L66-First Order Perturbation

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* Similar to the Frobenius method, perturbation theory is a method of solving a problem order by order.
  - except now we approximate the whole problem, not just the solution by a power series
  - solve one order at a time, no recursion relations
  - most problems in C.M. & Q.M. cannot be solved analytically, but often a restricted problem is solvable, and the rest can be treated as a perturbation.
  - example: treat electronic interactions in the atom as a perturbation.

* Perturbation theory, like much of mechanics, was developed to solve the 3-body problem:
  ex: Earth-Moon-Sun orbits:
  Solve the Earth-moon system, and add Sun-(Earth, Moon) Interactions as a perturbation

* Example: solve $x^2 - 1 = \varepsilon x$ http://www.cims.nyu.edu/~eve2/reg_pert.pdf

$x_0 \simeq \pm 1$ as $\underbrace{\varepsilon}_{\text{"book keeping parameter"}} \to 0$. let $x = x_0 + \varepsilon x_1 + \varepsilon^2 x_2 + \mathcal{O}(\varepsilon^3)$

$$x^2 = x_0^2 + \varepsilon(2x_0x_1) + \varepsilon^2(2x_0x_2 + x_1^2) + \mathcal{O}(\varepsilon^3)$$
$$\varepsilon x = \varepsilon(x_0) + \varepsilon^2(x_1) + \mathcal{O}(\varepsilon^3)$$

$$x^2 - 1 - \varepsilon x = \overbrace{(x_0^2 - 1)}^{0^{th}\text{ order}} + \varepsilon\overbrace{(2x_0x_1 - x_0)}^{1\text{st order}} + \varepsilon^2\overbrace{(2x_0x_2 + x_1^2 - x_1)}^{2\text{nd order}} + \mathcal{O}(\varepsilon^3)$$

$$x_0 = \pm 1 \qquad x_1 = 1/2 \qquad x_2 = \pm\frac{1}{8}$$

$$x = \pm 1 + \frac{\varepsilon}{2} \pm \frac{\varepsilon^2}{8} + \mathcal{O}(\varepsilon^3) \approx \frac{\varepsilon}{2} \pm \sqrt{1 + \left(\frac{\varepsilon}{2}\right)^2}$$

just application of power series to problem & solution

* Application to QM: $\mathcal{H} = \mathcal{H}^0 + \lambda\mathcal{H}'$ (divide up problem)

$$\Psi_n = \Psi_n^0 + \lambda \Psi_n^1 + \lambda^2 \Psi_n^2 + \dots$$
$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots$$

} λ serves as "book keeping" parameter to keep track of order

$$[\mathcal{H} - E_n]\Psi_n = \left[(\mathcal{H}^0 + \lambda \mathcal{H}') - (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 +)\right](\Psi_n^0 + \lambda \Psi_n^1 + \lambda^2 \Psi_n^2 + \dots) = 0$$

0th order: $(\mathcal{H}^0 - E_n^0)\Psi_n^0 = 0$ $\rightarrow$ E_n^0, Ψ_n^0 must be solved directly.

1st order: $(\mathcal{H}^0 - E_n^0)\Psi_n^1 + (\mathcal{H}' - E_n^1)\Psi_n^0 = 0$ $\rightarrow$ E_n^1, Ψ_n^1 in Ψ_n^0 basis

2nd order: $(\mathcal{H}^0 - E_n^0)\Psi_n^2 + (\mathcal{H}' - E_n^1)\Psi_n^1 + (-E_n^2)\Psi_n^0 = 0$ $\rightarrow$ E_n^2, Ψ_n^2

* write out matrices in the Ψ_n^0 basis: $|\Psi_n^1\rangle = \sum_{\ell \neq n} c_\ell^{(n)} |\Psi_\ell^0\rangle = C|\Psi_n^0\rangle$

- sandwitch $\langle \Psi_m^0|$ on left: $\langle \Psi_m^0 | \Psi_n^1\rangle = \sum_\ell \langle \Psi_m^0 | c_\ell^{(n)} | \Psi_\ell^0\rangle = \underbrace{c_m^{(n)}}_{m^{th} \text{ component of } \Psi_n^1} = \langle \Psi_m^0 | C | \Psi_n^0 \rangle$

- the component of Ψ_n^1 along $\Psi_n^0 = 0$
  just absorb it into Ψ_n^0 to get a better 0th order solution

- normalization: $c_\ell^{(m)}$ is the perturbation of a unitary matrix

$$\langle \Psi_m^0 + \lambda \Psi_m^1 | \Psi_n^0 + \lambda \Psi_n^1 \rangle \approx \cancel{\langle \Psi_m^0 | \Psi_n^0 \rangle}^{\delta_{mn}} + \lambda\Big[\underbrace{\langle \Psi_m^1 | \Psi_n^0 \rangle + \langle \Psi_m^0 | \Psi_n^1 \rangle}_{0!}\Big] + \mathcal{O}(\lambda^2) = \cancel{\delta_{mn}}$$

$$\langle \Psi_m^1 | \Psi_n^0 \rangle + \langle \Psi_m^0 | \Psi_n^1 \rangle = \sum_\ell c_\ell^{(m)*} \cancel{\langle \Psi_\ell^0 | \Psi_n^0 \rangle}^{\delta_{\ell n}} + c_\ell^{(n)} \cancel{\langle \Psi_m^0 | \Psi_\ell^0 \rangle}^{\delta_{m\ell}} = c_n^{(m)*} + c_m^{(n)} = 0$$

thus the matrix $c_m^{(n)}$ and its operator C are Antihermitian:
$c_m^{(n)} = -c_n^{(m)*}$, or $C = -C^\dagger$; the diagonal $c_n^{(n)} = 0$ (imaginary)

In terms of operators, $|\Psi_n\rangle \approx |\Psi_n^0\rangle + \lambda|\Psi_n^1\rangle = (1 + C)|\Psi_n^0\rangle$

$$\delta_{mn} = \langle \Psi_m | \Psi_n \rangle \approx \langle (1+\lambda C)\Psi_m^0 | (1 + \lambda C)\Psi_n^0 \rangle = \langle \Psi_m^0 | (1 + \lambda C^\dagger)(1 + \lambda C) | \Psi_n^0 \rangle = \delta_{mn}$$

so $\quad I + \lambda(C^\dagger + C) + \mathcal{O}(\lambda^2) = I \quad \Rightarrow \quad C^\dagger = -C$

We've seen these generators of rotations before! $i^* = -i$, $\times\vec{V} = -\vec{V}\times$

* 1st order matrix equation: $(\mathcal{H}^0 - E_n^0)\Psi_n^1 + (\mathcal{H}' - E_n^1)\Psi_n^0 = 0$

$$\underbrace{\langle \Psi_m^0 | (\cancel{\mathcal{H}^0}^{E_m^0} - E_n^0) | c_\ell^{(n)} \Psi_\ell^0 \rangle} + \langle \Psi_m^0 | (\mathcal{H}' - \underbrace{E_n^1) | \Psi_n^0 \rangle}_{0 \text{ if } m \neq n} = 0$$

$$\underbrace{\langle \psi_m^0 | (\cancel{\mathcal{H}^0} - E_n^0) | c_l^{(n)} \psi_l^0 \rangle}_{0 \text{ if } m=n} + \langle \psi_m^0 | (\mathcal{H}' - \underbrace{E_n^1) | \psi_n^0 \rangle}_{0 \text{ if } m\neq n} = 0$$

– when $m=n$, $\boxed{E_n^1 = \langle \psi_n^0 | \mathcal{H}' | \psi_n^0 \rangle \equiv V_{nn}}$ energy eigenvalue perturbation

– when $m \neq n$, $(E_m^0 - E_n^0) c_m^{(n)} = \langle \psi_m^0 | \mathcal{H}' | \psi_n^0 \rangle$

$$\boxed{|\psi_n^1\rangle = \sum_m c_m^{(n)} |\psi_m^0\rangle = \sum_n \frac{\langle \psi_m^0 | \mathcal{H}' | \psi_n^0 \rangle}{E_m^0 - E_n^0} |\psi_n^0\rangle \equiv \sum_n \frac{V_{mn}}{\Delta_{mn}} |\psi_n^0\rangle}$$

eigen-wavefunction perturbation

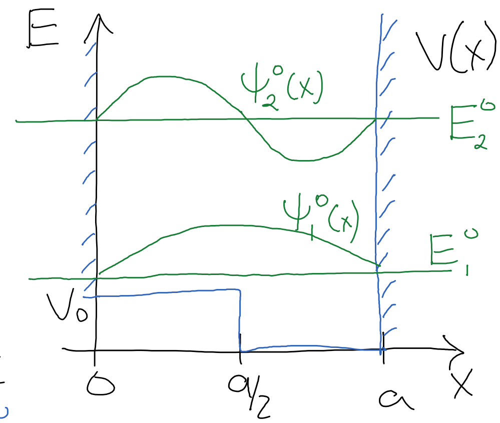
* 2nd order Energy: $(\mathcal{H}^0 - E_n^0)\psi_n^2 + (\mathcal{H}' - E_n^1)\psi_n^1 + (-E_n^2)\psi_n^0 = 0$

$$\langle \psi_n^0 | \cancel{\mathcal{H}^0}^{E_n^0} - E_n^0 | \psi_n^2 \rangle + \langle \psi_n^0 | \mathcal{H}' - \cancel{E_n^1} | \psi_n^1 \rangle - \langle \psi_n^0 | E_n^2 | \psi_n^0 \rangle = 0$$

$\langle \psi_n^0 | \psi_n^1 \rangle = 0$ const.

$$\boxed{E_n^2 = \langle \psi_n^0 | \mathcal{H}' | \psi_n^1 \rangle = \sum_m c_m^{(n)} \langle \psi_n^0 | \mathcal{H}' | \psi_m^0 \rangle = \sum_{m\neq n} \frac{|\langle \psi_n | \mathcal{H}' | \psi_m \rangle|^2}{E_m - E_n} = \sum_{m \neq n} \frac{|V_{mn}|^2}{\Delta_{mn}}}$$

* Example: perturbed inf. square well



$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}' = 0 + V_0\,\Theta(x - a/2)$$

$$\psi_n^0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad E_n^0 = \frac{\hbar^2 \pi^2}{2a^2} n^2$$

$$V_{mn} = \langle \psi_m^0 | \mathcal{H}' | \psi_n \rangle = \int_0^{a/2} dx\, V_0 \cdot \frac{2}{a} \sin \underbrace{\frac{n\pi x}{a}}_{N} \sin \underbrace{\frac{m\pi x}{a}}_{M}$$

$$= \frac{2V_0}{a} \int_0^{a/2} \frac{e^{iN} - e^{-iN}}{2i} \cdot \frac{e^{iM} - e^{-iM}}{2i} dx = \frac{2V_0}{a} \int_0^{a/2} \frac{e^{i(N+M)} + e^{-i(N+M)}}{-4} - \frac{e^{i(M-N)} + e^{-i(M-N)}}{-4}$$

$$= \frac{V_0}{a} \int_0^{a/2} \cos(M-N) - \cos(M+N)\, dx = \frac{V_0}{a} \left[\frac{\sin(M-N)}{(m-n)\pi/a} \Big|_0^{a/2} - \frac{\sin(M+N)}{(m+n)\pi/a} \Big|_0^{a/2} \right]$$

$$= \frac{V_0}{\pi} \left(\frac{\sin((m-n)\frac{\pi}{2})}{m-n} - \frac{\sin((m+n)\frac{\pi}{2})}{m+n} \right) \quad \text{if } m \neq n, \quad V_{nn} = \frac{V_0}{2}$$

$$E_n^1 = V_{nn} = V_0/2 \qquad \psi_n^1 = \sum_{m\neq n} \frac{V_{mn}}{E_m - E_n} \psi_m^0 \qquad E_n^2 = \sum_{m \neq n} \frac{|V_{mn}|^2}{E_m - E_n}$$

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Table[If[m == n, V0 / 2, V0 / Pi (Sin[(m - n) * Pi / 2] / (m - n) - Sin[(m + n) * Pi / 2] / (m + n))], {m, 1, 7}, {n, 1, 7}]
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$$\begin{pmatrix} \frac{V_0}{2} & \frac{4\,V_0}{3\,\pi} & 0 & -\frac{8\,V_0}{15\,\pi} & 0 & \frac{12\,V_0}{35\,\pi} & 0 \\ \frac{4\,V_0}{3\,\pi} & \frac{V_0}{2} & \frac{4\,V_0}{5\,\pi} & 0 & -\frac{4\,V_0}{21\,\pi} & 0 & \frac{4\,V_0}{45\,\pi} \\ 0 & \frac{4\,V_0}{5\,\pi} & \frac{V_0}{2} & \frac{8\,V_0}{7\,\pi} & 0 & -\frac{4\,V_0}{9\,\pi} & 0 \\ -\frac{8\,V_0}{15\,\pi} & 0 & \frac{8\,V_0}{7\,\pi} & \frac{V_0}{2} & \frac{8\,V_0}{9\,\pi} & 0 & -\frac{8\,V_0}{33\,\pi} \\ 0 & -\frac{4\,V_0}{21\,\pi} & 0 & \frac{8\,V_0}{9\,\pi} & \frac{V_0}{2} & \frac{12\,V_0}{11\,\pi} & 0 \\ \frac{12\,V_0}{35\,\pi} & 0 & -\frac{4\,V_0}{9\,\pi} & 0 & \frac{12\,V_0}{11\,\pi} & \frac{V_0}{2} & \frac{12\,V_0}{13\,\pi} \\ 0 & \frac{4\,V_0}{45\,\pi} & 0 & -\frac{8\,V_0}{33\,\pi} & 0 & \frac{12\,V_0}{13\,\pi} & \frac{V_0}{2} \end{pmatrix}$$