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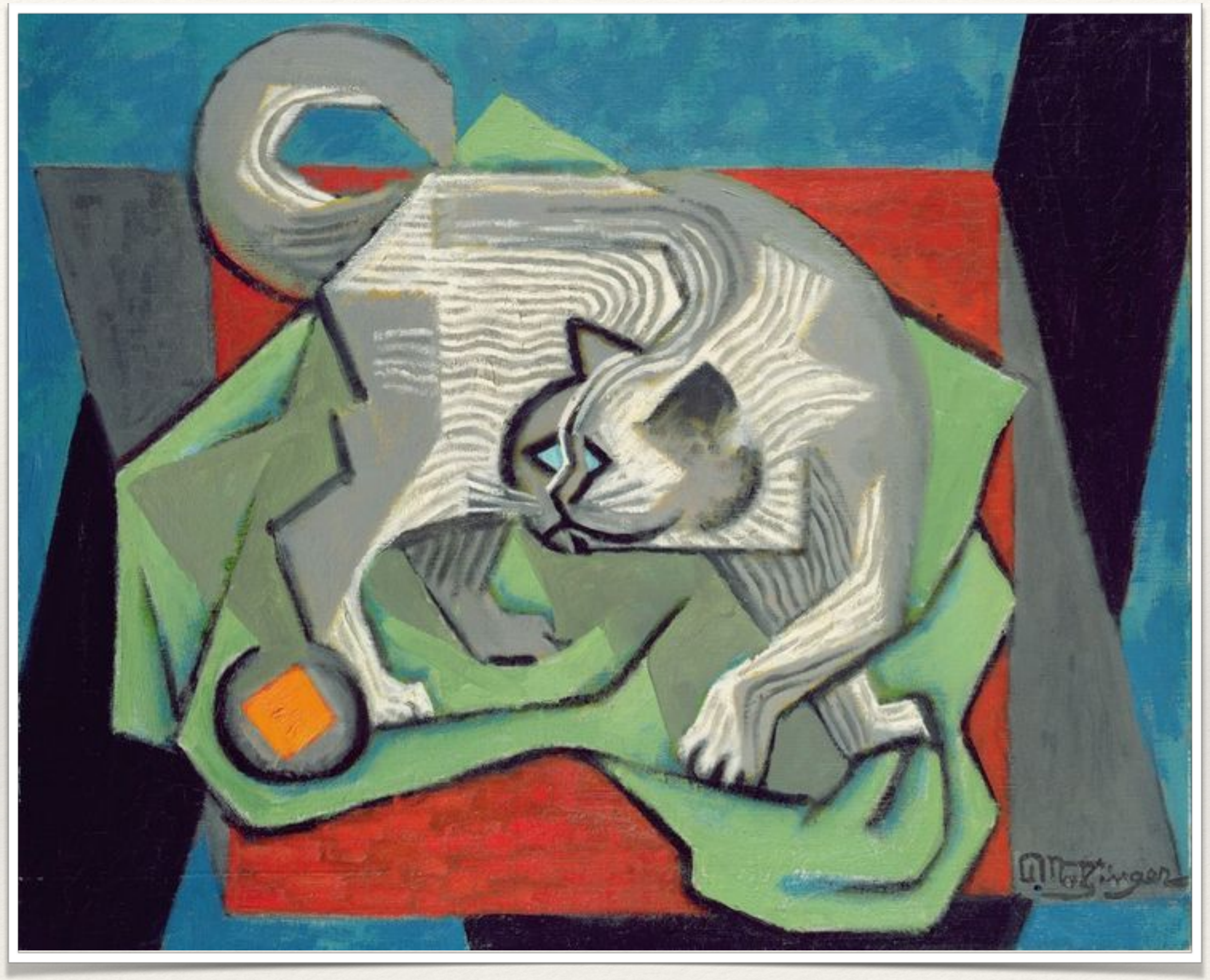
Quantum Mechanics

Lecture 9

Non-degenerate perturbation theory;
Example: quantum harmonic oscillator.



Weakly interacting systems

Consider a non-degenerate interacting system:

$$H = H_0 + \lambda H_1 \longleftarrow$$ complicating interactions

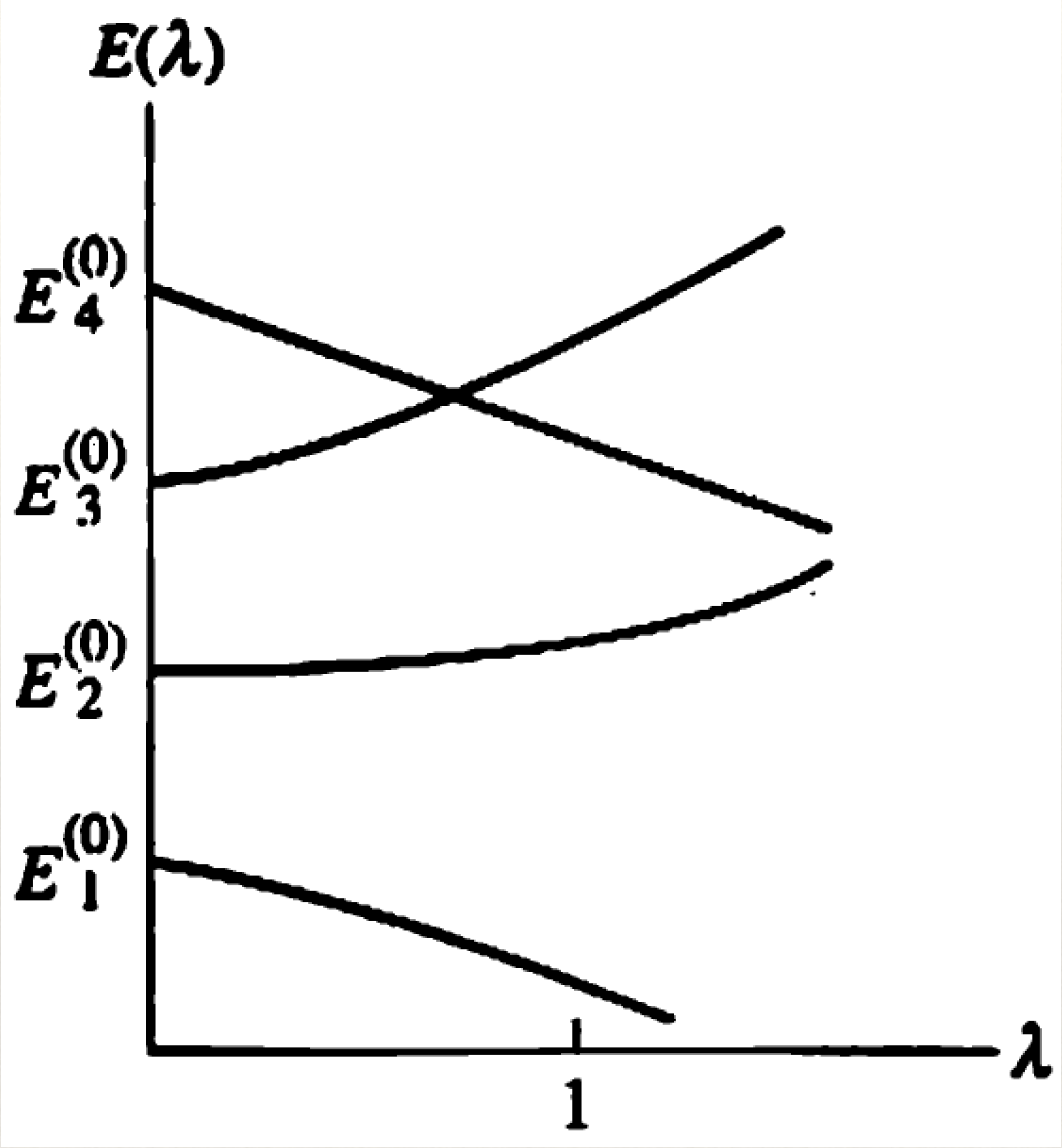
simple system

dimensionless parameter

We want to find all of the eigenstates:

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

Idea: suppose λ is small and expand as a power series:



bare system is solvable

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

energies and wave function depend smoothly on λ.

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

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

Matching term by term

Plug in the series expansion ansatz and define separate equations term by term:

$$\begin{aligned} H|\psi_n\rangle &= (H_0 + \lambda H_1)|\psi_n\rangle \\ &= (H_0 + \lambda H_1)(|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^2|\phi_n^{(2)}\rangle + \ldots) \\ &= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots)(|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^2|\phi_n^{(2)}\rangle + \ldots) \end{aligned}$$

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

Order λ^0

$$H_0|\phi_n^{(1)}\rangle + H_1|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}|\phi_n^{(0)}\rangle$$

Order λ^1

$$H_0|\phi_n^{(2)}\rangle + H_1|\phi_n^{(1)}\rangle = E_n^{(0)}|\phi_n^{(2)}\rangle + E_n^{(1)}|\phi_n^{(1)}\rangle + E_n^{(2)}|\phi_n^{(0)}\rangle$$

Order λ^2

$$\vdots$$

$\vdots$

First-order energy shift

Take the inner product with the zeroth-order eigenstates to derive:

$$H_0|\phi_n^{(1)}\rangle + H_1|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}|\phi_n^{(0)}\rangle$$

Use nth eigenstate

$$\langle\phi_n^{(0)}|H_0|\phi_n^{(1)}\rangle + \langle\phi_n^{(0)}|H_1|\phi_n^{(0)}\rangle = E_n^{(0)}\langle\phi_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}\langle\phi_n^{(0)}|\phi_n^{(0)}\rangle$$

$$\langle\phi_n^{(0)}|H_0 = \langle\phi_n^{(0)}|E_n^{(0)} \qquad \langle\phi_k^{(0)}|\phi_n^{(0)}\rangle = \delta_{nk}$$

$$\Rightarrow \quad E_n^{(1)} = \langle\phi_n^{(0)}|H_1|\phi_n^{(0)}\rangle$$

First-order correction to the eigenstates

Take the inner product with the zeroth-order eigenstates to derive:

$$H_0|\phi_n^{(1)}\rangle + H_1|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}|\phi_n^{(0)}\rangle$$

Use kth eigenstate, $k \neq n$.

$$\langle\phi_k^{(0)}|H_0|\phi_n^{(1)}\rangle + \langle\phi_k^{(0)}|H_1|\phi_n^{(0)}\rangle = E_n^{(0)}\langle\phi_k^{(0)}|\phi_n^{(1)}\rangle + E_n^{(1)}\langle\phi_k^{(0)}|\phi_n^{(0)}\rangle$$

$$\langle\phi_k^{(0)}|H_0 = \langle\phi_k^{(0)}|E_k^{(0)} \qquad \langle\phi_k^{(0)}|\phi_n^{(0)}\rangle = \delta_{nk}$$

$$E_k^{(0)}\langle\phi_k^{(0)}|\phi_n^{(1)}\rangle + \langle\phi_k^{(0)}|H_1|\phi_n^{(0)}\rangle = E_n^{(0)}\langle\phi_k^{(0)}|\phi_n^{(1)}\rangle$$

$$\Rightarrow \frac{\langle\phi_k^{(0)}|H_1|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} = \langle\phi_k^{(0)}|\phi_n^{(1)}\rangle \qquad (k \neq n)$$

First-order correction to the eigenstates

Now expand in the zeroth-order basis:

$$H_0 | \phi_n^{(1)} \rangle + H_1 | \phi_n^{(0)} \rangle = E_n^{(0)} | \phi_n^{(1)} \rangle + E_n^{(1)} | \phi_n^{(0)} \rangle$$

Use *k*th eigenstate, $k \neq n$.

$$| \phi_n^{(1)} \rangle = \left(\sum_k | \phi_k^{(0)} \rangle \langle \phi_k^{(0)} | \right) | \phi_n^{(1)} \rangle$$

Insert resolution of identity.

$$= | \phi_k^{(0)} \rangle \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle + \sum_{k \neq n} | \phi_k^{(0)} \rangle \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle$$

Isolate term *k*.

$$= | \phi_k^{(0)} \rangle \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle + \sum_{k \neq n} \frac{\langle \phi_k^{(0)} | H_1 | \phi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} | \phi_k^{(0)} \rangle$$

Follows from earlier.

First-order correction to the eigenstates

What about $\langle\phi_k^{(0)}|\phi_n^{(1)}\rangle$? Use normalization condition:

$$1 = \langle\psi_n|\psi_n\rangle = \langle\phi_n^{(0)}|\phi_n^{(0)}\rangle + \lambda\Big(\overset{=0}{\cancel{\langle\phi_n^{(0)}|\phi_n^{(1)}\rangle + \langle\phi_n^{(1)}|\phi_n^{(0)}\rangle}}\Big) + O(\lambda^2)$$

$$\Rightarrow \ \langle\phi_n^{(0)}|\phi_n^{(1)}\rangle = ia \ , \quad a \text{ real}$$

Therefore:

$$|\psi_n\rangle = |\phi_n^{(0)}\rangle + ia\lambda|\phi_n^{(0)}\rangle + \lambda\sum_{k\neq n}|\phi_k^{(0)}\rangle\langle\phi_k^{(0)}|\phi_n^{(1)}\rangle + O(\lambda^2)$$

$$= \mathrm{e}^{ia\lambda}|\phi_n^{(0)}\rangle + \lambda\sum_{k\neq n}|\phi_k^{(0)}\rangle\langle\phi_k^{(0)}|\phi_n^{(1)}\rangle + O(\lambda^2) \qquad \big(\mathrm{e}^{ia\lambda} = 1 + ia\lambda + O(\lambda^2)\big)$$

Re-phase to $a = 0$:

$$\Rightarrow \ \langle\phi_n^{(0)}|\phi_n^{(1)}\rangle = 0$$

Therefore:

$$\Rightarrow \ |\psi_n\rangle = |\phi_n^{(0)}\rangle + \lambda\sum_{k\neq n}|\phi_k^{(0)}\rangle\frac{\langle\phi_k^{(0)}|H_1|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} + O(\lambda^2)$$

Second-order energies

The second order energies follow from similar considerations:

$$H_0|\phi_n^{(2)}\rangle + H_1|\phi_n^{(1)}\rangle = E_n^{(0)}|\phi_n^{(2)}\rangle + E_n^{(1)}|\phi_n^{(1)}\rangle + E_n^{(2)}|\phi_n^{(0)}\rangle$$

Take the overlap with the zeroth-order eigenstate:

$$\underset{\text{cancels}}{\cancel{\langle\phi_n^{(0)}|H_0|\phi_n^{(2)}\rangle}} + \langle\phi_n^{(0)}|H_1|\phi_n^{(1)}\rangle = \overset{\text{cancels}}{\cancel{E_n^{(0)}\langle\phi_n^{(0)}|\phi_n^{(2)}\rangle}} + \overset{=0}{\cancel{E_n^{(1)}\langle\phi_n^{(0)}|\phi_n^{(1)}\rangle}} + E_n^{(2)}\underset{=1}{\underline{\langle\phi_n^{(0)}|\phi_n^{(0)}\rangle}}$$

$$\Rightarrow \quad \langle\phi_n^{(0)}|H_1|\phi_n^{(1)}\rangle = E_n^{(2)}$$

Now plug in the first-order corrected eigenstates to get:

$$\Rightarrow \quad E_n^{(2)} = \sum_{k\neq n} \frac{|\langle\phi_k^{(0)}|H_1|\phi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

In general, computing the *n*th order energy shift requires knowing the (*n*-1)th order corrections to the energy.

Example: perturbed harmonic oscillator

Consider a charged particle in a 1D harmonic potential, and an applied electric field that leads to a linear potential term:

$$H = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m^2\omega^2\hat{x}^2 - q\,|\,\mathbf{E}\,|\,\hat{x} \qquad H_0 = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m^2\omega^2\hat{x}^2 \qquad H_1 = -q\,|\,\mathbf{E}\,|\,\hat{x}$$

The unperturbed energies and states are simply:

$$E_n^{(0)} = \left(n + \frac{1}{2}\right)\hbar\omega \qquad |\,\phi_n^{(0)}\rangle = |\,n\rangle$$

Now recall the harmonic oscillator raising and lowering operators:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right)$$

$$\hat{a}^\dagger\,|\,n\rangle = \sqrt{n+1}\,|\,n+1\rangle$$

$$\hat{a}\,|\,n\rangle = \sqrt{n}\,|\,n-1\rangle$$

Example: perturbed harmonic oscillator

The first order energy corrections are: $E_n^{(1)} = \langle \phi_n^{(0)} | H_1 | \phi_n^{(0)} \rangle$

$$E_n^{(1)} = \langle n | H_1 | n \rangle \propto \langle n | \left(\hat{a} + \hat{a}^\dagger \right) | n \rangle = \sqrt{n} \langle n | n-1 \rangle + \sqrt{n+1} \langle n | n+1 \rangle = 0$$

We have to go to second order to see an effect: $E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_k^{(0)} | H_1 | \phi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$

Introduce:

$$C = \sqrt{\frac{\hbar q^2 |\mathbf{E}|^2}{2m\omega}}$$

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle k | -C(\hat{a} + \hat{a}^\dagger) | n \rangle|^2}{(n-k)\hbar\omega} = \frac{C^2}{\hbar\omega} \sum_{k \neq n} \frac{|\sqrt{n}\langle k | n-1 \rangle + \sqrt{n+1}\langle k | n+1 \rangle|^2}{(n-k)}$$

$$= \frac{C^2}{\hbar\omega} \left(\frac{|\sqrt{n}|^2}{(n-(n-1))} + \frac{|\sqrt{n+1}|^2}{(n-(n+1))} \right) = \frac{C^2}{\hbar\omega} \left(\frac{n}{1} + \frac{n+1}{-1} \right) = -\frac{q^2 |\mathbf{E}|^2}{2m\omega^2}$$

Example: perturbed harmonic oscillator

Thus the total corrected energies to second order are:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{q^2|\mathbf{E}|^2}{2m\omega^2}$$

We can check explicitly the accuracy in this case by completing the square:

$$\begin{aligned} H &= \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m^2\omega^2\hat{x}^2 - q|\mathbf{E}|\hat{x} \\ &= \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m^2\omega^2\left(\hat{x} - \frac{q^2|\mathbf{E}|^2}{m\omega^2}\right)^2 - \frac{q^2|\mathbf{E}|^2}{2m\omega^2} \end{aligned}$$

The eigenstates are just translated copies of the original number states.