Moment (Pade-via-Lanczos) Method for Electronic Structures

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[A.P. Horsfield et al., Phys. Rev. B $\underline{53}$, 12694 ('96)]

— Green's function

$$(z\hat{I} - \hat{H})\,\hat{G}(z) = \hat{I} \qquad (1)$$

— Lanczos recursion

Consider a Lanczos series $\{|0\rangle, |1\rangle, \ldots, |N\rangle\}$ and

$$\begin{cases} a_n = \langle n|\hat{H}|n\rangle & (n = 0, 1, \ldots, N) \\ b_n = \langle n-1|\hat{H}|n\rangle = \langle n|\hat{H}|n-1\rangle & (n = 1, 2, \ldots, N) \end{cases} \qquad (2)$$

$\langle 0| \times$ Eq. (1) $\times |0\rangle$

$$z\underbrace{\langle 0|\hat{G}(z)|0\rangle}_{\equiv G_{00}(z)} - \langle 0|\hat{H}\hat{G}|0\rangle = \underbrace{\langle 0|0\rangle}_{1}$$

$$zG_{00}(z) - \sum_i \underbrace{\langle 0|\hat{H}|i\rangle\langle i|G|0\rangle}_{\underbrace{\langle 0|\hat{H}|0\rangle}_{a_0} G_{00}(z) + \underbrace{\langle 0|\hat{H}|1\rangle}_{b_1} G_{10}(z)} = 1$$

$$\therefore\ (z - a_0)\,G_{00}(z) - b_1 G_{10}(z) = 1 \qquad (3)$$

where

$$G_{mn}(z) \equiv \langle m|\hat{G}(z)|n\rangle \qquad (4)$$

$\langle 1| \times$ Eq. (1) $\times |0\rangle$

$$z \underbrace{\langle 1|\hat{G}(z)|0\rangle}_{G_{10}(z)} - \langle 1|\hat{H}\hat{G}(z)|0\rangle = \underbrace{\langle 1|0\rangle}_{0}$$

$$z G_{10}(z) - \sum_i \underbrace{\langle 1|\hat{H}|i\rangle\langle i|G(z)|0\rangle}_{\underset{i=0}{b_1 G_{00}(z)} + \underset{i=1}{a_1 G_{10}(z)} + \underset{i=2}{b_2 G_{20}(z)}} = 0$$

$$\therefore (z-a_1)\, G_{10}(z) - b_2 G_{20}(z) = b_1 G_{00}(z) \qquad (5)$$

$\langle 2| \times$ Eq. (1) $\times |0\rangle$

$$z \underbrace{\langle 2|\hat{G}(z)|0\rangle}_{G_{20}(z)} - \langle 2|\hat{H}\hat{G}(z)|0\rangle = \underbrace{\langle 2|0\rangle}_{0}$$

$$z G_{20}(z) - \sum_i \underbrace{\langle 2|\hat{H}|i\rangle\langle i|\hat{G}(z)|0\rangle}_{\underset{i=1}{b_2 G_{10}(z)} + \underset{i=2}{a_2 G_{20}(z)} + \underset{i=3}{b_3 G_{30}(z)}} = 0$$

$$\therefore (z-a_2)\, G_{20}(z) - b_3 G_{30}(z) = b_2 G_{10}(z) \qquad (6)$$

In general,

$$(z-a_n)\, G_{n0}(z) - b_{n+1} G_{n+1,0}(z) = b_n G_{n-1\,0}(z) \quad (n \geq 1) \qquad (7)$$

In summary,

$$\boxed{\begin{array}{l} \left\{ \begin{array}{ll} (z-a_0)\, G_{00}(z) - b_1 \dfrac{G_{10}(z)}{G_{00}(z)} G_{00}(z) = 1 & (8) \\ (z-a_n) \dfrac{G_{n0}(z)}{G_{n-1,0}(z)} - b_{n+1} \dfrac{G_{n+1,0}(z)}{G_{n0}(z)} \cdot \dfrac{G_{n0}(z)}{G_{n-1,0}(z)} = b_n \quad (n \geq 1) & (9) \end{array} \right. \\ \text{where} \\ \quad G_{mn}(z) \equiv \langle m|\hat{G}(z)|n\rangle \qquad (4) \end{array}}$$

☺ Re-writing of Eqs. (3) & (7). //

– Continued fraction

Re-writing Eqs. (8) & (9),

$$\boxed{\begin{cases} G_{00}(z) = \dfrac{1}{z - a_0 - b_1 \dfrac{G_{10}(z)}{G_{00}(z)}} & (10) \\[2ex] \dfrac{G_{n0}(z)}{G_{n-1,0}(z)} = \dfrac{b_n}{z - a_n - b_{n+1}\dfrac{G_{n+1,0}(z)}{G_{n,0}(z)}} \quad (n \geq 1) & (11) \end{cases}}$$

Let $n=1$ in Eq. (11)

$$\frac{G_{10}(z)}{G_{00}(z)} = \frac{b_1}{z - a_1 - b_2 \dfrac{G_{20}(z)}{G_{10}(z)}} \tag{12}$$

Substituting Eq. (12) in (10),

$$G_{00}(z) = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - b_2 \cfrac{G_{20}(z)}{G_{10}(z)}}} \tag{13}$$

Let $n=2$ in Eq. (11)

$$\frac{G_{20}(z)}{G_{10}(z)} = \frac{b_2}{z - a_2 - b_3 \dfrac{G_{30}(z)}{G_{20}(z)}} \tag{14}$$

Substituting Eq. (14) in (13)

$$G_{00}(z) = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - b_3 \cfrac{G_{30}(z)}{G_{20}(z)}}}} \tag{15}$$

This leads to a recursive continued fraction,

$$\boxed{G_{00}(z) = \cfrac{1}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \cfrac{b_3^2}{\cdots}}}}} \qquad (16)$$

– Terminator

Let's consider the last term in the recursion,

$$t(z) = \cfrac{b_N^2}{z - a_N - \cfrac{b_{N+1}^2}{z - a_{N+1} - \cfrac{b_{N+2}^2}{\cdots}}} \qquad (17)$$

We approximate

$$\begin{cases} a_n \simeq a_N & (\forall n \geq N) \qquad (18) \\ b_n \simeq b_N & (\forall n \geq N) \qquad (19) \end{cases}$$

Then,

$$t(z) = \frac{b_N^2}{z - a_N - t(z)} \qquad (20)$$

$$\therefore \quad t(z)\left[z - a_N - t(z)\right] = b_N^2$$

$$t^2 - (z - a_N)\, t + b_N^2 = 0$$

$$t = \frac{(z - a_N) \pm \sqrt{(z - a_N)^2 - 4 b_N^2}}{2}$$

Near the pole $|z - a_N| \ll 2|b_N|$,

$$t = \frac{z - a_N \pm i|2b_N|\sqrt{1 - 4b^2/(z - a_N)^2}}{2}$$

We choose the pole, $z = t$, to be in the lower half plane.

we can always choose $b_N = \|r\| \geq 0$

$$\boxed{\therefore\ t(z) = \frac{z - a_N - i\,2b_N\sqrt{1 - \left(\frac{2b_N}{z - a_N}\right)^2}}{2}} \quad (21)$$