Lanczos method

(1) choose an initial vector $|\Phi_1\rangle$ (arbitrary)

normalize it $\quad |\phi_1\rangle = \dfrac{|\Phi_1\rangle}{\sqrt{\langle\Phi_1|\Phi_1\rangle}}$

(2) define projection operator

$P_1 = |\phi_1\rangle\langle\phi_1|$ so that $P_1|g\rangle = \langle\phi_1|g\rangle|\phi_1\rangle$

in particular $P_1|\phi_1\rangle = |\phi_1\rangle$

and $(1-P_1)|\phi_1\rangle = 0 \qquad (b)$

(3) define $|\Phi_2\rangle = (1-P_1)H|\phi_1\rangle$

$P_1^{+} = P_1 \quad \therefore$ from (b) $\quad \langle\phi_1|(1-P_1) = 0$

or $\langle\phi_1|\Phi_2\rangle = \underbrace{\langle\phi_1|(1-P_1)}_{0} H|\phi_1\rangle = 0$

$\therefore \langle\phi_1|\Phi_2\rangle = 0$, normalize $|\Phi_2\rangle \Rightarrow |\phi_2\rangle$

(4) examine $\quad H|\phi_1\rangle = P_1 H|\phi_1\rangle + (1-P_1)H|\phi_1\rangle$

from (a)

$= c_1|\phi_1\rangle + |\Phi_2\rangle$

$\therefore \quad H|\phi_1\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$

(5) to define $|\Phi_3\rangle$. We define $P_2 = |\phi_2\rangle\langle\phi_2|$

$$H|\phi_2\rangle = P_1 H|\phi_2\rangle + P_2 H|\phi_2\rangle + \underbrace{(1-P_1-P_2)H|\phi_2\rangle}_{|\Phi_3\rangle}$$

(6) We will show $|\Phi_3\rangle \perp |\phi_1\rangle$ and $|\phi_2\rangle$

$\because \langle\phi_2|\phi_1\rangle = 0 \quad \therefore P_2|\phi_1\rangle = 0$

$$\langle\phi_1|\Phi_3\rangle = \underbrace{\langle\phi_1|(1-P_1)H|\phi_2\rangle}_{\overset{\shortparallel}{0}\ \text{from (6)}} - \underbrace{\langle\phi_1|P_2}_{\overset{\shortparallel}{0}} H|\phi_2\rangle$$

$\because P_1|\phi_2\rangle = 0, \quad (1-P_2)|\phi_2\rangle = 0$

$\therefore \quad (1-P_1-P_2)|\phi_2\rangle = 0$

$$\langle\phi_3|\phi_2\rangle = \langle\phi_2|H\underbrace{(1-P_1-P_2)|\phi_2\rangle}_{\overset{\shortparallel}{0}} = 0$$

let $|\phi_3\rangle = |\Phi_3\rangle / \sqrt{\langle\Phi_3|\Phi_3\rangle}$

We have $|\phi_3\rangle, |\phi_2\rangle, |\phi_1\rangle$ they are orthogonal and normalized.

(7) matrix elements.

$\because \quad H|\phi_1\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle$

$\therefore \quad \langle\phi_3|H|\phi_1\rangle = 0$ and $\langle\phi_1|H|\phi_3\rangle = 0$ (C).

(8) define $P_3 = |\phi_3\rangle\langle\phi_3|$

$$|\Phi_4\rangle = (1 - P_2 - P_3) H |\phi_3\rangle$$

then $H|\phi_3\rangle = (1 - P_2 - P_3 + P_2 + P_3) H |\phi_3\rangle$

$$= P_2 H |\phi_3\rangle + P_3 H |\phi_3\rangle + (1 - P_2 - P_3) H |\phi_3\rangle$$

$$= c_2' |\phi_2\rangle + c_3' |\phi_3\rangle + |\Phi_4\rangle \qquad (d)$$

(9) $|\Phi_4\rangle \perp |\phi_2\rangle, |\phi_3\rangle$? yes.

$\because (1 - P_2)|\phi_2\rangle = 0, \quad P_3|\phi_2\rangle = 0 \quad \therefore (1 - P_2 - P_3)|\phi_2\rangle = 0$

$\therefore \langle\phi_4|\phi_2\rangle = \langle\phi_3| H \underbrace{(1 - P_2 - P_3)|\phi_2\rangle}_{0} = 0$

$\because (1 - P_3)|\phi_3\rangle = 0, \quad P_2|\phi_3\rangle = 0 \quad \therefore (1 - P_2 - P_3)|\phi_3\rangle = 0$

$\therefore \langle\phi_4|\phi_3\rangle = \langle\phi_3| H \underbrace{(1 - P_2 - P_3)|\phi_3\rangle}_{0} = 0$

(10) matrix element

from (c) $\langle\phi_1|H|\phi_3\rangle = 0$,

from (d) $\langle\phi_1|H|\phi_3\rangle = \langle\phi_1|\Phi_4\rangle = 0$

$\therefore |\Phi_4\rangle \perp |\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$.

$$\langle\phi_4|H|\phi_1\rangle = \langle\phi_4|(c_1|\phi_1\rangle + c_2|\phi_2\rangle) = 0$$

$$\langle\phi_4|H|\phi_2\rangle = \langle\phi_4|(c_1'|\phi_1\rangle + c_2'|\phi_2\rangle + c_3'|\phi_3\rangle) = 0$$

up to $|\Phi_4\rangle$, we have

$$H = \begin{pmatrix} \times & \times & 0 & 0 \\ \times & \times & \times & 0 \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \end{pmatrix}$$

We can proceed to define $|\Phi_5\rangle$ etc. to make H - matrix tridiagonal.

(11) in general, we have

$$H|\phi_n\rangle = C_{n-1}|\phi_{n-1}\rangle + C_n|\phi_n\rangle + C_{n+1}|\phi_{n+1}\rangle$$

tridiagonal form.

(12) What happens if $C_{n+1} \simeq 0$ for a large n?

a). different subspace $\begin{pmatrix} (\quad) & 0 \\ 0 & (\quad) \end{pmatrix}$

b). for very large n, accumulative error may make $C_{n+1} \simeq 0$.