FY2045 Quantum Mechanics I

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Week 10

Time-independent perturbation theory

General formulation

In most situations, a system is defined by a Hamiltonian H for which the Schrödinger equation cannot be solved exactly. However, if $H = H_0 + V$, where V is a small, time-independent term — a **perturbation** — and we know the solutions to

$$H_0|n\rangle = E_n^0|n\rangle, \tag{1}$$

we can find **approximate** solutions of

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \tag{2}$$

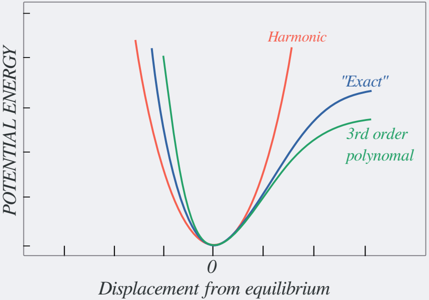
using **time-independent perturbation theory**.

Ø15, H7.1, G7

Examples of perturbations

Anharmonic oscillator:

$H = H_0 + \lambda x^4$



Zeemann effect, $H_Z = -\boldsymbol{\mu}_S \cdot \mathbf{B}$.

Relativistic energy correction

$$E = \sqrt{m^2c^4 + c^2p^2} \approx mc^2 + \frac{p^2}{2m} - \frac{p^4}{m^3c^2} + \dots$$

Spin-orbit coupling

$$H_{SO} = \xi \mathbf{L} \cdot \mathbf{S}.$$

Hyperfine splitting of atomic levels due to spin-spin interactions between electrons and nucleus.

Non-degenerate perturbation theory

Write

$$H = H_0 + \lambda V,$$

with "book keeping device" $\lambda \in [0, 1]$.

Analogy — Roots of polynomials

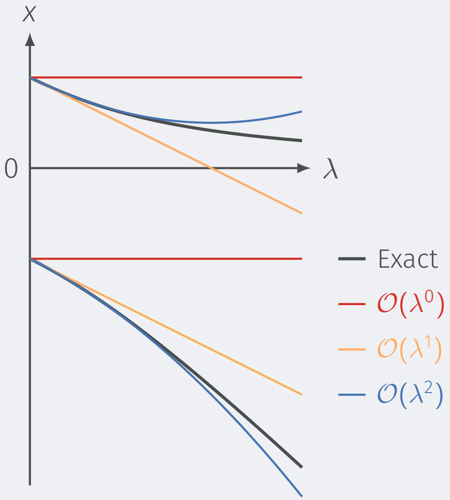
$$x^2 + \lambda x - c = 0.$$

If λ is small, we use ansatz

$$x = x_0 + \lambda x_1 + \lambda^2 x_2 + \ldots,$$

to get approximate solution

$$x \approx \pm\sqrt{c} - \frac{\lambda}{2} \pm \frac{\lambda^2}{8\sqrt{c}} + \mathcal{O}(\lambda^3).$$



Non-degenerate perturbation theory

We write $H = H_0 + \lambda V$, where $\lambda \in [0, 1]$. When $\lambda \to 0$, we should have

$$E_n \to E_n^0 \text{ and } |\psi_n\rangle \to |n\rangle.$$

We therefore write

$$E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots, \tag{3}$$
$$|\psi_n\rangle = |n\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \dots, \tag{4}$$

where we have assumed **non-degenerate** states. Inserting into the SE, eq. (2), and collecting like powers of λ, we get

$$\lambda^0 : \quad H_0|n\rangle = E_n^0|n\rangle,$$
$$\lambda^1 : \quad H_0|n^{(1)}\rangle + V|n\rangle = E_n^0|n^{(1)}\rangle + E_n^{(1)}|n\rangle, \tag{5}$$
$$\lambda^2 : \quad H_0|n^{(2)}\rangle + V|n^{(1)}\rangle = E_n^0|n^{(2)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(2)}|n\rangle. \tag{6}$$

Non-degenerate perturbation theory

First-order corrections

$$\underline{E_n^{(1)} = \langle n|V|n\rangle},$$

$$\underline{|n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle m|V|n\rangle}{E_n^0 - E_m^0}|m\rangle.}$$

Second-order energies

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

Summary

The solution to the eigenvalue problem

$$(H_0 + \lambda V)|\psi_n\rangle = E_n|\psi_n\rangle$$

is

$$|\psi_n\rangle = |n\rangle + \sum_{m\neq n} \frac{\langle m|\lambda V|n\rangle}{E_n^0 - E_m^0}|m\rangle + \mathcal{O}(\lambda^2),$$

$$E_n = E_n^0 + \langle n|\lambda V|n\rangle + \sum_{m\neq n} \frac{|\langle m|\lambda V|n\rangle|^2}{E_n^0 - E_m^0} + \mathcal{O}(\lambda^3).$$