Orthogonal Expansion of Wave Functions

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

Step #1:
- Hamiltonian: \( \mathcal{H} = \mathcal{H} - E_0 \) (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:
\[
|f_{k+1}\rangle = \mathcal{H} |f_k\rangle - a_k |f_k\rangle - b_k^2 |f_{k-1}\rangle, \quad k = 0, 1, 2, \ldots \quad (2a)
\]  
\[
a_k = \frac{\langle f_k | \mathcal{H} | f_k \rangle}{\langle f_k | f_k \rangle}, \quad b_k^2 = \frac{\langle f_k | f_k \rangle}{\langle f_{k-1} | f_{k-1} \rangle}. \quad (2b)
\]

Conditions: \( |f_{-1}\rangle = 0 \), \( |f_0\rangle = A |\phi_0\rangle \), \( b_0 = 0 \).

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]: \( \frac{d}{dt} |\psi(t)\rangle = \mathcal{H} |\psi(t)\rangle \).
- \( d/dt \) acts on \( D_k(t) \) and \( \mathcal{H} \) on \( |f_k\rangle \).

Comparison of coefficients in
\[
i \sum_{k=0}^{\infty} \dot{D}_k(t) |f_k\rangle = \sum_{k=0}^{\infty} D_k(t) \left[ \frac{|f_{k+1}\rangle + a_k |f_k\rangle + b_k^2 |f_{k-1}\rangle}{\mathcal{H} |f_k\rangle} \right] \] (3)
yields set of coupled, linear, first-order ODEs for functions \( D_k(t) \):
\[
i \dot{D}_k(t) = D_{k-1}(t) + a_k D_k(t) + b_k^2 D_{k+1}(t), \quad k = 0, 1, 2, \ldots \quad (4)
\]
Conditions: \( D_{-1}(t) = 0 \), \( D_k(0) = \delta_{k,0} \).

Normalized correlation function:
\[
D_0(t) = \frac{\langle f_0 | \psi(t) \rangle}{\langle f_0 | f_0 \rangle} = \frac{\langle \phi_0 | A(0)A(-t) |\phi_0 \rangle}{\langle \phi_0 | A(0)A(0) |\phi_0 \rangle} = \frac{\tilde{S}(t)}{\tilde{S}(0)} \equiv \tilde{S}_0(t). \quad (5)
\]