \sum_{m \neq n} c_{mn} \psi_m^{(0)}$$

$$c_{mn} = \frac{\langle \psi_m^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}}$$

- $m = n$ term excluded
- $\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)}$

Second-Order Energy Correction

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

- Considers interactions between different energy levels

Example: Infinite Square Well

$$V(x) = \begin{cases} V_0, & 0 < x < \frac{a}{2} \\ 0, & \frac{a}{2} < x < a \end{cases}$$

- V_0 is the perturbation strength
- a is the width of the well

Unperturbed Hamiltonian

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad n = 1, 2, 3, \ldots$$

First-Order Energy Correction Example

$$E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$$

$$E_n^{(1)} = \int_0^{a/2} \left(\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \right)^2 V_0 \, dx \tag{1}$$

$$= \frac{2}{a} \cdot V_0 \cdot \frac{a}{4} \tag{2}$$

$$= \frac{V_0}{2} \tag{3}$$

Degenerate Perturbation Theory

- Quantum systems with multiple eigenstates at identical energy levels
- Introduction of perturbation removes degeneracy

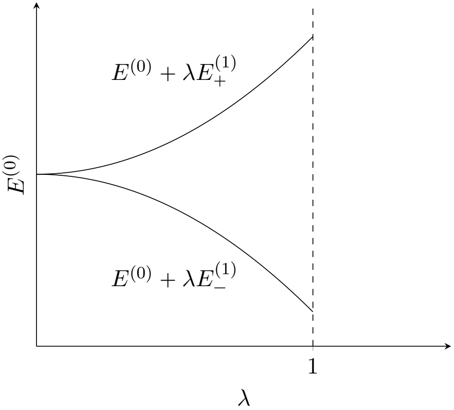
Energy Correction

- Degenerate eigenstates $\psi_a^{(0)}$ and $\psi_b^{(0)}$ with same eigenvalue $E^{(0)}$
- First-order energy correction:

$$E_{\pm}^{(1)} = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4W_{ab}^2}\right] \tag{4}$$

- $W_{ij} = \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle$

Lifting Degeneracy



Diagonalizing the W-Matrix

$$\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^{(1)} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

- Find eigenvalues of the matrix
- Non-zero W_{ab}: Lifts degeneracy, appropriate linear combination
- Zero W_{ab}: Perturbation fails to distinguish states, degeneracy preserved

Variational Principle

- Estimates ground state energy of a quantum system
- Useful for complex systems where Schrödinger equation is difficult to solve

Key Concept

- Ground state energy E_0 is the lowest expectation value of the Hamiltonian $\hat{H}$
- Approximated using a trial wave function ψ_{trial}

$$E_{gs} \leqslant \langle \psi_{\text{trial}} | \hat{H} | \psi_{\text{trial}} \rangle = E_{\text{approx}} \tag{5}$$

Application

- Select a trial wave function with adjustable parameters
- Minimize the expectation value of the Hamiltonian

$$E_{\text{approx}} = \min_{\{\text{parameters}\}} \langle \psi_{\text{trial}} | \hat{H} | \psi_{\text{trial}} \rangle \tag{6}$$

- The trial wave function yielding the minimum expectation value is the best approximation

Example: Particle in Infinite Square Well

- Trial wave function:

$$\psi_{\text{trial}}(x) = Ax(L - x) \tag{7}$$

Hamiltonian and Trial Energy

- For an infinite square well, $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$
- Trial energy:

$$E_{\text{approx}} = \langle \psi_{\text{trial}} | \hat{H} | \psi_{\text{trial}} \rangle \tag{8}$$

Calculation

- Expectation value of the Hamiltonian:

$$\langle\psi|\hat{H}|\psi\rangle = \frac{\hbar^2}{m}\frac{L^3}{6} \tag{9}$$

- Normalization constant A^2:

$$A^2 = \frac{L^5}{30} \tag{10}$$

- Trial energy:

$$E_{\text{approx}} = \frac{5\hbar^2}{mL^2} \tag{11}$$

Comparison with True Ground State Energy

- Known ground state energy:

$$E_{gs} = \frac{\hbar^2\pi^2}{2mL^2} \tag{12}$$

- Ratio:

$$\frac{E_{\text{trial}}}{E_{gs}} = \frac{10}{\pi^2} \tag{13}$$

- Since $\pi^2 \approx 9.87$, the ratio is:

$$\frac{10}{\pi^2} < 5 \tag{14}$$

- Indicates a "good" guess

Perturbation Theory vs Variational Principle

Perturbation Theory

- Know answer to similar problem
- Gives corrections to E_n and ψ_n
- Language to look for is:
  - Estimate to first order...
  - Consider the perturbation

Variational Principle

- No need to know anything
- Gives estimate of E_{gs}
- Language to look for is:
  - Estimate E_{gs}...
  - Use trial function...

Exercises

Exercise 1

Really important, must do!

Exercise 2

Really important, must do!

Exercise 3

Interesting! There is a good video on Youtube

Questions?

THANK YOU all for coming!