Orthogonal Expansion of Wave Functions [nln90]

$$|\psi(t)\rangle = \sum_{k=0}^{\infty} D_k(t)|f_k\rangle. \tag{1}$$

Step #1:

- Hamiltonian: $\bar{\mathcal{H}} \doteq \mathcal{H} - E_0$ (generator of new directions).
- Ground state: $|\phi_0\rangle$.
- Dynamical variable of interest: A.
- Orthogonal basis, $|f_0\rangle, |f_1\rangle, \ldots$, with initial condition, $|f_0\rangle = A|\phi_0\rangle$.

Recurrence relations for basis vectors:

$$|f_{k+1}\rangle = \bar{\mathcal{H}}|f_k\rangle - a_k|f_k\rangle - b_k^2|f_{k-1}\rangle, \quad k = 0, 1, 2, \ldots \tag{2a}$$

$$a_k = \frac{\langle f_k|\bar{\mathcal{H}}|f_k\rangle}{\langle f_k|f_k\rangle}, \quad b_k^2 = \frac{\langle f_k|f_k\rangle}{\langle f_{k-1}|f_{k-1}\rangle}. \tag{2b}$$

Conditions: $|f_{-1}\rangle \doteq 0, \quad |f_0\rangle \doteq A|\phi_0\rangle, \quad b_0 \doteq 0.$

First three iterations spelled out in [nln91].

Step #2: (setting $\hbar = 1$)

- Time-dependent coefficients of basis vectors: $D_k(t)$.
- Substitute (1) into eq. of motion from [nln81]: $\imath\frac{d}{dt}|\psi(t)\rangle = \bar{\mathcal{H}}|\psi(t)\rangle$.
- d/dt acts on $D_k(t)$ and $\bar{\mathcal{H}}$ on $|f_k\rangle$.

Comparison of coefficients in

$$\imath\sum_{k=0}^{\infty} \dot{D}_k(t)|f_k\rangle = \sum_{k=0}^{\infty} D_k(t)\big[\underbrace{|f_{k+1} + a_k|f_k\rangle + b_k^2|f_{k-1}\rangle}_{\bar{\mathcal{H}}|f_k\rangle}\big] \tag{3}$$

yields set of coupled, linear, first-order ODEs for functions $D_k(t)$:

$$\imath\dot{D}_k(t) = D_{k-1}(t) + a_k D_k(t) + b_k^2 D_{k+1}(t), \quad k = 0, 1, 2, \ldots \tag{4}$$

Conditions: $D_{-1}(t) \equiv 0, \quad D_k(0) = \delta_{k,0}.$

Normalized correlation function:

$$D_0(t) = \frac{\langle f_0|\psi(t)\rangle}{\langle f_0|f_0\rangle} = \frac{\langle\phi_0|A(0)A(-t)|\phi_0\rangle}{\langle\phi_0|A(0)A(0)|\phi_0} = \frac{\tilde{S}(t)}{\tilde{S}(0)} \doteq \tilde{S}_0(t). \tag{5}$$