20190521 Ch5

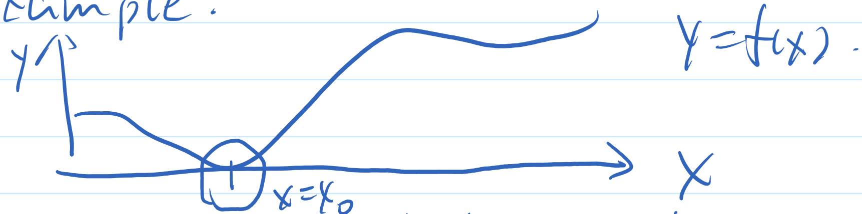
Tuesday, May 21, 2019 5:25 PM

Chapter 5 approximation methods

§1 time-independent perturbation theory.

philosophy: we start with the problem really close to a solved problem, then we can use the solution at hand to do approximation.

example.



↑ would like to look at behavior at bottom.

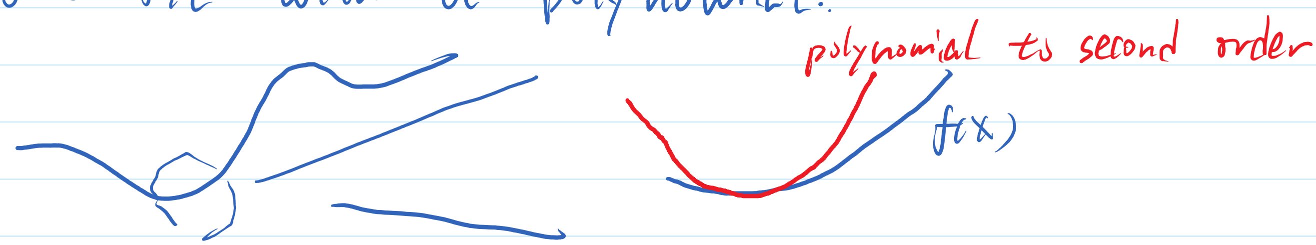
to begin with assume polynomials are good.

Taylor-expansion 泰勒展开.

$$f(x) \simeq f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \cdots$$

if keep all the way to $(x-x_0)^2$

→ do a fit with a polynomial.



Quantum: time independent perturbation theory.

① $H = H_0 + H'$

H_0 has a know solution for eigen energy $E_n^{(0)}$, and eigenstate $\{|n^{(0)}\rangle\}$

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

$H' = \lambda V$, V is another part of Hamiltonian.
but λ a number, $\lambda \ll 1$

② try to find $H|n\rangle = E_n |n\rangle$.
E_n must be a function of H, which is a function of λ, so as $|n\rangle$. $\rightarrow E_n(\lambda)$, $|n(\lambda)\rangle$

we can make a Taylor expansion of $E_n(\lambda)$

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

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

$\lambda E_n^{(1)}$ is first order energy shift
$\lambda E_n^{(2)}$ second 〃

plug it back to $H|n\rangle = E|n\rangle$ with $H = H_0 + \lambda V$

$(H_0 + \lambda V)(|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots) =$
$(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots) \cdot (|n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle + \cdots)$

λ^0, or not containing λ

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

$\lambda^1 \Rightarrow H_0 |n^{(1)}\rangle + V|n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle$.
if we apply $\langle n^{(0)}|$ to the left.

$\underline{\langle n^{(0)} | n^{(0)}\rangle = 1}$, $\underline{\langle n^{(0)} | H} |n^{(1)}\rangle = E_n^{(0)} \langle n^{(0)} | n^{(1)}\rangle$

$\Rightarrow \langle n^{(0)} | H_0 | n^{(1)}\rangle + \langle n^{(0)} | V | n^{(0)}\rangle = E_n^{(0)} \langle n^{(0)} | n^{(1)}\rangle + E_n^{(1)} \langle n^{(0)} | n^{(0)}\rangle$

$\Rightarrow E_n^{(0)} \cancel{\langle n^{(0)} | n^{(1)}\rangle} + \langle n^{(0)} | V | n^{(0)}\rangle = E_n^{(0)} \cancel{\langle n^{(0)} | n^{(1)}\rangle} + E_n^{(1)}$

$\Rightarrow \boxed{E_n^{(1)} = \langle n^{(0)} | V | n^{(0)}\rangle}$

[illegible]

$\Rightarrow \boxed{E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle}$

$\Rightarrow$ first order perturbation for E_n

$E_n = E_n^{(0)} + \lambda E_n^{(1)} = E_n^{(0)} + \langle n^{(0)} | \lambda V | n^{(0)} \rangle$

$$\boxed{E_n = E_n^{(0)} + \langle n^{(0)} | H' | n^{(0)} \rangle}$$

$H = H_0 + \lambda V$, we can express it in the energy representation in the basis of $\{|n^{(0)}\rangle\}$

$$H_0 = \begin{pmatrix} E_0^{(0)} & & & & \\ & E_1^{(0)} & & 0 & \\ & & E_2^{(0)} & & \\ & 0 & & \ddots & \\ & & & & E_n^{(0)} & \\ & & & & & \ddots \end{pmatrix}$$

λV in the same basis

$$\lambda V = \begin{pmatrix} \lambda V_{11} & \lambda V_{12} & \lambda V_{13} & \cdots \\ \lambda V_{21} & \lambda V_{22} & \lambda V_{23} & \cdots \\ & & \cdots & \\ & & & \ddots \end{pmatrix}$$

for $n=0$ $\quad E_0 \simeq E_0^{(0)} + \lambda V_{11}$

1^{st} order perturbation is just n^{th} row, n^{th} column for matrix $H_0 + \lambda V$ in $\{|n^{(0)}\rangle\}$ basis.

1^{st} order perturbation for state

$$\begin{cases} H_0 |n^{(1)}\rangle + V|n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + \underline{E_n^{(1)}} |n^{(0)}\rangle \\ E_n^{(1)} = \langle n^{(0)} | V | n^{(0)} \rangle . \end{cases}$$

$\checkmark$

we try to solve for $|n^{(1)}\rangle$.

we apply $\langle k^{(0)}|$ to left, with $\underline{k \neq n}$. $\langle k^{(0)} | n^{(0)} \rangle = 0$

also require $E_n^{(0)} \neq E_k^{(0)}$

) also require $E_n^{(0)} \neq E_k^{(0)}$

$$\langle k^{(0)} | H_0 | n^{(1)} \rangle + \langle k^{(0)} | V | n^{(0)} \rangle = E_n^{(0)} \langle k^{(0)} | n^{(1)} \rangle + \underbrace{E_n^{(1)} \langle k^{(0)} | n^{(0)} \rangle}_{0}$$

$$E_k^{(0)} \langle k^{(0)} | n^{(1)} \rangle + \langle k^{(0)} | V | n^{(0)} \rangle$$
$$= E_n^{(0)} \langle k^{(0)} | n^{(1)} \rangle .$$

$\langle k^{(0)} | n^{(1)} \rangle$ — inner product between an unknown state $|n^{(1)}\rangle$ and a state in the known basis — amplitude.

$|n^{(1)}\rangle = \sum_m C_m |m^{(0)}\rangle$, since $\{ |m^{(0)}\rangle \}$ form a basis.

$$\langle k^{(0)} | n^{(1)} \rangle = \sum_m C_m \underbrace{\langle k^{(0)} | m^{(0)} \rangle}_{=0 \text{ unless } k=m} = C_k$$

$$\Rightarrow \boxed{C_k = \frac{\langle k^{(0)} | V | n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}} \quad , k \neq n.$$

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

the 1st order perturbation for state

$$\boxed{|n\rangle = |n^{(0)}\rangle + \sum_{k \neq n} \frac{\langle k^{(0)} | H' | n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle}$$

$\langle k^{(0)} | H' | n^{(0)} \rangle$ — matrix element in the k^{th} row and n^{th} column of matrix H' in the basis of $\{ |n^{(0)}\rangle \}$

$H_0 + H' \xrightarrow{\text{matrix in } \{|n^{(0)}\rangle\}}$

$$\begin{array}{cc} \begin{array}{ccc} k^{th} & n^{th} \text{ column} & \end{array} & \\ \begin{pmatrix} - - E_k^{(0)} - H'_{kn} - - - - \end{pmatrix} & k^{th} \text{ row} \end{array}$$

$$H_0 + H' \longrightarrow \begin{array}{c} \left(\begin{array}{ccccc} \cdots & E_k^{(0)} & \cdots & H'_{kn} & \cdots \\ \cdots & & & E_n^{(0)} & \cdots \end{array}\right) \end{array} \begin{array}{l} k^{th} \text{ row} \\ n^{th} \end{array}$$

$$H_{kn} = \langle k^{(0)} | H' | n^{(0)} \rangle$$

- example spin-$\frac{1}{2}$ system.

$$H_0 = \Omega \sigma_z \longrightarrow \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}$$

$$H' = \lambda \sigma_x \longrightarrow \begin{pmatrix} 0 & \lambda \\ \lambda & 0 \end{pmatrix}$$

$$H = H_0 + H' = \begin{pmatrix} \Omega & \lambda \\ \lambda & -\Omega \end{pmatrix}$$

$\Omega \gg \lambda$

$$\Rightarrow E = \Omega + \frac{\lambda^2}{2\Omega}, \quad |\psi\rangle = \begin{pmatrix} 1 - \frac{\lambda^2}{2\Omega^2} \\ \frac{\lambda}{2\Omega} \end{pmatrix}. \quad \text{keep } \lambda \text{ to second order}$$

$$E = -\Omega - \frac{\lambda^2}{2\Omega}, \quad |\psi\rangle = \begin{pmatrix} -\frac{\lambda}{2\Omega} \\ 1 - \frac{\lambda^2}{2\Omega^2} \end{pmatrix}.$$