

Gram-Schmidt Orthogonalization I [nl83]

First three iterations in step #1 of [nl82].

Initial condition:

$$|f_0\rangle = A.$$

First iteration:

$$\imath L|f_0\rangle = |f_1\rangle \quad \Rightarrow \quad \langle f_0|f_1\rangle = \langle f_0|\imath L|f_0\rangle = 0.$$

Second iteration:

$$\begin{aligned} \imath L|f_1\rangle = |f_2\rangle - \Delta_1|f_0\rangle &\Rightarrow \langle f_1|f_2\rangle = \underbrace{\langle f_1|\imath L|f_1\rangle}_0 + \Delta_1 \underbrace{\langle f_1|f_0\rangle}_0 = 0, \\ &\Rightarrow \langle f_0|f_2\rangle = \underbrace{\langle f_0|\imath L|f_1\rangle}_{-\langle f_1|f_1\rangle} + \Delta_1 \langle f_0|f_0\rangle = 0 \\ &\quad \text{if } \Delta_1 = \frac{\langle f_1|f_1\rangle}{\langle f_0|f_0\rangle}. \end{aligned}$$

Third iteration:

$$\begin{aligned} \imath L|f_2\rangle = |f_3\rangle - \Delta_2|f_1\rangle - \Gamma_2|f_0\rangle \\ \Rightarrow \langle f_2|f_3\rangle = \underbrace{\langle f_2|\imath L|f_2\rangle}_0 + \Delta_2 \underbrace{\langle f_2|f_1\rangle}_0 + \Gamma_2 \underbrace{\langle f_2|f_0\rangle}_0 = 0, \\ \Rightarrow \langle f_1|f_3\rangle = \underbrace{\langle f_1|\imath L|f_2\rangle}_{-\langle f_2|f_2\rangle} + \Delta_2 \langle f_1|f_1\rangle + \Gamma_2 \underbrace{\langle f_1|f_0\rangle}_0 = 0 \\ \quad \text{if } \Delta_2 = \frac{\langle f_2|f_2\rangle}{\langle f_1|f_1\rangle}, \\ \Rightarrow \langle f_0|f_3\rangle = \underbrace{\langle f_0|\imath L|f_2\rangle}_{\langle f_1|f_2\rangle=0} + \Delta_2 \underbrace{\langle f_0|f_1\rangle}_0 + \Gamma_2 \langle f_0|f_0\rangle = 0 \\ \quad \text{if } \Gamma_2 = 0. \end{aligned}$$