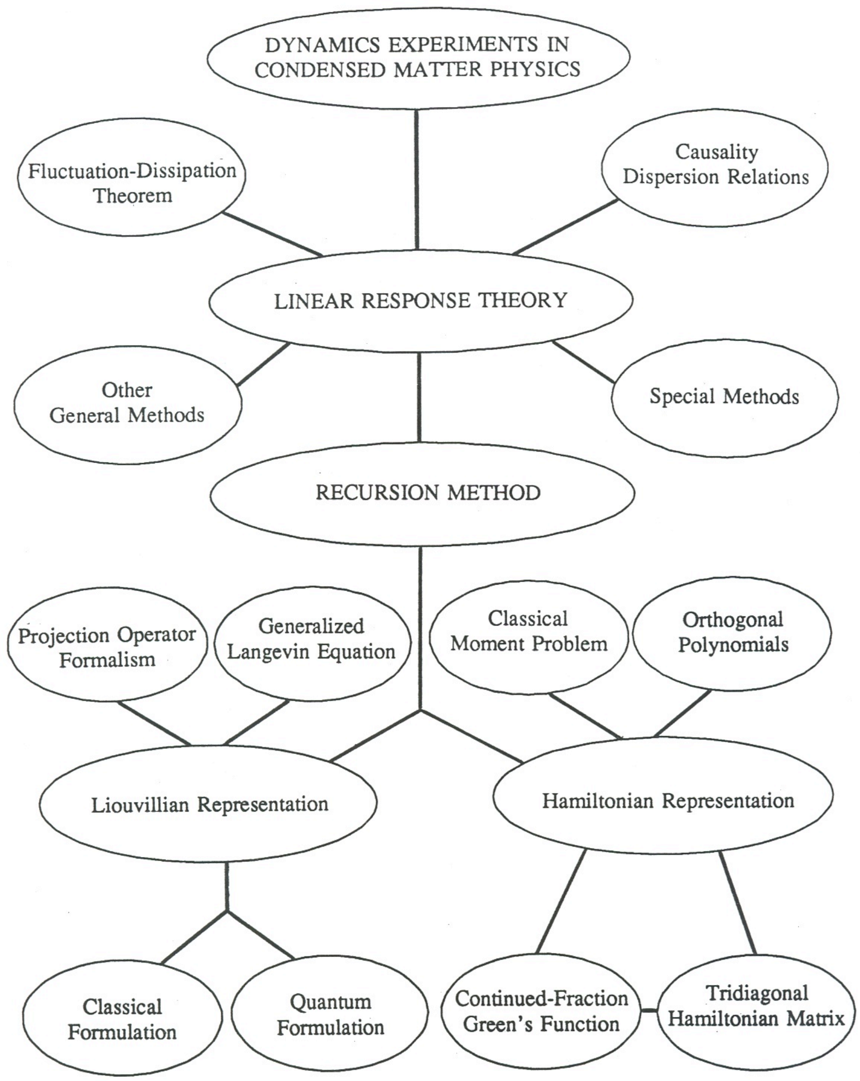
Contents of this Document [ntc10]

11. Recursion Method: Concepts

Stage for Recursion Method [nln79]

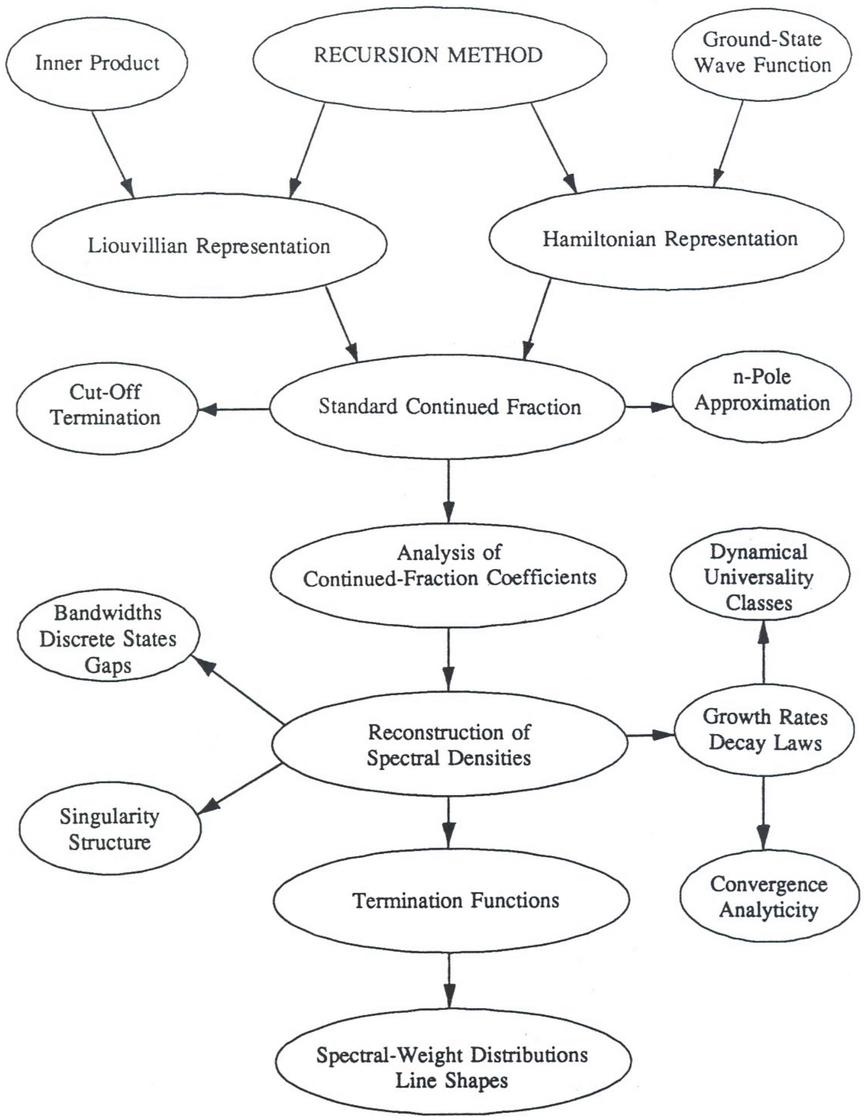
Recursion method as applied to many-body dynamics:
backdrop, props, protagonists.



[from Viswanath and Müller 1994]

Modules of Recursion Method [nln80]

Recursion method as applied to many-body dynamics:
main lines of formal development.



[from Viswanath and Müller 1994]

Representations of Recursion Method [nln81]

Object of interest: time-dependent correlation function $\langle A(t)A\rangle$.

Recursive part of method: orthogonal expansion of carrier of time evolution.

Heisenberg picture:

- time evolution prescribed by Heisenberg (or Hamilton) equation,
- time evolution carried by dynamical variable,
- Liouvillian operator generates new directions.

Schrödinger picture:

- time evolution prescribed by Schrödinger equation,
- time evolution carried by wave function,
- Hamiltonian operator generates new directions.

Liouvillian representation	**Hamiltonian representation**
$\frac{d}{dt}A(t) = \imath L_{\mathrm{qu}}A(t) = \frac{\imath}{\hbar}[\mathcal{H}, A(t)]$ $\frac{d}{dt}A(t) = \imath L_{\mathrm{cl}}A(t) = -\{\mathcal{H}, A(t)\}$	$\imath\hbar\frac{d}{dt}\lvert\psi(t)\rangle = \mathcal{H}\lvert\psi(t)\rangle$
$A(t) = e^{\imath Lt}A(0) = \sum_{k=0}^{\infty} C_k(t)\lvert f_k\rangle$	$\lvert\psi(t)\rangle = e^{-\imath\mathcal{H}t/\hbar}\lvert\psi(0)\rangle = \sum_{k=0}^{\infty} D_k(t)\lvert f_k\rangle$
$\lvert f_0\rangle = A(0), \quad \lvert f_{k+1}\rangle = \imath L\lvert f_k\rangle - \ldots$	$\lvert f_0\rangle = \lvert\psi(0)\rangle = A\lvert\phi_0\rangle, \quad \lvert f_{k+1}\rangle = \mathcal{H}\lvert f_k\rangle - \ldots$
$\tilde{\Phi}(t) = \langle[A(t), A(0)]_+\rangle - \langle A\rangle^2$	$\tilde{S}(t) = \langle A(t)A(0)\rangle - \langle A\rangle^2$
$\mathrm{Tr}\left[e^{-\beta\mathcal{H}} \underbrace{e^{\imath\mathcal{H}t/\hbar}Ae^{-\imath\mathcal{H}t/\hbar}}_{A(t)} A\right]$	$e^{\imath E_0 t/\hbar}\left\langle\phi_0\right\rvert A \underbrace{e^{-\imath\mathcal{H}t/\hbar}A\lvert\phi_0\rangle}_{\lvert\psi(t)\rangle}$

Orthogonal Expansion of Dynamical Variables [nln82]

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

Step #1: [M.H. Lee]

- Orthogonal basis, $|f_0\rangle, |f_1\rangle, \ldots$, with initial condition, $|f_0\rangle = A(0)$.
- Quantum statistics: $|f_k\rangle$ form orthogonal set of operators.
- Classical statistics: $|f_k\rangle$ form orthogonal set of phase-space functions.
- Generation of orthogonal directions: $\langle f_k|\imath L|f_k\rangle = 0$.

Recurrence relations for basis vectors $|f_k\rangle$:

$$|f_{k+1}\rangle = \imath L|f_k\rangle + \Delta_k|f_{k-1}\rangle, \quad \Delta_{k+1} = \frac{\langle f_{k+1}|f_{k+1}\rangle}{\langle f_k|f_k\rangle}, \quad k = 0, 1, 2, \ldots \tag{2}$$

Conditions: $|f_{-1}\rangle \doteq 0, \quad |f_0\rangle \doteq A, \quad \Delta_0 \doteq 0.$

First three iterations spelled out in [nln83].

Step #2: [M.H. Lee]

- Time-dependent coefficients of basis vectors: $C_k(t)$.
- Substitute (1) into equation of motion from [nln81]: $dA/dt = \imath LA$.
- d/dt acts on $C_k(t)$ and L acts on $|f_k\rangle$.

Comparison of coefficients in

$$\sum_{k=0}^{\infty} \dot{C}_k(t)|f_k\rangle = \sum_{k=0}^{\infty} C_k(t)\big[\underbrace{|f_{k+1}\rangle - \Delta_k|f_{k_1}|\rangle}_{\imath L|f_k\rangle}\big] \tag{3}$$

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

$$\dot{C}_k(t) = C_{k-1}(t) - \Delta_{k+1}C_{k+1}(t), \quad k = 0, 1, 2, \ldots \tag{4}$$

Conditions: $C_{-1}(t) \equiv 0, \quad C_k(0) = \delta_{k,0}, \quad k = 0, 1, 2, \ldots$

Normalized fluctuation function (see [nln39]):

$$C_0(t) = \frac{\langle A(t)|A(0)\rangle}{\langle A(0)|A(0)\rangle} = \frac{\tilde{\Phi}(t)}{\tilde{\Phi}(0)}. \tag{5}$$

Gram-Schmidt Orthogonalization I [nln83]

First three iterations in step #1 of [nln82].

Initial condition:

$$|f_0\rangle = A.$$

First iteration:

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

Second iteration:

$$\imath L|f_1\rangle = |f_2\rangle - \Delta_1|f_0\rangle \quad \Rightarrow \; \langle f_1|f_2\rangle = \underbrace{\langle f_1|\imath L|f_1\rangle}_{0} + \Delta_1 \underbrace{\langle f_1|f_0\rangle}_{0} = 0,$$

$$\Rightarrow \; \langle f_0|f_2\rangle = \underbrace{\langle f_0|\imath L|f_1\rangle}_{-\langle f_1|f_1\rangle} + \Delta_1\langle f_0|f_0\rangle = 0$$

$$\text{if } \Delta_1 = \frac{\langle f_1|f_1\rangle}{\langle f_0|f_0\rangle}.$$

Third iteration:

$$\imath L|f_2\rangle = |f_3\rangle - \Delta_2|f_1\rangle - \Gamma_2|f_0\rangle$$

$$\Rightarrow \; \langle f_2|f_3\rangle = \underbrace{\langle f_2|\imath L|f_2\rangle}_{0} + \Delta_2 \underbrace{\langle f_2|f_1\rangle}_{0} + \Gamma_2 \underbrace{\langle f_2|f_0\rangle}_{0} = 0,$$

$$\Rightarrow \; \langle f_1|f_3\rangle = \underbrace{\langle f_1|\imath L|f_2\rangle}_{-\langle f_2|f_2\rangle} + \Delta_2\langle f_1|f_1\rangle + \Gamma_2 \underbrace{\langle f_1|f_0\rangle}_{0} = 0$$

$$\text{if } \Delta_2 = \frac{\langle f_2|f_2\rangle}{\langle f_1|f_1\rangle},$$

$$\Rightarrow \; \langle f_0|f_3\rangle = \underbrace{\langle f_0|\imath L|f_2\rangle}_{\langle f_1|f_2\rangle = 0} + \Delta_2 \underbrace{\langle f_0|f_1\rangle}_{0} + \Gamma_2\langle f_0|f_0\rangle = 0$$

$$\text{if } \Gamma_2 = 0.$$

Relaxation Function and Spectral Density [nln84]

Relaxation function via Laplace transform:

$$c_k(z) \doteq \int_0^\infty dt\, e^{-zt} C_k(t). \tag{1}$$

Coupled ODEs for $C_k(t)$ become coupled algebraic equations for $c_k(z)$:[1]

$$zc_k(z) - \delta_{k,0} = c_{k-1}(z) - \Delta_{k+1} c_{k+1}(z), \quad k = 0, 1, 2, \ldots \tag{2}$$

Condition: $c_{-1}(z) \equiv 0$.

Recursive construction of continued fraction representation for $c_0(z)$:

$$k = 0: \; zc_0(z) - 1 = -\Delta_1 c_1(z) \quad \Rightarrow \; c_0(z) = \frac{1}{z + \Delta_1 \dfrac{c_1(z)}{c_0(z)}},$$

$$k = 1: \; zc_1(z) = c_0(z) - \Delta_2 c_2(z) \quad \Rightarrow \; \frac{c_1(z)}{c_0(z)} = \frac{1}{z + \Delta_2 \dfrac{c_2(z)}{c_1(z)}},$$

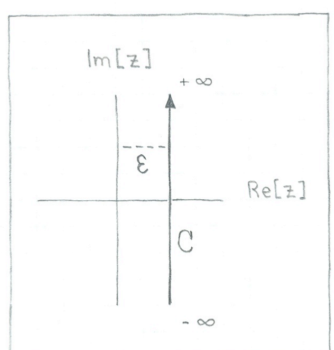
$$\Rightarrow \; c_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots}}} \tag{3}$$

Spectral density $\Phi(\omega)$ from relaxation function $c_0(z)$: combine Fourier transform with inverse Laplace transform.

$$\Phi_0(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t} C_0(t),$$

$$C_0(t) = \frac{1}{2\pi\imath} \int_{\mathcal{C}} dz\, e^{zt} c_0(z)$$

$$\Rightarrow \; \Phi_0(\omega) = 2 \lim_{\epsilon \to 0} \mathrm{Re}[c_0(\epsilon - \imath\omega)]. \tag{4}$$



[1] Use $\int_0^\infty dt\, e^{-zt} \dot{C}_k(t) = \Big[e^{-zt} C_k(t)\Big]_0^\infty - \int_0^\infty dt (-z) e^{-zt} C_k(t) = zc_k(z) - C_k(0)$.

Moment Expansion vs Continued Fraction I [nln85]

Moment expansions of fluctuation function (see [nln78]):

$$C_0(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} M_{2k} t^{2k}, \quad M_0 = 1. \tag{1}$$

Asymptotic expansion and continued-fraction representation of relaxation function:

$$c_0(z) \doteq \int_0^\infty dt\, e^{-zt} C_0(t) = \sum_{k=0}^{\infty} M_{2k} z^{-(2k+1)} = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots}}}. \tag{2}$$

Transformation relations between $\{M_{2k}\}$ and $\{\Delta_n\}$ extracted from inspecting the two representations of $c_0(z)$, using the algebraic equations in [nln84].

Forward direction: $\{M_{2k}\} \to \{\Delta_n\}$

Set values: $M_{2k}^{(0)} \doteq M_{2k}, \quad M_{2k}^{(-1)} \doteq 0, \quad k = 1, 2, \ldots, K; \quad \Delta_{-1} = \Delta_0 \doteq 1.$

Then evaluate

$$M_{2k}^{(n)} = \frac{M_{2k}^{(n-1)}}{\Delta_{n-1}} - \frac{M_{2k-2}^{(n-2)}}{\Delta_{n-2}}, \quad \Delta_n = M_{2n}^{(n)} \tag{3}$$

sequentially for $k = n, n+1, \ldots, K$ and $n = 1, 2, \ldots, K$.

Reverse direction: $\{\Delta_n\} \to \{M_{2k}\}$

Set values: $M_{2k}^{(k)} \doteq \Delta_k, \quad M_{2k}^{(-1)} \doteq 0, \quad k = 1, 2, \ldots, K; \quad \Delta_{-1} = \Delta_0 \doteq 1.$

Then evaluate

$$M_{2k}^{(n-1)} = \Delta_{n-1} M_{2k}^{(n)} + \frac{\Delta_{n-1}}{\Delta_{n-2}} M_{2k-2}^{(n-2)}, \quad M_{2k} = M_{2k}^{(0)} \tag{4}$$

sequentially for $n = k, k-1, \ldots, 1$ and $k = 1, 2, \ldots, K$.

Forward direction: $\{M_{2k}\} \rightarrow \{\Delta_n\}$

$k \backslash n$	0	1	2	3	4
0	1	M_2	M_4	M_6	M_8
1		M_2	M_4	M_6	M_8
2			$\frac{M_4}{M_2} - M_2$	$\frac{M_6}{M_2} - M_4$	$\frac{M_8}{M_2} - M_6$
3				$\frac{\frac{M_6}{M_2} - M_4}{\frac{M_4}{M_2} - M_2} - \frac{M_4}{M_2}$	$\frac{\frac{M_8}{M_2} - M_6}{\frac{M_4}{M_2} - M_2} - \frac{M_6}{M_2}$

Reverse direction: $\{\Delta_n\} \rightarrow \{M_{2k}\}$

$n \backslash k$	0	1	2	3
0	1	Δ_1	$\Delta_1(\Delta_1 + \Delta_2)$	$\Delta_1[\Delta_2\Delta_3 + (\Delta_1 + \Delta_2)^2]$
1		Δ_1	$\Delta_1(\Delta_1 + \Delta_2)$	$\Delta_1[\Delta_2\Delta_3 + (\Delta_1 + \Delta_2)^2]$
2			Δ_2	$\Delta_2(\Delta_1 + \Delta_2 + \Delta_3)$
3				Δ_3

First two steps in forward directions spelled out:

- $c_0(z) = z^{-1} - M_2 z^{-3} + M_4 z^{-5} - M_6 z^{-7} + \ldots$
- $\Delta_1 c_1(z) = 1 - z c_0(z) = \underbrace{M_2}_{\Delta_1} z^{-2} - M_4 z^{-4} + M_6 z^{-6} - \ldots$
- $c_1(z) = z^{-2} - \frac{M_4}{M_2} z^{-4} + \frac{M_6}{M_2} z^{-6} - \frac{M_8}{M_2} z^{-8} + \ldots$
- $\Delta_2 c_2(z) = c_0(z) - z c_1(z) = \underbrace{\left(\frac{M_4}{M_2} - M_2\right)}_{\Delta_2} z^{-3} - \left(\frac{M_6}{M_2} - M_4\right) z^{-5} + \ldots$

Link to Generalized Langevin Equation [nln86]

Define two functions from the $c_k(z)$ introduced in [nln84]:

$$\Sigma(z) \doteq \Delta_1 \frac{c_1(z)}{c_0(z)}, \quad b_k(z) \doteq \frac{c_k(z)}{c_0(z)}. \tag{1}$$

Rewrite algebraic equations (2) for $k = 0$ of [nln84] using $\Sigma(z)$ and $b_k(z)$:

$$zc_0(z) + \Sigma(z)c_0(z) = 1, \tag{2a}$$
$$zc_k(z) + \Sigma(z)c_k(z) = b_k(z), \quad k = 1, 2, \ldots \tag{2b}$$

Inverse Laplace transforms of these functions then satisfy

$$\dot{C}_0(t) + \int_0^t dt' \tilde{\Sigma}(t - t')C_0(t') = 0, \tag{3a}$$
$$\dot{C}_k(t) + \int_0^t dt' \tilde{\Sigma}(t - t')C_k(t') = B_k(t), k = 1, 2, \ldots \tag{3b}$$

Recall orthogonal expansion (1) in [nln82] of dynamical variable:

$$A(t) = \sum_{k=0}^{\infty} C_k(t)|f_k\rangle. \tag{4}$$

From (3) and (4) follows generalized Langevin equation [M. H. Lee 1983]:[1]

$$\dot{A}(t) + \int_0^{\infty} dt' \tilde{\Sigma}(t - t')A(t') = F(t). \tag{5}$$

Orthogonal exapnsion of random force:

$$F(t) = \sum_{k=1}^{\infty} B_k(t)|f_k\rangle, \quad B_k(0) = \delta_{k,1}. \tag{6}$$

Absence of correlations between dynamical variable and random force:

$$\langle F(t)|A(0)\rangle = \sum_{k=1}^{\infty} B_k(t)\langle f_k|f_0\rangle = 0. \tag{7}$$

Fluctuation-dissipation relation between $\tilde{\Sigma}(t)$ (memory function) and $F(t)$:

$$\langle F(t)|F(0)\rangle = B_1(t)\langle f_1|f_1\rangle = \Delta_1 B_1(t)\langle f_0|f_0\rangle = \tilde{\Sigma}(t)\langle f_0|f_0\rangle. \tag{8}$$

[1]Lower integration boundary is specific to initial-value problem under consideration.

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]: $\imath \dfrac{d}{dt}|\psi(t)\rangle = \bar{\mathcal{H}}|\psi(t)\rangle$.
- 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:

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

Gram-Schmidt Orthogonalization II [nln91]

First three iterations in step #1 of [nln90].

Initial condition:

$$|f_0\rangle = A|\phi_0\rangle.$$

First iteration:

$$|f_1\rangle = \bar{\mathcal{H}}|f_0\rangle - a_0|f_0\rangle$$

$$\Rightarrow \ \langle f_0|f_1\rangle = \langle f_0|\bar{\mathcal{H}}|f_0\rangle - a_0\langle f_0|f_0\rangle = 0$$

$$\text{if } a_0 = \frac{\langle f_0|\bar{\mathcal{H}}|f_0\rangle}{\langle f_0|f_0\rangle}.$$

Second iteration:

$$|f_2\rangle = \bar{\mathcal{H}}|f_1\rangle - a_1|f_1\rangle - b_1^2|f_0\rangle$$

$$\Rightarrow \ \langle f_0|f_2\rangle = \underbrace{\langle f_0|\bar{\mathcal{H}}|f_1\rangle}_{\langle f_1|f_1\rangle} - a_1 \underbrace{\langle f_0|f_1\rangle}_{0} - b_1^2\langle f_0|f_0\rangle = 0$$

$$\text{if } b_1^2 = \frac{\langle f_1|f_1\rangle}{\langle f_0|f_0\rangle},$$

$$\Rightarrow \ \langle f_1|f_2\rangle = \langle f_1|\bar{\mathcal{H}}|f_1\rangle - a_1\langle f_1|f_1\rangle - b_1^2 \underbrace{\langle f_1|f_0\rangle}_{0} = 0$$

$$\text{if } a_1 = \frac{\langle f_1|\bar{\mathcal{H}}|f_1\rangle}{\langle f_1|f_1\rangle}.$$

Third iteration:

$$|f_3\rangle = \bar{\mathcal{H}}|f_2\rangle - a_2|f_1\rangle - b_2^2|f_0\rangle - c_2|f_0\rangle$$

$$\Rightarrow \ \langle f_0|f_3\rangle = \cdots = 0 \quad \text{if } c_2 = 0,$$

$$\Rightarrow \ \langle f_1|f_3\rangle = \cdots = 0 \quad \text{if } b_2^2 = \frac{\langle f_2|f_2\rangle}{\langle f_1|f_1\rangle},$$

$$\Rightarrow \ \langle f_2|f_3\rangle = \cdots = 0 \quad \text{if } a_2 = \frac{\langle f_2|\bar{\mathcal{H}}|f_2\rangle}{\langle f_2|f_2\rangle}.$$

Structure Function [nln92]

Laplace transform (with $\imath\zeta = -z$):

$$d_k(\zeta) \doteq \int_0^\infty dt\, e^{\imath\zeta t} D_k(t). \qquad (1)$$

Coupled ODEs for $D_k(t)$ become coupled algebraic equations for $d_k(\zeta)$:

$$(\zeta - a_k) d_k(\zeta) - \imath\delta_{k,0} = d_{k-1}(\zeta) + b_{k+1}^2 d_{k+1}(\zeta), \quad k = 0, 1, 2, \ldots \qquad (2)$$

Condition: $d_{-1}(\zeta) \equiv 0$.

Recursive construction of continued fraction representation for $d_0(\zeta)$:

$$k = 0: \;\; (\zeta - a_0) d_0(\zeta) - \imath = b_1^2 d_1(\zeta) \quad \Rightarrow \; d_0(\zeta) = \frac{\imath}{\zeta - a_0 - b_1^2 \dfrac{d_1(\zeta)}{d_0(\zeta)}},$$

$$k = 1: \;\; (\zeta - a_1) d_1(\zeta) = d_0(\zeta) + b_2^2 d_2(\zeta) \quad \Rightarrow \; \frac{d_1(\zeta)}{d_0(\zeta)} = \frac{1}{\zeta - a_1 - b_2^2 \dfrac{d_2(\zeta)}{d_1(\zeta)}},$$

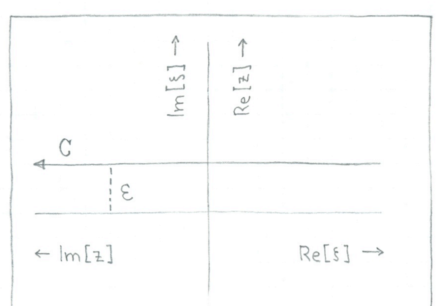
$$\Rightarrow \; d_0(\zeta) = \cfrac{\imath}{\zeta - a_0 - \cfrac{b_1^2}{\zeta - a_1 - \cfrac{b_2^2}{\zeta - a_2 - \cdots}}} \qquad (3)$$

Structure function $S(\omega)$ from $d_0(\zeta)$: combine Fourier transform with inverse Laplace transform.

$$S_0(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t} D_0(t),$$

$$D_0(t) = -\frac{1}{2\pi} \int_{\mathcal{C}} d\zeta\, e^{-\imath\zeta t} d_0(\zeta)$$

$$\Rightarrow \; S_0(\omega) = 2 \lim_{\epsilon \to 0} \mathrm{Re}[d_0(\omega + \imath\epsilon)]. \qquad (4)$$



Moment Expansion vs Continued Fraction II [nln96]

Moment expansion of correlation function (see [nln78]):

$$D_0(t) = \sum_{n=0}^{\infty} M_n \frac{(-\imath t)^n}{n!}, \quad M_{2k} \text{ as in [nln85].} \tag{1}$$

Asymptotic expansion and continued-fraction representation:

$$d_0(\zeta) \doteq \int_0^\infty dt\, e^{\imath\zeta t} D_0(t) = \imath \sum_{n=0}^{\infty} M_n \zeta^{-(n+1)} = \cfrac{\imath}{\zeta - a_0 - \cfrac{b_1^2}{\zeta - a_1 - \cdots}} \tag{2}$$

Transformation relations between $\{M_n\}$ and $\{a_n, b_n^2\}$ extracted from inspection of the two representation in (2).

- Conversion $\{a_n, b_n^2\} \leftrightarrow \{\Delta_k\}$ in two steps.
- First step: $\{a_n, b_n^2\} \leftrightarrow \{M_n\}$ here.
- Second step: $\{M_{2k}\} \leftrightarrow \{\Delta_k\}$ in [nln85].

Calculating $\{a_n, b_n^2\}$ first is most practical in many applications. Key features of dynamical quantities (bandwidth, gap, singularity structure) are most effectively extracted from $\{\Delta_k\}$.

Forward direction: $\{M_n\} \rightarrow \{a_n, b_n^2\}$

Initialize auxiliary quantities:

$$M_k^{(0)} = (-1)^k M_k, \quad L_k^{(0)} = (-1)^{k+1} M_{k+1}, \quad k = 0, \ldots, 2K. \tag{3}$$

Evaluate sequentially for $k = n, \ldots, 2K-n+1$ (in two successive inner loops) and $n = 1, \ldots, 2K$ (outer loop):

$$M_k^{(n)} = L_k^{(n-1)} - L_{n-1}^{(n-1)} \frac{M_k^{(n-1)}}{M_{n-1}^{(n-1)}}, \qquad L_k^{(n)} = \frac{M_{k+1}^{(n)}}{M_n^{(n)}} - \frac{M_k^{(n-1)}}{M_{n-1}^{(n-1)}}. \tag{4}$$

Identify continued-fraction coefficients among auxiliary quantities:

$$b_n^2 = M_n^{(n)}, \quad a_n = -L_n^{(n)}, \quad n = 0, \ldots, K. \tag{5}$$

Reverse direction: $\{a_n, b_n^2\} \rightarrow \{M_n\}$

Initialize auxiliary quantities, setting $b_0^2 = b_{-1}^2 \doteq 1$:

$$M_n^{(n)} = b_n^2, \quad L_n^{(n)} = -a_n, \quad n = 0, \ldots, K; \tag{6a}$$

$$M_k^{(-1)} = 0, \quad k = 0, \ldots, 2K+1. \tag{6b}$$

Evaluate sequentially for $n = 0, \ldots, \min(K, 2K - j)$ (inner loop) and $j = 0, \ldots, 2K+1$ (outer loop):

$$M_{n+j+1}^{(n)} = b_n^2 L_{n+j}^{(n)} + \frac{b_n^2}{b_{n-1}^2} M_{n+j}^{(n-1)}, \quad L_{n+j+1}^{(n)} = M_{n+j+1}^{(n+1)} - \frac{a_n}{b_n^2} M_{n+j+1}^{(n)}. \tag{7}$$

Identify moments among auxiliary quantities:

$$M_n = (-1)^n M_n^{(0)}, \quad n = 0, \ldots, 2K+1. \tag{8}$$

Results of a few iterations in the forward sequence (left) and in the reverse sequence (right):

$a_0 = M_1$	$M_1 = a_0$
$b_1^2 = M_2 - M_1^2$	$M_2 = a_0^2 + b_1^2$
$a_1 = \dfrac{M_3 - M_1^3}{M_2 - M_1^2} - 2M_1$	$M_3 = (a_0^3 + 2a_0 b_1^2 + b_1^2 a_1)$
$b_2^2 = \dfrac{M_4 - M_1 M_3}{M_2 - M_1^2} - M_2$ $- \left[\dfrac{M_1^3 - M_3}{M_2 - M_1^2} - 2M_1\right] \left[\dfrac{M_1^3 - M_3}{M_2 - M_1^2} + M_1\right]$	$M_4 = b_1^2 \left[a_0^2 + a_1^2 + a_0 a_1 + b_1^2 + b_2^2\right]$ $+a_0 \left[a_0^3 + 2a_0 b_1^2 + b_1^2 a_1\right]$

Genetic Code of Spectral Densities [nln98]

Justification of biological term used for analogy:

- Spectral densities, structure functions, dissipation functions, and Green's functions for any given classical or quantum many-body system and any choice of dynamical variable are related to each other by rigorous relations (see [nln39] and nln88]).
- The (symmetric) spectral density is fully characterized by a Δ_k-sequence of continued-fraction coefficients [nln84].
- The recursion method presents a user-friendly and systematic way to calculate coefficients Δ_k sequentially, either directly (Liouvillian representation [nln83]) or indirectly (Hamiltonian representation [nln91]).
- Hence the Δ_k-sequence is a genetic code of sorts: (i) it is a *code* of retrievable information about key features of spectral densities as listed below; (ii) it is *generative* in nature in the sense that it can be used to produce spectral densities with these very features in conjunction with specific termination schems of continued fractions.

Features of spectral densities that can be identified in Δ_k-sequences (incomplete list):

- Position and intensity of individual spectral lines [nln99].
- Bandwidth of spectral densities with compact support [nln100].
- Band-edge singularity of spectral densities with compact support [nln100].
- Infrared singularity of spectral density with compact support [nln100].
- Bandwidth and gap size of spectral densities with bounded support [nln101].
- Infrared singularity of spectral densities with unbounded support [nln102].
- Large-ω asymptotics of spectral densities with unbounded support [nln102].
- Gap size of spectral densites with unbounded support [nln103].

Spectral Lines from Finite Δ_k-Sequences [nln99]

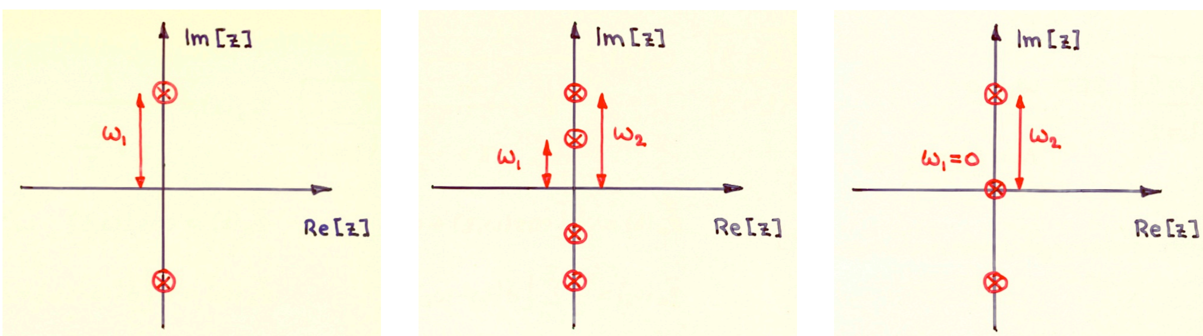
Orthogonal expansion in [nln83] comes natural stop: $|f_{K+1}\rangle = 0$.

Relaxation function has $K+1$ poles on imaginary z-axis.

$$\Rightarrow c_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots \cdots + \cfrac{\Delta_K}{z}}}} = \frac{p_K(z)}{q_{K+1}(z)}.$$

Spectral density: $\Phi_0(\omega) = \pi \sum_{l=1}^{L} u_l \big[\delta(\omega - \omega_l) + \delta(\omega + \omega_l)\big].$

- K: number of nonzero continued-fraction coefficients Δ_k.
- L: number of spectral lines (with frequencies ω_l).
- Relation: $K = \begin{cases} 2L-1 \text{ (odd)} & \text{if all } \omega_l > 0, \\ 2L-2 \text{ (even)} & \text{if } \omega_l = 0 \text{ occurs.} \end{cases}$



Special case $u_1 = u_2$ for $L = 2$:

$$\Delta_1 = \frac{1}{2}(\omega_1^2 + \omega_2^2), \quad \Delta_2 = \Delta_1 - \Delta_3, \quad \Delta_3 = \frac{2\omega_1^2\omega_2^2}{\omega_1^2 + \omega_2^2}.$$

Limit $\omega_1 \to 0$ implies $\Delta_3 \to 0$ and $\Delta_2 \to \Delta_1$.

Spectral Densities with Bounded Support [nln100]

Consider spectral densities with convergent Δ_k-sequences.

Bandwidth:

If $\lim_{k\to\infty} \Delta_k = \frac{1}{4}\omega_0^2$ then $\Phi_0(\omega)$ has compact support on the interval $|\omega| \leq \omega_0$.

Band edge singularity:

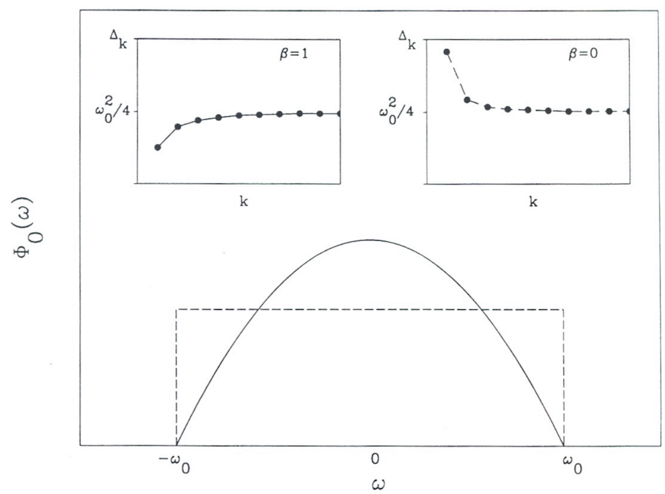
Model spectral density with singularities only at the band edges:[1]

$$\Phi_0(\omega) = \frac{2\pi\omega_0^{2\beta+1}}{B(1/2, 1+\beta)} \left(\omega_0^2 - \omega^2\right)^\beta, \quad |\omega| < \omega_0, \quad \beta > -1. \tag{1}$$

Associated Δ_k-sequence [Magnus 1985] and its asymptotic expansion:

$$\Delta_k = \frac{\omega_0^2 k(k+2\beta)}{(2k+2\beta-1)(2k+2\beta+1)} = \frac{1}{4}\omega_0^2 \left[1 + \frac{1-4\beta^2}{4k^2} + \cdots\right]. \tag{2}$$

Graphical representations for two cases [Viswanath and Müller 1994]:



Analysis of limiting cases in [nex69]:

- $\beta = \frac{1}{2}$: $\Delta_1 = \Delta_2 = \ldots = \frac{1}{4}\omega_0^2 \quad \Rightarrow \Phi_0(\omega) = \frac{4}{\omega_0^2}\sqrt{\omega_0^2 - \omega^2}$.
- $\beta = -\frac{1}{2}$: $\Delta_1 = \frac{1}{2}\omega_0^2,\ \Delta_2 = \Delta_3 \ldots = \frac{1}{4}\omega_0^2 \quad \Rightarrow \Phi_0(\omega) = \frac{2}{\sqrt{\omega_0^2 - \omega^2}}$.

[1] $B(x,y) \doteq \Gamma(x)\Gamma(y)/\Gamma(x+y)$.

Infrared singularity:

Model spectral density with infrared singularity added:

$$\Phi_0(\omega) = \frac{2\pi\omega_0^{-(\alpha+2\beta+1)}}{B\big((1+\alpha)/2, 1+\beta\big)}|\omega|^\alpha(\omega_0^2-\omega^2)^\beta, \quad |\omega|<\omega_0, \quad \alpha,\beta>-1. \quad (3)$$

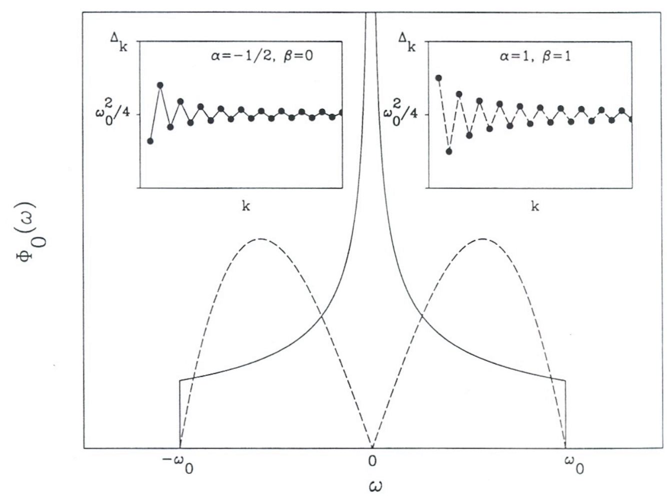
Associated Δ_k-sequence [Magnus 1985]:

$$\Delta_{2k} = \frac{4\omega_0^2 k(k+\beta)}{(4k+2\beta+\alpha-1)(4k+2\beta+\alpha+1)},$$
$$\Delta_{2k+1} = \frac{\omega_0^2(2k+\alpha+1)(2k+2\beta+\alpha+1)}{(4k+2\beta+\alpha+1)(4k+2\beta+\alpha+3)}. \quad (4)$$

Asymptotic expansion:

$$\sqrt{\Delta_k} = \frac{1}{2}\omega_0\left[1-(-1)^k\frac{\alpha}{2k}+\frac{1-4\beta^2+2(-1)^k\alpha(2\beta+\alpha)}{8k^2}+\cdots\right]. \quad (5)$$

Graphical representations for two cases [Viswanath and Müller 1994]:



Signature of divergent infrared singularity ($\alpha<0$): the Δ_{2k+1} converge from below and the Δ_{2k} from above toward the same limit.

Bandwith and Gap in Spectral Density [nln101]

Consider a model Δ_k-sequence that is periodic with period two:

$$\Delta_{2k-1} = \Delta_\mathrm{o}, \quad \Delta_{2k} = \Delta_\mathrm{e}, \quad k = 1, 2, \ldots \tag{1}$$

Relaxation function with this genetic code:

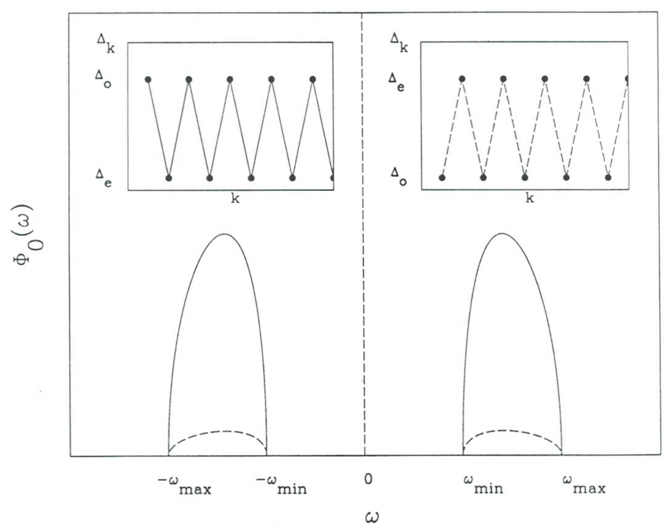
$$\begin{aligned} c_0(z) &= \cfrac{1}{z + \cfrac{\Delta_\mathrm{o}}{z + \Delta_\mathrm{e} c_0(z)}} \\ &= \frac{1}{2\Delta_\mathrm{e}}\left[\sqrt{2(\Delta_\mathrm{o}+\Delta_\mathrm{e}) + z^2 + \frac{(\Delta_\mathrm{o}-\Delta_\mathrm{e})^2}{z^2}} - z - \frac{\Delta_\mathrm{o}-\Delta_\mathrm{e}}{z}\right]. \end{aligned} \tag{2}$$

Spectral density has bounded support and gap:

$$\begin{aligned} \Phi_0(\omega) &= \frac{1}{\Delta_\mathrm{e}}\sqrt{2(\Delta_\mathrm{o}+\Delta_\mathrm{e}) - \omega^2 - \frac{(\Delta_\mathrm{o}-\Delta_\mathrm{e})^2}{\omega^2}}\,\theta\big(|\omega| - \omega_\mathrm{min}\big)\theta\big(\omega_\mathrm{max} - |\omega|\big) \\ &\quad + \frac{\pi}{\Delta_\mathrm{e}}\Big[|\Delta_\mathrm{o}-\Delta_\mathrm{e}| - (\Delta_\mathrm{o}-\Delta_\mathrm{e})\Big]\delta(\omega), \end{aligned} \tag{3}$$

$$\omega_\mathrm{min} = \left|\sqrt{\Delta_\mathrm{o}} - \sqrt{\Delta_\mathrm{e}}\right|, \quad \omega_\mathrm{max} = \left|\sqrt{\Delta_\mathrm{o}} + \sqrt{\Delta_\mathrm{e}}\right|.$$

Graphical representation for two cases [Viswanath and Müller 1994]:



- $\Delta_\mathrm{o} > \Delta_\mathrm{e}$: continuum only (solid lines).
- $\Delta_\mathrm{o} < \Delta_\mathrm{e}$: continuum plus central δ-peak (dashed lines).

Spectral Densities with Unbounded Support

Spectral densities with unbounded support are encoded by Δ_k-sequences that grow to infinity as $k \to \infty$. The growth law of the Δ_k-sequence determines the high-frequency decay law of the spectral density [Magnus 1985]:

$$\Delta_k \sim k^\lambda \quad \Rightarrow \quad \Phi_0(\omega) \sim \exp\left(-\omega^{2/\lambda}\right). \tag{1}$$

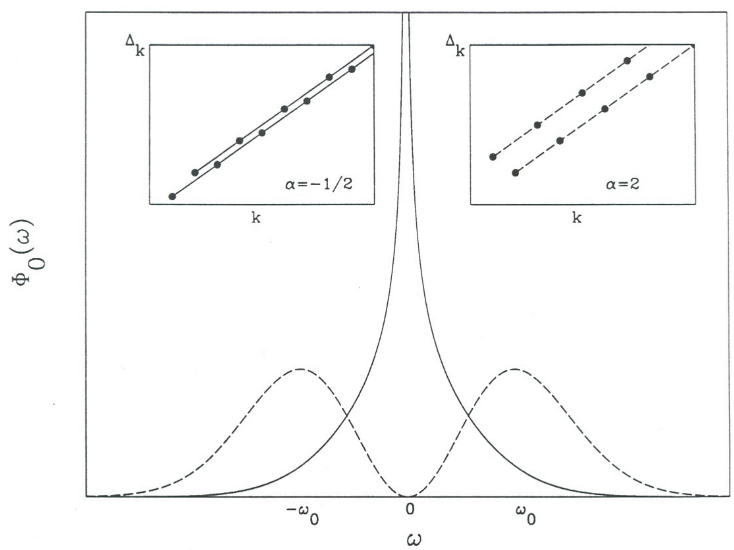
Model spectral density with Gaussian decay and infrared singularity:

$$\Phi_0(\omega) = \frac{2\pi}{\omega_0 \Gamma\big((\alpha+1)/2\big)} \left|\frac{\omega}{\omega_0}\right|^\alpha e^{-(\omega/\omega_0)^2}. \tag{2}$$

Associated Δ_k-sequence has linear growth law. The intercept of the Δ_{2k-1} is governed by the exponent of the infrared singularity.

$$\Delta_{2k-1} = \frac{1}{2}\omega_0^2(2k-1+\alpha), \quad \Delta_{2k} = \frac{1}{2}\omega_0^2(2k). \tag{3}$$

Graphical representations for two cases [Viswanath and Müller 1994]:



Model spectral density with Δ_k-sequence of different growth laws:

$$\Phi_0(\omega) = \frac{2\pi/(\lambda\omega_0)}{\Gamma\big(\lambda(\alpha+1)/2\big)} \left|\frac{\omega}{\omega_0}\right|^\alpha e^{-|\omega/\omega_0|^{2/\lambda}}, \quad M_{2k} = \omega_0^2 \frac{\Gamma\big(\lambda(1+\alpha+2k)/2\big)}{\Gamma\big(\lambda(1+\alpha)/2\big)},$$

where the Δ_k must be determined numerically from the moment M_{2k} as described in [nln85].

Unbounded Support and Gap [nln103]

The presence of a gap in spectral densities with unbounded support is encoded in sequences of Δ_{2k-1} and Δ_{2k} that have the same growth-law exponent λ but grow with different (asymptotic) amplitudes.

Model spectral density with Gaussian decay and a gap:

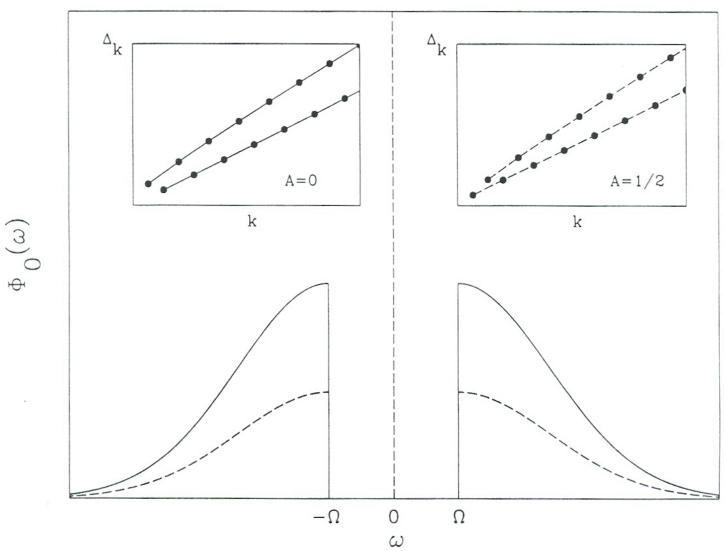
$$\Phi_0(\omega) = 2\pi A\delta(\omega) + \frac{2\sqrt{\pi}}{\omega_0}(1-A)\theta\big(|\omega|-\Omega\big)e^{-(|\omega|-\Omega)^2/\omega_0^2}. \qquad (1)$$

Frequency moments:

$$M_{2k} = 2\pi(1-A)\sum_{m=0}^{k}\binom{2k}{2m}\omega_0^{2m}\Omega^{2(k-m)}2^{-m}(2m-1)!!$$
$$+ 2\sqrt{\pi}(1-A)\sum_{m=0}^{k-1}\binom{2k}{2m+1}\Omega^{2(k-m)-1}\omega_0^{2m+1}m!, \quad k=1,2,\ldots \qquad (2)$$

with the Δ_k to be determined from the M_{2k} as described in [nln85].

Graphical representations for two cases [Viswanath and Müller 1994]:



In the cases shown the asymptotics set in early.

- $A = 0$: Δ_{2k+1} grow more steeply: spectral density consists of continuum split by gap alone.
- $A = \frac{1}{2}$: Δ_{2k+1} grow less steeply: spectral density consists of continuum split by gap and a central spectral line.