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

$$H_0|n\rangle = E_n^0|n\rangle, \tag{1}$$
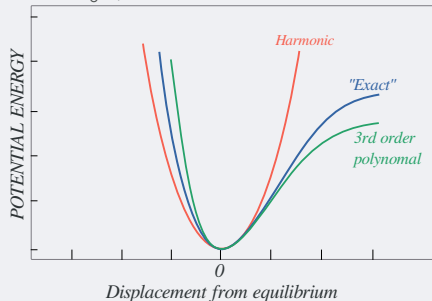
we can find **approximate** solutions of

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

using **time-independent perturbation theory**.

Ø15, H7.1, G7

Anharmonic oscillator:

$H = H_0 + \lambda x^4$

Displacement from equilibrium

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

Relativistic energy correction

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

Spin-orbit coupling

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

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

Write

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

with "book keeping device" $\lambda \in [0, 1]$.
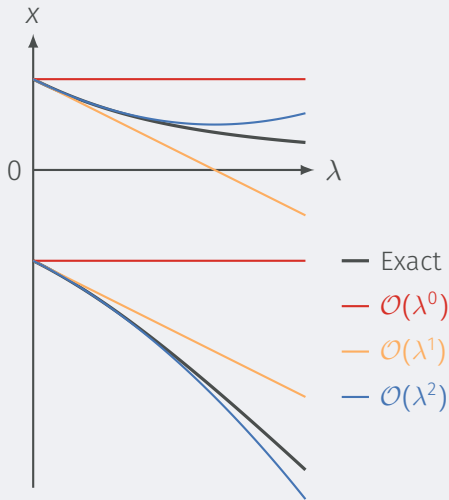
Analogy — Roots of polynomials

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

If λ is small, we use ansatz

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

to get approximate solution

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

- Exact
- $\mathcal{O}(\lambda^0)$
- $\mathcal{O}(\lambda^1)$
- $\mathcal{O}(\lambda^2)$

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

$$E_n = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots, \tag{3}$$

$$|\psi_n\rangle = |n\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \ldots, \tag{4}$$

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

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

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

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

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

$$E_n = E_n^0 + \langle n|\lambda V|n \rangle + \sum_{m \neq n} \frac{|\langle m|\lambda V|n \rangle|^2}{E_n^0 - E_m^0} + \mathcal{O}(\lambda^3).$$
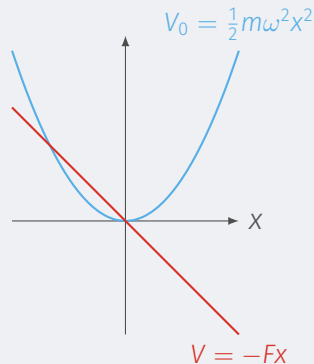
A harmonic oscillator is perturbed by force F in positive x-direction:

$$V = -Fx.$$

The perturbed Hamiltonian is

$$H = H_0 + V = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 - Fx.$$

What are the corrections to the energies and eigenstates?

$V_0 = \frac{1}{2}m\omega^2 x^2$

x

$V = -Fx$

Example — Perturbed harmonic oscillator

To second order in F we find the energies

$$E_n = E_n^0 + E_n^{(1)} + E_n^{(2)}$$
$$= \hbar\omega \left[n + \frac{1}{2} \right] - \frac{F^2}{2m\omega^2},$$

and to first order the state vectors

$$|\psi_n\rangle = \left(1 - \frac{ix_0\hat{p}_x}{\hbar} \right) |n\rangle,$$
$$\Rightarrow \psi_n(x) = \left(1 - x_0 \frac{d}{dx} \right) \psi_n^{(0)}(x),$$

with $x_0 = \frac{F}{m\omega^2}$.

Example — Perturbed harmonic oscillator

Exact solution

Rewrite perturbed Hamiltonian

$$H = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2(x - x_0)^2 - \frac{F^2}{2m\omega^2}.$$

Hence, we have exact solution

$$E_n = \hbar\omega\left[n + \frac{1}{2}\right] - \frac{F^2}{2m\omega^2},$$

$$\psi_n(x) = \psi_n^{(0)}(x - x_0) = \psi_n^{(0)}(x) - x_0\frac{d}{dx}\psi_n^{(0)}(x)\ldots,$$

which agrees exactly with the second order energy correction, and to first order with the wavefunction correction.