Let's now work on finding a more general prescription for PT expansions. This approach will work for any dimension of Hilbert space and as long as the pertubation is small, it will produce a reasonable approx. 1

The method relies on having an exactly solvable zeroth order problem,

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$$

no pertubation at all.

The problem we want to solve is the one where the pertubation, H', is present.

$$(H_0 + H')|n\rangle = E_n |n\rangle$$

we seek approximate solutions to E_n & $|n\rangle$ that will rely on $E_n^{(0)}$ and $|n^{(0)}\rangle$. To keep track of the order of approx, we introduce λ, and set equal to 1 at the end,

$$(H_0 + \lambda H')|n\rangle = E_n |n\rangle$$

We look for a power series solution, 2

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

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \lambda^3 |n^{(3)}\rangle + \ldots$$

To do so, we pop our solution into the eigenvalue equation and match terms of the same λ order,

$$(H_0 + \lambda H')\left(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \ldots\right)$$

$$= \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots\right)\left(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \ldots\right)$$

Doing so gives us,

λ^0: $H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$ just the original problem

λ^1: $H_0|n^{(1)}\rangle + H'|n^{(0)}\rangle = E_n^{(0)}|n^{(1)}\rangle + E_n^{(1)}|n^{(0)}\rangle$

λ^2: $H_0|n^{(2)}\rangle + H'|n^{(1)}\rangle = E_n^{(0)}|n^{(2)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle$

etc.

We collect terms based on their $|n^{(i)}\rangle$ ket.

$$\lambda^0: \left(H_0 - E_n^{(0)}\right)|n^{(0)}\rangle = 0$$

$$\lambda^1: \left(H_0 - E_n^{(0)}\right)|n^{(1)}\rangle = \left(E_n^{(1)} - H'\right)|n^{(0)}\rangle$$

$$\lambda^2: \left(H_0 - E_n^{(0)}\right)|n^{(2)}\rangle = \left(E_n^{(1)} - H'\right)|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle$$

etc.

This is why the original problem,

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$$

needs a solution. the rest of the expansion relies on it.

McIntyre goes through an excellent matrix tracing argument (read it!) to show,

$$\boxed{\begin{aligned} E_n^{(1)} &= H'_{nn} = \langle n^{(0)}|H'|n^{(0)}\rangle \\ |n^{(1)}\rangle &= \sum_{m \neq n} \frac{\langle m^{(0)}|H'|n^{(0)}\rangle}{\left(E_n^{(0)} - E_m^{(0)}\right)}|m^{(0)}\rangle \end{aligned}}$$

Basically, to first order, the energy correction, $E_n^{(1)}$, is equal to the diagonal matrix elements of H'.

To first order, the contribution of a state $|m^{(0)}\rangle$ to the state correction, $|n^{(1)}\rangle$, is proportional to the off diagonal elements of H' and inversely proportional to the energy difference between $E_n^{(0)}$ & $E_m^{(0)}$.

Through a second matrix tracing example, McIntyre shows the second order correction to the energy, $E_n^{(2)}$, is proportional to the square of the off diag. elements of H' scaled by their energy differences with $E_n^{(0)}$.

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

A few notes:

- This only works for a system where $H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$ is solvable.
- It assumes each correction (λ order) is smaller than H^0's contribution $\rightarrow$ preferably smaller contributions as λ increases. (to converge)
- It does not work for degenerate problems $\Rightarrow (E_n^{(0)} - E_m^{(0)}) = 0$ ✓
- We typically don't look beyond 2nd order for E_n or first order for $|n\rangle$