Lanczos Tridiagonalization

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Let $\hat{H}$ be Hermitian ($\langle m|\hat{H}|n\rangle = \langle n|\hat{H}^\dagger|m\rangle = \langle n|H|m\rangle$)
and $|0\rangle$ a normalized ($\langle 0|0\rangle = 1$) vector.
Then the Lanczos recursion is defined as follows:

$$\begin{cases} b_1|1\rangle = \underbrace{(\hat{H}-a_0)|0\rangle}_{\text{residual}} & (1) \\ b_{n+1}|n+1\rangle = \underbrace{(\hat{H}-a_n)|n\rangle}_{\text{residual}} - \underbrace{b_n|n-1\rangle}_{\text{tridiagonalizing constrained force}} \quad (n=1,2,\ldots,N-1) & (2) \end{cases}$$

where

$$a_n \equiv \langle n|\hat{H}|n\rangle \qquad (n=0,1,\ldots,N) \qquad (3)$$

is the diagonal Hamiltonian element, and

$$b_n \equiv \langle n-1|\hat{H}|n\rangle \qquad (n=1,2,\ldots,N) \qquad (4)$$

is determined to normalized $|n\rangle$ each time a new $|n\rangle$ is obtained by Eq.(2). The arbitrary phase in determined such that b_n is real.

$$\begin{array}{c|cccccc|}
 & 0 & 1 & 2 & & n\text{-}1 & n \\
\hline
0 & a_0 & b_1 & & & & \\
1 & b_1 & a_1 & b_2 & & & \\
2 & & b_2 & a_2 & b_3 & & \\
 & & & \ddots & \ddots & \ddots & \\
N\text{-}1 & & & & b_{n-1} & a_{n-1} & b_n \\
N & & & & & b_n & a_n \\
\hline
\end{array}$$

(Th)

① $\langle m | n \rangle = \delta_{mn}$ (orthonormality) (5)

② $\langle n-\delta | \hat{H} | n \rangle = \emptyset \quad (\delta \geq 2)$ (tridiagonality) (6)

(Proof by mathematical induction)

$$\begin{cases} \langle i | j \rangle = \delta_{ij} \quad \text{for } \forall i,j \leq n & (7) \\ \langle i-\delta | \hat{H} | i \rangle = \emptyset \quad \text{for } \forall i \leq n, \forall \delta \geq 2 & (8) \end{cases}$$

(Basis step: $n=2$)

By assumption $\langle 0|0 \rangle = 1$

$\langle 0| \times (1)$:

$$b_1 \langle 0|1 \rangle = \underbrace{\langle 0|\hat{H}|0 \rangle}_{\equiv a_0} - a_0 \underbrace{\langle 0|0 \rangle}_{1} = \emptyset$$

$\therefore \langle 0|1 \rangle = 0$

$\langle 1| \times (1)$:

$$\cancel{b_1} \langle 1|1 \rangle = \underbrace{\langle 1|\hat{H}|0 \rangle}_{\equiv b_1^* = \cancel{b_1}} - a_0 \underbrace{\langle 1|0 \rangle}_{\emptyset}$$

$\therefore \langle 1|1 \rangle = 1$

Let $n=2$ in Eq. (2):

$$b_2 |2\rangle = (\hat{H} - a_1)|1\rangle - b_1 |0\rangle \tag{9}$$

$\langle 0| \times (9)$:

$$b_2 \langle 0|2 \rangle = \underbrace{\langle 0|\hat{H}|1 \rangle}_{\equiv b_1} - a_1 \underbrace{\langle 0|1 \rangle}_{\emptyset} - b_1 \underbrace{\langle 0|0 \rangle}_{1} = 0$$

$\therefore \langle 0|2 \rangle = 0$

$\langle 1| \times (9)$:

$$b_2 \langle 1|2 \rangle = \underbrace{\langle 1|\hat{H}|1 \rangle}_{\equiv a_1} - a_1 \underbrace{\langle 1|1 \rangle}_{1} - b_1 \underbrace{\langle 1|0 \rangle}_{\emptyset} = \emptyset$$

$\therefore \langle 1|2 \rangle = \emptyset$

$\langle 2| \times (9)$:

$$\cancel{b_2} \langle 2|2 \rangle = \underbrace{\langle 2|\hat{H}|1 \rangle}_{\cancel{b_2}} - a_1 \underbrace{\langle 2|1 \rangle}_{\emptyset} - b_1 \underbrace{\langle 2|0 \rangle}_{\emptyset}$$

$\therefore \langle 2|2 \rangle = 1$

$\langle 2| \times (1)$:

$$b_1 \underbrace{\langle 2|1\rangle}_{\emptyset} = \langle 2|\hat{H}|0\rangle - a_0 \underbrace{\langle 2|0\rangle}_{\emptyset}$$

$$\therefore \langle 0|\hat{H}|2\rangle = \emptyset$$

(Inductive step)

Assume the inductive hypothesis (7) & (8) for n.

Now consider $n+1$.

$\langle n-1| \times (2)$

$$b_{n+1} \langle n-1|n+1\rangle = \cancel{\underbrace{\langle n-1|\hat{H}|n\rangle}_{\equiv b_n}} - a_n \underbrace{\langle n-1|n\rangle}_{\emptyset} - \cancel{b_n \underbrace{\langle n-1|n-1\rangle}_{1}} = 0$$

$$\therefore \langle n-1|n+1\rangle = 0$$

$\langle n| \times (2)$

$$b_{n+1} \langle n|n+1\rangle = \cancel{\underbrace{\langle n|\hat{H}|n\rangle}_{\equiv a_n}} - \cancel{a_n \underbrace{\langle n|n\rangle}_{1}} - b_n \underbrace{\langle n|n-1\rangle}_{0} = 0$$

$$\therefore \langle n|n+1\rangle = 0$$

$\langle n+1| \times (2)$

$$\cancel{b_{n+1}} \langle n+1|n+1\rangle = \cancel{\underbrace{\langle n+1|\hat{H}|n\rangle}_{\equiv b_{n+1}^* = b_{n+1}}} - a_n \underbrace{\langle n+1|n\rangle}_{\emptyset} - b_n \underbrace{\langle n+1|n-1\rangle}_{\emptyset}$$

$$\therefore \langle n+1|n+1\rangle = 1$$

$\langle n-\delta| \times (2) \quad (\delta \geq 2)$

$$b_{n+1} \langle n-\delta|n+1\rangle = \underbrace{\langle n-\delta|\hat{H}|n\rangle}_{\emptyset \text{ by the inductive hypothesis (8)}} - a_n \underbrace{\langle n-\delta|n\rangle}_{\emptyset \text{ by the inductive hypothesis (7)}} - b_n \underbrace{\langle n-\delta|n-1\rangle}_{\emptyset} = \emptyset$$

$$\therefore \langle n-\delta|n+1\rangle = 0$$

Let $n = n+1-\delta$ $(\delta \geq 2)$ in Eq.(2):

$$b_{n+2-\delta} |n+2-\delta\rangle = (\hat{H} - a_{n+1-\delta}) |n+1-\delta\rangle - b_{n+1-\delta} |n-\delta\rangle \qquad (10)$$

$\langle n+1| \times (10)$

$$b_{n+2-\delta} \underbrace{\langle n+1|n+2-\delta\rangle}_{\emptyset} = \langle n+1|\hat{H}|n+1-\delta\rangle - a_{n+1-\delta} \underbrace{\langle n+1|n+1-\delta\rangle}_{\emptyset} - b_{n+1-\delta} \underbrace{\langle n+1|n-\delta\rangle}_{\emptyset}$$

$$\therefore \langle n+1-\delta|\hat{H}|n+1\rangle = \emptyset \quad \text{for } \forall \delta \geq 2$$

Thus the inductive hypotheses, (7) & (8), are T for $n+1$.

$\therefore$ The propositions, (7) & (8), are T for $\forall n$. //

(Lanczos algorithm)

Given $|0\rangle$ $(\langle 0|0\rangle = 1)$

$b_0 = 0$, $|-1\rangle = 0$ // Non-existance of constrained force @ $j = \emptyset$

for $j = 0$ to $N-1$

$a_j \leftarrow \langle j|\hat{H}|j\rangle$

$r \leftarrow (\hat{H} - a_j)|j\rangle - b_j|j-1\rangle$

$b_{j+1} \leftarrow \|r\|$

$|j+1\rangle \leftarrow r / b_{j+1}$

endfor

$a_N \leftarrow \langle N|\hat{H}|N\rangle$